Spring 2013

Chemistry & Chemical Biology 2013 APR Self-Study & Documents

University of New Mexico

THE UNIVERSITY *of* NEW MEXICO

Department of Chemistry and Chemical Biology

Self Study for Academic Program Review

April, 2013

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Executive Summary

The department of Chemistry and Chemical Biology (CCB) at UNM has been in a period of transition and upheaval for several years.

Historically, the department has had several overlapping missions and goals- service teaching for science and engineering majors, professional training of chemistry majors and graduate students and ambitions for a nationally-recognized research program. CCB teaches ~3% of the student credit hours taught on main campus, and at one point had over 20 tenured and tenure track faculty and ~80 graduate students.

The department continues to teach a major service load, but the number of research active faculty, graduate students and funded research grants are at or near record low points. Several underlying problems have contributed to the current situation: CCB's main teaching and research laboratory building, Clark Hall, has needed major renovations since at least 1988, and recurring problems with utilities and lab space may have contributed to faculty departures. As noted by the graduate review committee in 2003, governance issues have hampered smooth operations and led to a departmental atmosphere which does not necessarily focus on the common good. The department has had 4 different chairs since 2007, and has also had several changes to graduate and undergraduate programs which have contributed to confusion among students and faculty alike. For the last 10 years, CCB has had a poor track record of retaining junior faculty, and the number of tenure-track faculty recently reached a historic low of 13 in 2009 (it is now just 16).

Real and potential improvements are underway, however. Ongoing facility improvements include a Science and Math Learning Center (SMLC), recently constructed and now scheduled for expansion, and $16 million in funds allocated for the renovation of Clark Hall. The SMLC now houses general chemistry teaching labs, and the expansion will accommodate organic chemistry teaching labs as well. The Clark Hall renovation should provide modern utilities and some refurbished lab space, although funds will not cover a complete renovation. Six new faculty hires over the last six years have brought new ideas and energy, and the first of these should receive tenure this year. Changes in faculty governance and in the graduate program are underway- a new faculty handbook has been approved and a new graduate program is being drafted.

The ability of the department to recover stability and fulfill its mission will depend on several mutually dependent tasks- the successful design and renovation of Clark Hall, improved interactions with other units on campus, development of a collegial and productive departmental working environment, and the successful mentoring of junior faculty.

I. Background

A. History

The modern version of the UNM Chemistry department (now the department of Chemistry and Chemical Biology) emerged in the 1980's under the leadership of Riley Schaeffer. To quote W. Litchman's departmental history, "Around 1980, the UNM chemistry faculty decided that to maintain currency in the mainstream of chemical education and research (with its trend towards biochemical specialties) a new direction in hiring, promotion, tenure, and pay was needed, one which emphasized the role of research over the role of undergraduate education as a determinant for tenure. To this end, they recruited a new department chairman to implement these changes: Riley Schaeffer, who came from the University of Indiana with a significant reputation in research and graduate education. One of his first actions as chairman was to create a two-tier faculty: those who were significantly and successfully engaged in graduate education and research, and those who were more involved in the undergraduate curriculum. Emphasis on research productivity, funding, and graduate recruitment meant that departmental resources (funds, space, and personnel) were stretched tight, and caused friction through the following years." Some faculty recall a decision to create two research foci- one in biological chemistry and one in materials. According to Litchman, in 1988 the department had "…22 tenure-track faculty members, plus lecturers, laboratory supervisors, and technicians."

Litchman goes on to describe the 1990's as a period in which successful hires of senior faculty (Christie Enke, Patrick Mariano, Debra Dunaway-Mariano, Hua Guo, Richard Kemp) were counterbalanced by a failure to keep overall faculty hiring even with retirements and departures, and the departures of several faculty who have since reached positions of distinction (including Vincent Ortiz, Thomas Bein, Su-Moon Park, Richard Crooks, Mark Hampden-Smith, Peter Ogilby and Carlos Bustamonte). By 2002, the department had only 18 tenure-track faculty, two of whom were partially committed to university service in the offices of the Dean of Arts and Sciences and the Provost.

The list of department chairs and graph of faculty numbers illustrate two of the problems that CCB has encountered since that time.

Table 1. Chairs of Chemistry and Chemical Biology since 1988

Richard Willis Holder (1 Jan 1988 -- 31 Dec 1990)
Cary Jacks Morrow (1 Jan 1991 -- 30 Jun 1995)
Fritz Schreyer Allen (1 Jul 1995 -- 30 Jun 2000)
Thomas M Niemczyk (1 Jul 2000 – 30 June 2006)
Cary Jacks Morrow (1 Jul 2006 -- 30 Jun 2008)
Martin L Kirk (acting) (1 Jul 2008 – 30 June 2009)
David Bear (1 July 2009- July 15, 2012)
Stephen Cabaniss (16 July, 2012-present)

Although CCB had only 3 chairs for the 15-year period 1991-2006, it has had 4 chairs in the 7-year period 2006-2013. This instability in the chair's position started during an acrimonious period which began with a divisive failed search and which ended with the retirement of two analytical chemistry faculty (Enke, Niemczyk) and the departure of a third (John Engen). The remaining faculty voted not to make re-hiring into the analytical division a priority.

Morrow's chairmanship of 2006-2008 (his second) was intended to allow the department to find and hire an external chair, but chair searches were not successful, and he was succeeded for one year (2008-2009) by Martin Kirk. During this time, the Provost and Dean, at the direction of the President, made a conscious decision to hire an external chair and dynamic young faculty to rejuvenate a shrinking department.

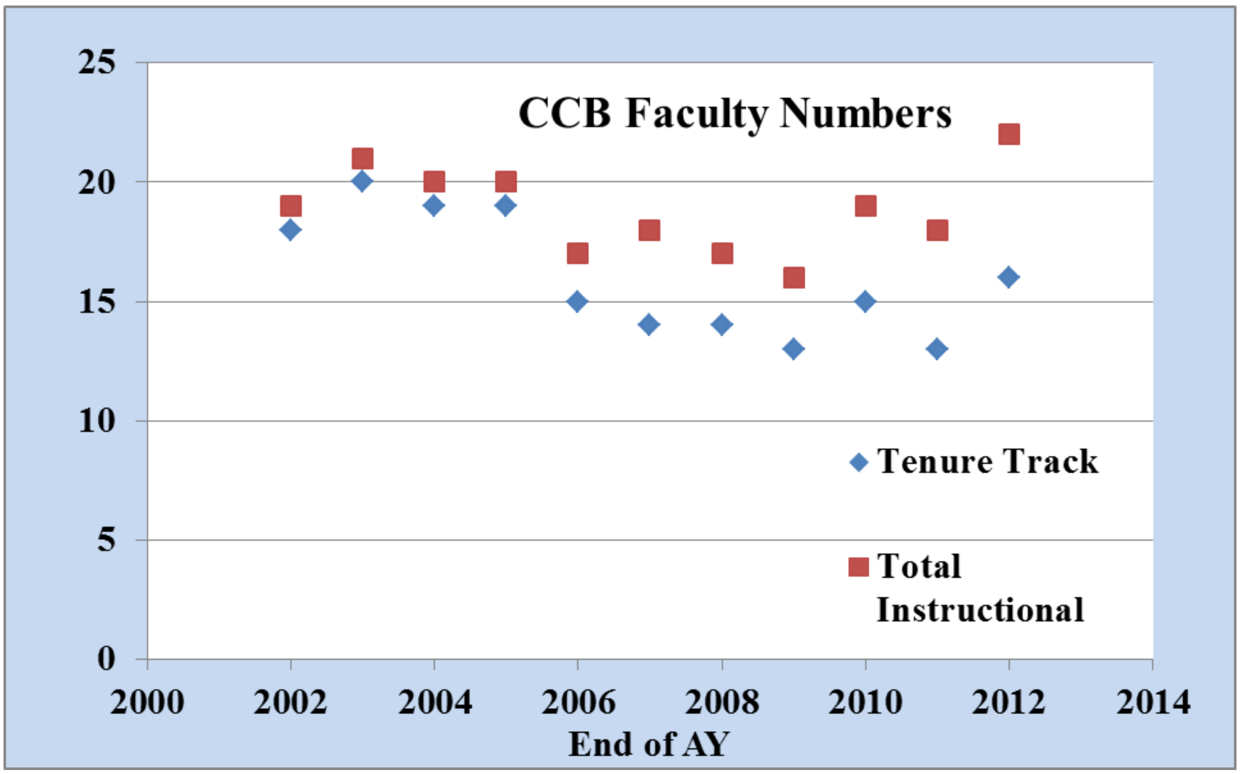

Figure 1. CCB faculty since 2002. Tenure track faculty reached a low of 13 in 2009.

In 2009, the Dean of A&S appointed David Bear, a professor and former chair of Cell Biology and Physiology at the School of Medicine, as department chair. Bear set out to simultaneously reform degree programs, increase faculty numbers and improve laboratory facilities. Bear persuaded the university to make renovations to Clark Hall a top priority, and although a bond request for renovation funds was rejected in the November 2010 election, he obtained several million dollars from the UNM Regents to upgrade labs and other space; the bond issue passed in 2012, and more extensive renovations are now planned (see section VIII, page 20). During Bear's chairmanship, three new faculty (Yang Qin, Chad Melancon and Fu-Sen Liang) started in CCB and two more (Ramesh Giri and Terefe Habteyes) were hired.

Several sets of changes were implemented to the BA, BS and PhD programs. However, internal disagreements within the department contributed to his decision to step down as chair in the summer of 2012.

The current chair, Steve Cabaniss, has been in office since July 2012.

B. Governance and Organization

The department has remarkably few written records of organizational procedures on file, either because they have been lost or because until recently many procedures were perpetuated through the memory of senior faculty. The department traditionally has had a chair, an elected 'executive committee' of tenured faculty and a set of standing committees (graduate studies, undergraduate studies, etc.). It has not traditionally had an associate chair, formal mentoring arrangements for junior faculty or written rules for the conduct of faculty meetings.

In view of the impending retirement of senior faculty and the perceived need for more stable rules and procedures, the department decided to create a written handbook this academic year (AY 12-13). Drafted by the chair and senior faculty last summer, the handbook was discussed, modified as necessary, and approved section by section in a series of faculty meetings from September 2012 to February 2013.

The entire handbook was approved April 3, 2013 (Appendix A2), and continues the traditions of a chair and appointed standing committees, formally re-institutes the practice of electing a faculty advisory committee (which had not occurred for several years), and adds several new features, including

Formalizing the position of associate chair (created by Bear);

Specifying a required super-majority (2/3) for faculty votes on important issues;

Requiring distribution of agendas and written summaries for all regular faculty meetings;

Requiring the formation of 3-member mentoring committees for junior faculty with one external (non-CCB) member;

Codifying tenure procedures and expectations.

Although this departmental handbook will not "officially" go into effect until AY 13-14, the department has attempted to abide by many of its features this year. Specifically, a faculty advisory committee (Wei Wang, Marty Kirk, David Keller and Richard Holder) has met approximately bi-weekly since being elected at the end of the Fall 2012, Richard Holder has served as Associate Chair since August 2012, written tenure guidelines have been submitted to the college of Arts and Sciences, and the handbook sections each have been passed by a minimum 2/3 majority. Mentoring committees should be in place by the end of the Spring 2013 term.

Standing committees for this year include the undergraduate committee chaired by director of undergraduate education Joe Ho, the graduate recruitment committee chaired by Hua Guo (Fall) and John Grey (Spring) and the building committee chaired by Marty Kirk. This last committee is especially important now due to the passage of general obligation bonds last November which will enable extensive (though not comprehensive) renovations of Clark Hall.

The graduate studies committee is being chaired by Steve Cabaniss by default, since several senior faculty declined to serve on the committee due to recent tensions and disagreements among the faculty.

C. External Accreditation

The American Chemical Society (ACS) Committee on Professional Training (CPT) determines and publishes guidelines for undergraduate degree program approval and also reviews and approves programs from various departments. The complete ACS CPT document, "Undergraduate Professional Education in Chemistry" is included as Appendix A3. The program approval guidelines cover a range of areas including the institutional environment, faculty and staff, infrastructure, curriculum, undergraduate research, specific student skills to be taught and program self-evaluation.

As noted in the CPT guidelines (page 1), *"ACS authorizes the chair of the ACS approved program to certify graduating students who complete a bachelor's degree meeting the ACS guidelines. Graduates who attain a certified degree must often complete requirements that exceed those of the degree-granting institution…"* Thus in contrast to some other disciplines and departments, completing a degree from an ACS-approved program does not guarantee an ACS-certified degree. This is the case for the B.S. degree from CCB. The ACS requires foundational work in 5 sub-disciplines of chemistry, including biochemistry, but CCB does not require a biochemistry course for graduation (it is an elective). ACS certification also requires 400 contact hours of chemistry laboratory beyond the general chemistry level, but B.S. requires only 330 contact hours (although this can be met by performing undergraduate research or taking the advanced synthesis lab).

The most recent periodic report for departmental approval was submitted to the ACS in 2011, and UNM CCB is currently an approved program.

In general, the CCB undergraduate program meets or exceeds ACS expectations for faculty and program size, resources and course offerings. However, a few of the requirements indicate a need for improvement:

Page 4- "The collective expertise of the faculty should reflect the breadth of the major areas of modern chemistry."

"Because faculty members serve as important professional role models, a program should have a faculty that is diverse in gender, race, and ethnic background."

Since the department has lacked an analytical division since 2006, it cannot be said that the faculty "reflect the breadth of the major areas of modern chemistry". Similarly, a UNM department with no Hispanic or native American members (and only two female tenure-track faculty) does not meet the diversity guideline. Starting in Fall 2013, Julia Fulghum will become the third female tenure-track faculty member and the only analytical chemist in the faculty.

Page 4- "Full-time, permanent faculty should teach the courses leading to student certification in an approved chemistry program. Programs may occasionally engage highly qualified individuals outside the regular faculty when permanent faculty members are on *sabbatical leaves or to deliver special courses. The Committee strongly discourages, however, excessive reliance on temporary, adjunct, or part-time faculty in an ACS-approved program and will review such situations carefully."*

Most sections of general chemistry (CHEM 121 and 122) offered since 2006 have been taught by temporary or part-time instructors.

Page 13- Original research culminating in a comprehensive written report provides an effective means for integrating undergraduate learning experiences, and allows students to participate directly in the process of science.

While some of our students participate in undergraduate research, the percentage is relatively low and written reports have not been systematically documented by the department.

D. Previous Review

The previous external review of this department, conducted in 2003, was intended to evaluate the graduate program. However other aspects of the department, including faculty governance, staff function and morale, facilities, and teaching, are necessarily linked to the graduate program and were considered by the committee. The Graduate Review Committee (GRC) had one internal member, Prof. Kathryn Vogel of Biology, and four external members- Ignacio Tinoco, Isiah Warner, Gary Molander and John Fackler, Jr. (chair). The full text of their report is in Appendix A4.

GRC comments and recommendations in the executive summary and the departmental reaction/implementation since then:

GRC1. Given the focus of the Chemistry Department over the past decade, there are distinct recruiting advantages in changing the name of the department. Perhaps the appropriate name would be the Department of Chemistry and Chemical Biology.

The department's name has been changed as suggested.

GRC2. With the proximity of the University to several key US Government laboratories, the UNM Mission plays well into the manifold opportunities these laboratories provide for collaboration and synergy with chemical education and research. This effort appears to be producing an excellent model for building bridges to the significant resources of the state's national laboratories.

The department has lost some faculty (e.g., Niemczyk, Brozik) who interacted extensively with the national labs, but other interactions have appeared (Grey is on the users board for the Center for Integrated Nano-Technology, CINT, operated by LANL and SNL; Fulghum will join the CCB faculty as co-chair of the CINT Science Advisory board). The CCB chair is encouraging faculty participation in current efforts by the Advanced Materials Laboratory (AML) leadership to broaden and deepen collaborative relationships through regular seminars and sharing of facilities (The AML building is owned by UNM, but half of the space is rented and operated by SNL. In this document, AML-SNL refers to the Sandia wing and personnel, AML-UNM to the wing operated by UNM, and AML to the entire facility, which is jointly operated.)

GRC3. A key to future success of the Chemistry Department is significant improvement in faculty governance.

Systematic reform of faculty governance was not a priority until this year, when the department established a written faculty handbook- see section B above and Appendix A2.

GRC4. Unfortunately little progress appears to have been made since the last graduate review in 1993 on the issues of research space and facilities. Short term space needs for research appear to be adequate but not optimally organized. In the long term, new facilities are essential.

The condition of Clark Hall has been an issue since 1988, and several attempts to raise awareness of the problems had been unsuccessful until Martin Kirk and David Bear began to champion the cause. Although an initial bond was rejected in 2010, some renovations were funded internally and a new $16 million renovation project is in the planning stages following the 2012 bond approval. The state legislature has also approved $5 million to expand the Science and Math Learning Center (SMLC) to accommodate the organic teaching labs. According to the present schedule, Clark Hall renovations should begin summer of 2014 and finish summer of 2015; planning for the expansion of the SMLC has only begun in the last month.

GRC5. The lack of proper facilities maintenance protocols has raised serious issues of health and safety within the Chemistry Department. The Chair, in consultation with other chairs and Administrators, should establish a protocol and communication network that will allow discussion of any physical plant maintenance that will disrupt electricity, water, or hoods CONSIDERABLY BEFORE such work is undertaken, so that researchers can plan their activities around these job actions.

Communications with Physical Plant have improved considerably since 2003, and these surprise maintenance operations are no longer a major issue.

GRC6. The support staff organization appears to have been developed nicely under good leadership. A positive morale has been created that appears to have overcome problems that existed in 1993. Even so, the standard of staff support for the Chemistry Department is far below that of peer institutions, particularly as research active faculty numbers increase.

CCB office staff number have increased since 2002, but the department has lost 2 full-time technical staff (Dr. Eileen Duesler, Mike Davenport) and gained a part-time mass spectrometry technician dedicated to the MS facility. CCB currently does not have enough technical staff to make efficient use of existing departmental instrumentation.

GRC7. The hiring of many excellent junior faculty and four well established senior faculty, all supporting the departmental thrust areas, has been a significant positive development. However, retention of junior faculty is one of the most important roles needed to be done by the senior faculty and administration.

The untenured junior faculty in 2003 were Richard Watt, David Tierney, James Brozik and John Engen. None of these remains at UNM; clearly, the department has not found the right approach to retaining "*excellent junior faculty*". Formalized mentoring, as suggest by the GRC, is currently being implemented as required by the new faculty handbook.

GRC8. The Chemistry Department is to be commended for its policy on post tenure review. This is really a model for other institutions.

Post-tenure review is a UNM policy and not specific to CCB. The policy has not been used or much discussed since 2002.

GRC9. The departmental web page should be professionally produced, be up to date, and have links to the faculty web pages, which should list research interests and publications.

The departmental website has been updated and is undergoing a redesign by the Arts and Science information technology team and a contract web designer. The office of Graduate Studies (OGS) has also posted an RFP for a third-party contractor to provide online graduate application software which can be customized for each department. The website re-design (except the online application) has a scheduled completion date of August 1, 2013.

GRC10. The Chemistry Department must find a mechanism to increase graduate student stipends. The current stipend for graduate students in chemistry at UNM ($15,400) is well below the stipends in the peer schools, and in research universities in the west. The Chemistry Department must strengthen its recruitment of quality domestic students and especially Hispanics, Native Americans, and other minorities.

Graduate student teaching stipends have been increased to over $21,000 annually, which is much closer to current norms than $15,400 in 2003. However, most incoming graduate students are non-domestic, and Hispanic and Native American students are under-represented within the domestic student population relative to NM demographics.

GRC11. Procedures for early identification of outstanding undergraduate students who may later be approached as potential undergraduate assistants (and potential graduate assistants) must be implemented.

The undergraduate education director (Joseph Ho) has improved and expanded the recruitment of undergraduate teaching assistants. Although some of our better undergraduates have been recruited into the graduate program by individual advisors, no formal department-wide mechanism exists for recruiting these students.

GRC 12. The graduate students in the chemistry department seem to be satisfied with the program although the number of graduate students is well below the desirable number for the size of the faculty.

Although the number of graduate students increased from 2003 to 2006, reaching a maximum of nearly 80 students, CCB now has <60 students, fewer than in 2003.

GRC 13. A core set of courses should be required of all students in each discipline that ensures the students to obtain the requisite knowledge. This means that core courses must be given regularly.

A single core course system was implemented for all graduate students regardless of division or sub-discipline. This gave rise to a number of problems, including disagreements between disciplines. The number and nature of required core courses was the subject of a faculty meeting last year which had a catastrophic effect on faculty morale. A "super-committee" (graduate studies + graduate recruiting) is currently working to revise the graduate program in a more widely acceptable manner. Although the revision is not yet complete, it appears the formal core course requirement will be dropped in favor of a system of regularly scheduled courses which provide greater flexibility to the students.

GRC 14a. The Chemistry Department must aggressively pursue funding to upgrade departmental facilities and equipment.
GRC14b. The committee recommends that an instrumentation committee be established to coordinate efforts in the Chemistry Department to submit proposals annually.

Since 2003, CCB has significantly upgraded X-ray crystallography, molecular mass spectrometry and NMR facilities through multi-user grants. One CCB faculty member has contributed to acquisition of elemental mass spectrometry equipment for the geo-analytical laboratory in Earth and Planetary Sciences. The mechanisms for these proposals have not consistently involved a facilities committee, however, but instead grew out of individual faculty research requirements.

The main text of the GRC report contained some other noteworthy comments, including the need (p. 7) to move quickly to re-establish the materials 'wing' of the department; the hiring of Grey, Qin and Habteyes represents a significant effort in this direction, and the department is currently pursuing one senior hire in photonic materials and closer research ties with Sandia NL through the AML.

The GRC also recognized the need to improve the equipment available in teaching laboratories (p. 16), which has been greatly enhanced following the implementation of a lab fee which exceeds reagent costs.

Finally, a discouraging section of the GRC report (page 9 of that document) remains a departmental challenge:

"The Chemistry Department at the University of New Mexico (UNM), consistently indicated that one of their highest priority is recruiting and retaining better graduate students. However, with few exceptions, it appears that the department has elected not to participate in the graduate recruiting competition.

"In spite of what is said the recruiting of graduate students does not appear to be a high priority of the department; it is definitely not effective. Some faculty seem to think that obtaining more students is impossible, and thus a waste of their time. Other faculty recruit students vigorously, but only for their research groups. A concerted effort should be made to obtain more students, and more U.S.-born students, while keeping the quality of the students high. It will require more time from the faculty, and more state and federal funding."

Graduate student recruiting remains a serious problem for the department, although last year's dip in applications has been reversed. New procedures instituted by the recruiting committee (on-line applications, department-funded recruiting at ACS meetings) and the graduate recruiting committee's proposed procedures for AY 13-14 may begin to make a difference over the next few years.

II. Program Goals

A. Departmental Mission The CCB departmental mission statement reads:
"The primary mission of the Department of Chemistry and Chemical Biology is to deliver a quality education to traditional and nontraditional graduate and undergraduate students in the College of Arts and Sciences, and to the University at large. The Department provides a robust educational environment that fosters the acquisition of chemical knowledge and the use of chemical principles to give students deeper insight into understanding how Chemistry will play a fundamental role in molecular science discovery and the development of new technologies in the 21st century. Therefore, we view Chemistry as the central science, and the Department as a community of scholars whose research and educational activities focus on understanding the fundamental properties of materials, and chemical and biological reactions at the molecular level. The faculty is committed to the development of a nationally prominent and internationally recognized graduate research program. This program will be fully engaged in efforts to ensure success of the mission. To this end, the Department will actively seek mutual partnerships with the University community, the National Laboratories in New Mexico, and the greater national and international scientific communities in order to fully contribute to the fundamental molecular science needs of our society."

This departmental commitment addresses all four points of the UNM mission statement (Appendix A5), by (1) offering undergraduate and graduate educational programs, (2) emphasizing a graduate research mission, (3) partnering with the scientific community locally and nationally to serve the public of New Mexico, and (4) providing training and research support for the fields of medicine and public health in New Mexico.

B. Program Learning Goals The published learning goals of CCB's Bachelor of Arts (B.A.), Bachelor of Science (B.S.) and Master of Science (M.S.) degrees (Appendix A6) date from 2009 and emphasize

1. Understanding major chemical concepts, theoretical principles and experimental findings in the field of chemistry,
2. Employing critical thinking and hypothesis-driven methods of scientific inquiry,
2a. (BS but not BA) Constructing and testing hypotheses using modern laboratory equipment and appropriate quantitative methods,
3. Presenting scientific data and arguments in an oral and written format,
4. Preparing for a career which utilizes this scientific training.

The MS degree further emphasizes a significant and deep-rooted knowledge of a sub-discipline within Chemistry and Chemical Biology. The Ph.D. degree emphasizes both a deep-rooted subject knowledge and the ability to plan and carry out independent research in chemistry. The assessment plan and learning goals for the Ph.D. were modified in January 2009, but have not been approved or published. The lack of approval may be due to the numerous changes the program has undergone in the last four years (see section III below).

These goals are typically presented to the students within the CCB curriculum through syllabi, course learning objectives and course assessment (tests, lab reports, etc.).

C. Constituents The department of Chemistry and Chemical Biology serves a variety of often interrelated groups both on- and off-campus. On-campus constituencies include the general undergraduate student body, through general education courses; the science and engineering majors who require CCB service courses as part of their degrees; the chemistry majors who rely upon CCB for upper division coursework and academic and career, advising; CCB graduate students who rely upon faculty for advanced coursework, research support and professional training; and our colleagues in other UNM departments whose research programs rely upon our chemical expertise, student training and specialized facilities. Off-campus constituencies include the people of the Albuquerque area and New Mexico at large, who rely upon access to chemical expertise in public matters; chemical educators in NM secondary schools and UNM branch campuses who rely upon our department for guidance in curriculum and standards in their courses; NM community colleges, whose students will transfer to UNM to complete their degrees; local and NM industry which may employ CCB graduates and/or require advanced technical expertise or facility access; and the national and international science communities, which rely upon UNM (and other schools, of course) to produce the trained professionals and the research-derived knowledge that these communities employ.

CCB faculty lead and participate in a number of outreach and community activities. In Albuquerque, faculty (Ho, Qin, Whalen) work with local schools to provide lab access and demonstration and provide expertise on local environmental problems like the Kirtland AFB jet fuel plume (Cabaniss). Statewide, the department's summer workshop for high school chemistry teachers (Ho) has helped improve secondary instruction. Nationally, faculty organize symposia and edit prominent scholarly journals (e.g., Guo, Kirk and Dunaway-Mariano). These activities show how chemistry and CCB integrate with the intellectual and civic life of New Mexico and the nation.

III. Teaching and Learning: Curriculum

CCB offers two undergraduate degrees- the B.A. and B.S.- and two graduate degrees, the M.S. and Ph.D.

The undergraduate degree requirements follow the traditional pattern of many ACS-certified chemistry degrees, and are specified in Appendix A7, which also includes sample 4-year plans for graduation. For both the B.A. and the B.S., students must fulfill the UNM general education requirements, and pass one year of calculus and one year of calculus-based physics, two semesters each of General Chemistry plus lab and Organic Chemistry plus lab, and one year of quantitative analysis plus lab. The B.A. degree, which is intended for pre-professional students (mostly medicine and pharmacy) and students with a strong interest or double major in biology, further requires a single semester of physical chemistry emphasizing biological systems and 7 hours of approved electives (the biologically oriented courses CHEM 421 and 425 are often selected for this, since they meet the UNM medical school's matriculation requirement). The B.S. degree requires a two-semester calculus-based physical chemistry sequence with one semester of lab, a senior-level inorganic course, advanced lecture/lab courses in chemical synthesis and instrumental analysis and 4 credit hours of approved electives.

The graduate program requirements are currently in a state of flux. The most recent graduate handbook (Appendix 8) requires that students take four "core courses" from a list of 5, perform a laboratory rotation to select an advisor, and take an individualized, literature-based written candidacy exam. This handbook is not consistent with the published UNM catalog or the recollection of several faculty who believe it was modified during the 2011-2012 AY (though no specific modifications were recorded). The department is in the process of developing a new graduate program handbook, which will change the coursework requirements and advisor selection procedures and may also change the written and oral candidacy exams. A complete draft of this new handbook should be available by the time the review committee convenes at UNM.

CCB teaches courses required by other science and engineering programs which increase enrollment far beyond that needed for chemistry majors alone. Physics and most engineering majors require the general chemistry sequence (CHEM 121 and 122) with lab (123L and 124L). Biology, biochemistry and chemical engineering majors are also required to take the organic chemistry sequence (CHEM 301 and 302) with lab (303L and 304L). Chemical engineering and biochemistry majors also take one semester of physical chemistry, and many of the biology majors opt for a minor in chemistry which typically leads to enrollment in quantitative analysis (CHEM 253L) and/or physical chemistry (CHEM 315).

CCB also teaches two service courses intended for allied health majors- nursing, physical therapy, etc. The first semester (CHEM 111) is a 4-CH survey of general chemistry topics. The second semester (CHEM 212) is a 3-CH combined organic and biochemistry course. These courses are not recommended to either A&S science majors or to majors in non-health-related fields, although CHEM 111 can be counted toward the UNM general education requirement.

The department has requested permission to begin offering a course targeting non-science majors. The course (CHEM 101) would use the ACS textbook “Chemistry in Context” which teaches chemical concepts, scientific literacy and critical thinking through an unusual curricular approach. Unlike traditional textbooks, which are organized by chemical concept (one chapter on reaction kinetics, one chapter on photoprocesses, etc.), “Chemistry in Context” is organized by macroscopic issues or problems (the ozone hole, energy and alternative fuels, etc.). Chemical concepts are taught by repeated exposure in multiple contexts throughout the semester, rather by in-depth coverage over a 1-3 week period. If the current curricular application is approved, the course will commence in Spring 2014. The request has been approved by both undergraduate and curriculum committees, and awaits approval by the Faculty Senate on April 23.

IV. Teaching and Learning: Continuous Improvement

A. Assessment and Evaluation

Systematic assessment plans were designed and approved for the B.A., B.S., M.S. and Ph.D. degree programs (Appendix A6), and the plans for the first three have been approved. However, no records indicate the plan was carried out, and formal course assessment has not been a departmental priority for AY 2012-2013.

B. Actions to Improve Learning

CCB faculty have pursued a variety of strategies to improve pedagogy and student learning, particularly in lower level courses.

General Chemistry labs (123L and 124L) were modified by lab director Joe Ho to minimize written lab hand-outs and instead require the students to observe lab technique and procedures. The technique of calibrated peer review of written reports was also tested in these labs, although the results did not show a clear benefit to student learning.

CCB has also introduced a “parachute” mechanism into General Chemistry I (CHEM 121) which encourages students who fare poorly on the first test or two in CHEM 121 to move into a smaller section to review fundamentals (designated CHEM 120). These “parachuted” students thus remain enrolled in a science course and receive additional preparation to improve their chances of passing CHEM 121 should they re-take it. Preliminary data from 2010-2012 shows that “parachuted” students have significantly greater chances of re-taking and passing CHEM 121 than students who remained in CHEM and received a W or F. Appendix A9 contains additional material on the motivation for the course and preliminary results.

Another ongoing project is the redesign of General Chemistry II (CHEM 122) to employ active learning pedagogy. This project, sponsored by the UNM Office for Support of Effective Teaching (OSET) and Title V for Gateway Course Redesign, has been underway for less than one year but shows promising improvements in student learning (Appendix A10). As of March 29 2013, Drs. Ho, Knottenbelt and colleagues have submitted a follow-up proposal for the redesign of General Chemistry I along similar lines; preliminary response from OSET indicates it will be funded starting this summer.

V. Students

Undergraduates

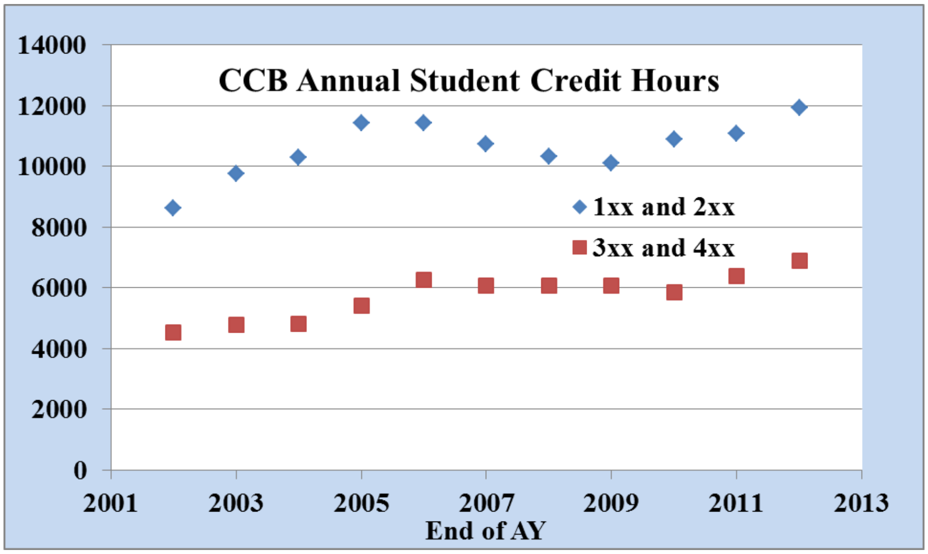

Fig. 2. Undergraduate credit hours taught by CCB

The department plays a central role in educating UNM undergraduates, and awards more PhD degrees than all but two other departments in A&S. CCB teaches a very large service load of undergraduates majoring in science, engineering and the allied health sciences. In AY 2011-2012, CCB taught ~20,000 student credit hours (19,950), or over 3% of the SCH taught on main campus. This represents a ~50% increase in credit hours taught over the last 10 years while tenure-track faculty numbers have declined.

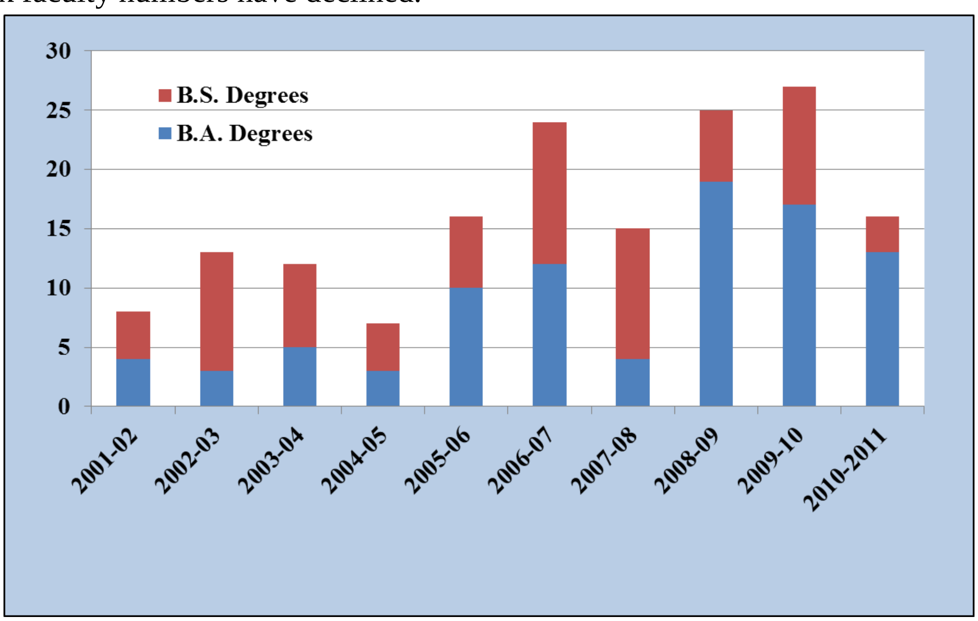

Fig. 3. Undergraduate degrees awarded by CCB (OIR data)

Discerning historical trends in undergraduate degrees is problematic, since the UNM OIR(Office of Institutional Research), UNM A&S (College of Arts and Sciences) and ACS databases are not mutually consistent. Based on enrollments in B.S.-only courses, it would appear that the number of B.S. degrees may have peaked in the period 2005-2009, but the increased number of B.A. degrees has led to increases in total degrees awarded (Fig. 3). In AY 2011-2012, CCB graduated 8 B.S. and 36 B.A. students according to departmental records. (Note: the departmental BA count includes all BA double-majors and not just those who listed CCB first on the graduation form, which differs from OIR and A&S counting statistics).

CCB majors are a diverse mixture of ethnicities mirroring the ethnic composition of the state. The principal minority student groups are Hispanic (~40%), American Indian (~10%) and Asian (~8-10%), with smaller numbers (<5%) of African-American students. Since 2004, women have been a majority of the enrolled chemistry majors, generally between 50-60% female and currently 52% female chemistry majors.

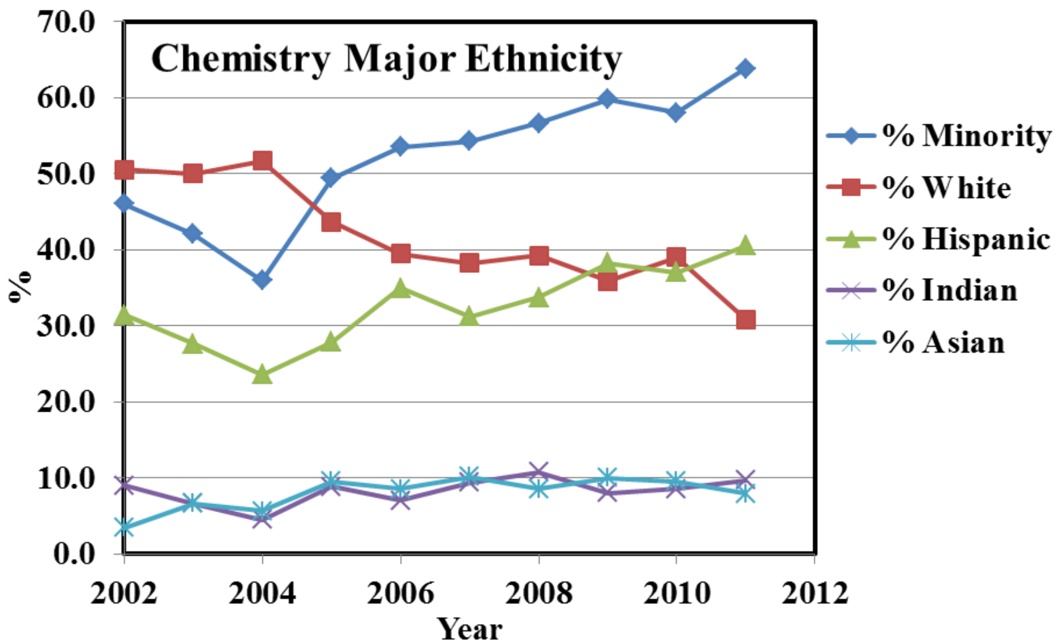

Figure 4. Ethnicity of declared chemistry majors by year.

CCB has not traditionally made systematic efforts to recruit undergraduate students, relying instead on the perceived market value of the chemistry degree and its utility in preparing students for graduate and professional schools. For the past several years, all formal undergraduate advising has been handled by a single staff member, who also handles aspects of graduate student advising and record-keeping. This system may soon be changed, as the department has been told to expect an additional undergraduate staff advisor who will spend ~2 days per week advising chemistry majors (but who will report to A&S). We are also recruiting faculty to act as career advisors for junior and senior chemistry majors starting Fall 2013.

CCB has also not traditionally kept consistent records of student placement, which has hampered our ability to contact departmental alumni.

Graduate students

In contrast to the increasing undergraduate enrollments, the CCB graduate education program has been shrinking since 2006, reaching its smallest size in a decade as defined by numbers of students enrolled (45 in Fall 2011) or by student credit hours taught (453 in AY 2011-2012) (Fig. 5).

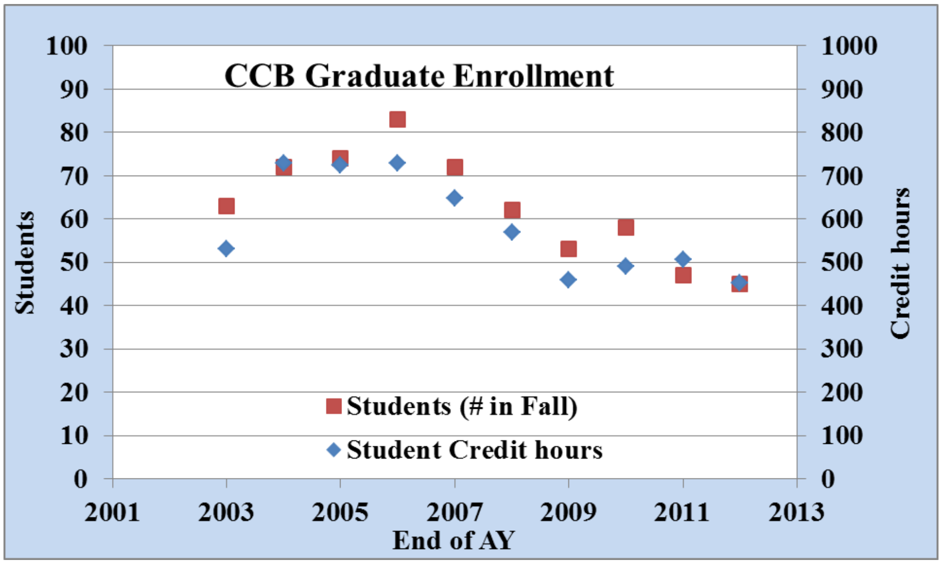

Fig. 5. Numbers of graduate students enrolled and credit hours since 2003.

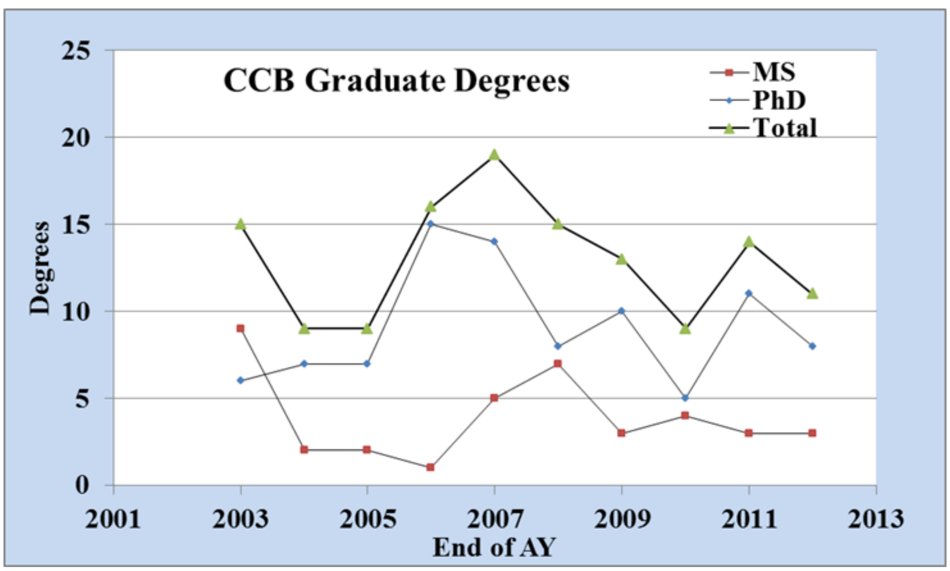

Fig. 6. Number of graduate degrees awarded since 2003.

The trend in degrees awarded is less clear, perhaps due to the more stochastic nature of this metric, but also indicates significant shrinking over the last 5 years (Fig. 6). In 2011-2012, CCB awarded 8 PhD and 3 MS degrees. As recently as Fall 2007, the department had >60 graduate students, and in 2005 over 80. The number of degrees is approaching the same percentage decrease. In AY 2010-2011, CCB ranked 2nd in A&S in number of PhD degrees awarded, behind History but ahead of all other natural sciences; it is not clear if this will continue over the next few years.

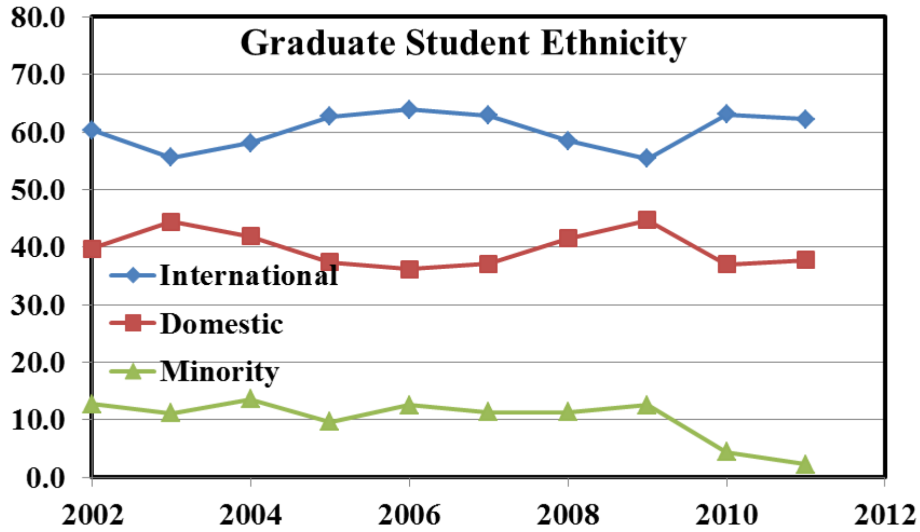

Fig. 7. Source and ethnicity of CCB graduate students since 2002.

The department has traditionally admitted a large number of international students, principally from the People's Republic of China (PRC). Over the last decade, the percentage of international students has averaged ~60% (see Fig. 6). In recent years, the fraction of domestic students has dropped from above to below 40%, and the fraction of domestic minority students has dropped below 10%.

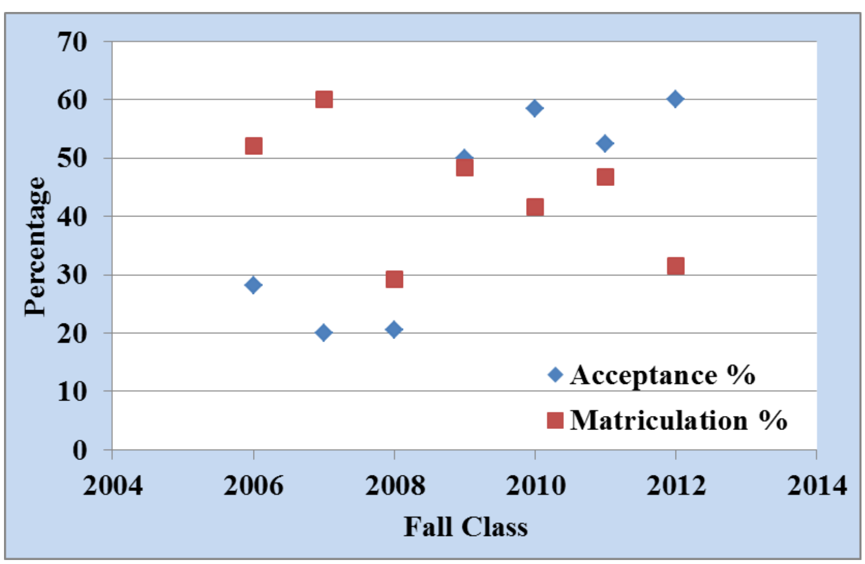

Fig. 8. Percentage of graduate applicants accepted and the percentage arriving at UNM

Recent trends in graduate student recruitment have also been problematic (Fig. 8). Since 2006, the number of applicants for Fall admission has dropped from ~90 to ~60-65 for Fall 2012, while the percentage accepted has increased from <30% to >50%. At the same time, the percentage of accepted students arriving at UNM (matriculation % or yield) has dropped (47% in Fall 2011 and 32% in Fall 2012). The applicant pool for Fall 2013 is higher- over 90 applications were received; this may be due to the implementation of on-line application on the CCB website.

Several possible explanations for the shrinkage in the graduate program must be considered:

i) As previously argued by David Bear and others, CCB TA stipends are ~$2000 lower than other flagship universities.

ii) The overall decrease in faculty size reduces the number of prospective advisers for new students and the number of RA positions available.

iii) The decision not to hire analytical faculty eliminates a popular sub-discipline for prospective students (analytical chemistry is the third largest division of the American Chemical Society).

iv) Continued reliance on Chinese graduate students at a time when the economy of the PRC has been stronger than that of the USA complicates recruiting.

v) The graduate education program fails to excite and attract students.

This last possibility has led to several proposals to re-organize the graduate program. Unfortunately, serious disagreements within the faculty have prevented any consensus on the best path forward, and the political fallout from this process has severely undermined departmental morale and cooperation.

VI. Faculty

As noted in the history section above (Fig. 1), the size of the (tenured+tenure track) faculty is only now recovering from its lowest point in 20+ years. CCB currently has 16.5 tenured or tenure-track faculty, four permanent lecturer positions and two visiting assistant professors (Table 2). All faculty with permanent (non-visiting) appointments are voting members charged with long-terrn guidance and improvement of the department. All faculty hold the Ph.D. except for senior Lecturer II Alisha Ray, who holds an M.S.

Table 2. CCB Faculty by rank

Professor

- Steve Cabaniss (chair)
- Debora Dunaway-Mariano
- Hua Guo
- Richard Holder
- Rick Kemp (0.5 appt in CCB)
- Martin Kirk
- Patrick Mariano
- Robert Paine (Distinguished Prof.)
- Wei Wang

Associate Professor

- Deborah Evans
- David Keller

Assistant Professor

- John Grey
- Ramesh Giri
- Terefe' Habteyes
- Fu-Sen Liang
- Yang Qin
- Chad Melancon

Lecturer

- Donald Bellew
- K. Joseph Ho
- Alisha Ray
- Lisa Whalen

Visiting Assistant Professor

- Sushilla Knottenbelt
- John McBride

Historically, the faculty have been split into four divisions- analytical, inorganic, organic and physical. Since 2006, the analytical division has disappeared and been replace by a division of chemical biology. However useful these divisions may be for managing undergraduate teaching assignments, they do not necessarily reflect the research directions and focus areas. For example, both Kirk (inorganic) and Keller (physical) work on biological systems, while Grey (physical) and Qin (organic) study photovoltaic polymers. Table 3 lists faculty by affinity groups. Most faculty appear in more than one group.

The 15 research-active tenure-track faculty can be divided into approximately three groups: Members of the most active group have published 10 or more papers over the last 3 years and have multiple external grants (Table 4). Five of these and Patrick Mariano (no current independent funding) have published over 100 journal articles apiece. A smaller, less research active group of tenured faculty has <10 publications over this time period and less independent grant support. Finally, the five most recently hired assistant professors have published fewer than five articles apiece over the 2010-2012 period and are relying on internal UNM funding.

CCB faculty composition will change next year when Robert Paine retires and Julia Fulghum (Ph.D. Analytical Chemistry) moves her tenure from Chemical and Nuclear Engineering into CCB. Jeremy Edwards (Ph.D. Bioengineering) has requested to move his tenure from the UNM Health Sciences Medical School into CCB, and deliberations are ongoing with an anticipated decision in May.

Table 3. Faculty by Research Focus

Catalysis
- Debora Dunaway-Mariano
- Ramesh Giri
- Rick Kemp
- Wei Wang

Chemical Biology and Biochemistry
- Debora Dunaway Mariano
- Martin Kirk
- David Keller
- Fu-Sen Liang
- Chad Melancon
- Wei Wang

Chemical Education
- K. Joseph Ho
- Sushilla Knottenbelt

Environmental Chemistry
- Steve Cabaniss

Inorganic Chemistry
- Ramesh Giri
- Rick Kemp
- Martin Kirk
- Robert Paine

Materials Chemistry
- John Grey
- Terefe' Habteyes
- Rick Kemp
- Yang Qin

Physical Chemistry
- Deborah Evans
- John Grey
- Hua Guo
- Terefe Habteyes
- David Keller

Synthesis
- Ramesh Giri
- Rick Kemp
- Fu-Sen Liang
- Robert Paine
- Wei Wang

Theory and Computation
- Deborah Evans
- Hua Guo
- Martin Kirk

More complete information on individual faculty can be found in Appendix A12 and at http://chemistry.unm.edu/faculty.html.

Table 4. Research Activity for CCB Faculty

Faculty	Rank	Grants	Recent Pubs	Total Pubs
Cabaniss	Prof	1	6	60
Dunaway-Mariano	Prof	4	16	188
Evans	Assoc	4	5	40
Giri	Asst	A	4	20
Grey	Asst	2	11	30
Guo	Prof	4	45	260
Habteyes	Asst	A	2	11
Keller	Assoc	1	2	63
Kemp	Prof	3	18	73
Kirk	Prof	3	17	106
Liang	Asst	A	2	12
Melancon	Asst	A	0	12
Paine	Prof	1	12	243
Qin	Asst	A	3	23
Wang	Prof	3	38	113

A = Assistant professor with internal funding only
Recent Pubs = Journal articles published 2010-2012

VII. Resources and Planning

In recent years, resource allocation and planning has been performed principally by the chair and on a year-to-year basis. This method of operation may be partly in response to political disarray within the department and low faculty numbers, but it should not be allowed to continue. Unfortunately, the department has not recently had a strategic planning committee or an external advisory board, and the elected faculty advisory committee was only recently re-constituted. Assembling an external advisory board which will represent departmental alumni, the local and national scientific community and local business leaders is a priority for AY 2013-2014.

The department has three principal revenue sources. “Hard money” support from the university coming from tuition and state formula revenue is used for instructional, administrative and general expenditures (I&G). In AY 2011-2012 CCB received $3.7M in I&G funds to cover faculty and staff salaries, TA’s, operating expenses, etc. A more flexible sub-category of this I&G funding is derived from the extended university (EU), and until recently this amount was linked directly to enrollment in CCB online courses. In AY 2011-2012, the department received $165K in EU funds. Last year, the proportionality between EU funds and enrollment was removed and it is not clear how EU monies will be allocated in the future. “Soft money” support is derived from funded grant overhead (F&A for facilities and administration), and has been used principally to support research efforts and start-up packages for new faculty. In AY 2011-2012, CCB faculty generated ~$650K in F&A for UNM, although only $70K was returned to the department. Until recently, some of the F&A retained at the Provost’s level was contributed to start-up packages for new faculty, but that policy has been suspended; the financing of junior faculty hires remains uncertain. Endowment funds are derived from a variety of accounts overseen by the UNM Foundation, mostly donations for specific scholarships.

The 13 full-time CCB staff positions can be approximately divided into office staff and technical staff, with the latter group being subdivided into teaching and research groups.

The departmental administrator (DA) is the departmental office manager, chief fiscal agent and chief human resources agent; the position is currently vacant (search underway and may be complete by the time of the site visit), and requires a highly responsible individual with a variety of skills and expertise. All other office staff report to the DA, including a departmental accountant, a fiscal technician, an advisement coordinator, a receptionist/administrative assistant and a building manager (see Appendix A13 for specific job descriptions of office and technical staff). This group is often assisted by one or more student employees.

The department facilities and instrumentation director, Dr. Karen Ann Smith, is charged with managing CCB shared instrumentation and supervising one instrumental technician (research scientist) and one electronic/computer technician (research engineer). Shared instrumentation includes 3 NMR instruments and the mass spectrometry facility, as described in section VIII.B below.

The CCB director of undergraduate education, Principal Lecturer K. Joseph Ho, oversees the teaching laboratory staff. Three teaching lab technicians report to the supervising lab technician, Gary Bush. Currently, James Almand and Nancy Boldt support the general chemistry labs taught in the SMLC, Sharon Boyd supports the organic labs taught in Clark Hall, and Bush directly supports the analytical and physical laboratory sections.

The UNM library system provides direct access to numerous electronic and print journals, databases and other information resources relevant to chemical teaching and research (see http://libguides.unm.edu/chemistry). CCB has a designated librarian, Donna Cromer, who assists with student training and chemical acquisitions. Students and faculty have electronic access to all ACS, Elsevier, Pergamon and other journals, and to the Web of Science and SciFinder Scholar search services. Data librararians are also available to assist with NSF- and NIH-mandated data plans.

VIII. Facilities

A. Space The department of Chemistry and Chemical Biology is centered in Clark Hall, where the department offices are located, but occupies space in several other buildings as well. Clark Hall currently has ~10,000 ft^2 of office space (faculty offices + departmental offices), 14,000 ft^2 of instructional lab and support space, ~2000 ft^2 of shop and basement utility space, and 24,000 ft^2 of research lab space. Unfortunately, Clark has been in need of major renovations since at least 1988, and much of the lab space is greatly underutilized due to inadequate electrical supply, plumbing and/or air handling. Several research labs are currently unoccupied due in part to inadequate hood space and ventilation.

Recent passage of a general obligation bond has generated $16 million for renovation of Clark Hall, which is currently in the planning stage. Clark is comprised of two wings; the older, 2-story Clark wing is ~60 years old, while the newer 3-story Riebsomer wing is ~40 years old. Current estimates for upgrade of utilities alone are $7-10 million for hard costs (add ~30% for soft costs), so it is unclear how much money will be allocated to visible lab renovation and re-configuration.

The Science and Math Learning Center currently houses all the general chemistry teaching labs and has offices for lab personnel and TA office hours. Recently-passed legislation would provide $5 million (of $6 million needed) to expand the SMLC to include organic chemistry teaching space. This would not only improve the learning environment for hundreds of organic lab students per semester, but will allow re-purposing of a large Clark Hall laboratory (room 150).

Several CCB faculty have their principal lab spaces outside of Clark Hall. Hua Guo's theoretical and computational group is located in Bandelier East, while Cabaniss has shared space with environmental engineering in Centennial Engineering. These buildings are each a short walk from Clark Hall, but Rick Kemp has space at AML and Terefe Habteyes has his principal lab at the Center for High Tech Materials (CHTM), both located on South campus ~1 mile from Clark Hall.

B. Equipment

CCB has equipment available in individual research group laboratories, through teaching facilities (when not being used for instruction) and via the Analytical Chemistry Service directed by Dr. Karen Ann Smith. The Analytical Chemistry Service facilities are equipped with modern, state-of-the art equipment and operated by well trained staff. The facilities include magnetic resonance, x-ray and mass spectrometry instruments to support investigators wishing to analyze compounds ranging from organic small molecules to large proteins.

The Nuclear Magnetic Resonance (NMR) Facility contains 3 spectrometers, all with temperature control and multiple RF channels and housed in the basement of Clark Hall:
a Bruker Avance 500 used primarily for liquids with 3 solution probes;
a Bruker Avance 300 widebore used primarily for solids with 8 probes;
a Bruker Avanc 300 standard for liquid only with 2 probes.

The X-ray facility consists of a Kappa Apex II diffractometer with a 4-circle Kappa goniometer and CCD detector, and is housed at the Advanced Materials Lab.

The Mass Spectrometry and Proteomics Facility includes an Applied Biosystems 4700 Proteomics Analyzer (Mass range: m/z 200,000 for MS, m/z ~2,000 for MS/MS, MALDI ionization) and a Water/Micromass LCT Premier (Mass range: m/z 12,000+, with electrospray, APCI and APPI ionization). The facility occupies several labs on the 2nd floor of the Riebsomer wing of Clark Hall.

Appendix A14 lists equipment in individual and teaching labs.

The department does not maintain significant computing facilities besides workstations and groups of workstations, but relies upon other sources including the UNM Center for Advanced Research Computing (CARC) for compute-intensive applications.

IX. Program Comparisons

The New Mexico Division of Higher Education (HED) has recently designated a new set of 27 peer institutions for UNM. The chemistry departments at these universities range from highly-regarded "top 20" programs to much smaller departments which do not offer a Ph.D.

UNM Chemistry is ranked 10-11th out of these 27 chemistry departments based on its annual graduating class of B.A. and B.S. students and 12-14th of 27 based on the number of Ph.D. degrees awarded (Table 5). Based on undergraduate degrees awarded, UNM CCB is much smaller (2X) than flagships in Texas, Arizona, and Colorado and neighboring Arizona State, and somewhat smaller than (<2X) than Texas A&M, Texas Tech, and Utah. CCB awards more bachelors' degrees in chemistry than NMSU, Colorado State, Utah State and Kansas State.

However, UNM has only 20.5 permanent faculty members, including 16.5 tenure-track faculty and four lecturers (but not two visiting assistant professors or any emeritus faculty). The CCB faculty size is only 24th of the 27 departments in this category even though the UNM faculty count includes lecturers while many of the other departments do not. While the current CCB faculty size is larger than in recent years (see Fig. 1), it is on average a factor of two smaller than chemistry faculties at the other flagship institutions. Only two of the peer institutions, one without a Ph.D. program, have fewer faculty.

While ranking departments by size may be relatively unambiguous, size alone does not ensure high quality research and education. On the other hand, ranking the "quality" of academic department is a highly contentious process, one with as many rankings as there are rankers. Table 6 shows rankings of the local group of chemistry graduate programs obtained in several ways. The first ranking, "USNews" (published by US News and World Report), is based on surveys which reflect reputation in the field. The other rankings were all compiled by the National Research Council based on a set of 21 metrics. S-rankings emphasize those metrics which scholars in the field consider most important, while research rankings use subsets of the metrics related to research productivity. The range between high and low for a particular ranking can be thought of as a confidence interval.

Although the program rankings (USNews, S-rank and Research rank) were obtained through different mechanisms, the same pattern emerges in each. The UNM department of Chemistry and Chemical Biology is ranked 17-18th by the US News and World Report, 13th of 27 by a mean of the S-rankings, and 14-15th of 27 by the mean R-ranking. This department is thus seen as significantly weaker than the departments at other flagship universities in the Four Corners states and Texas, although stronger than departments at NMSU and Texas Tech.

The NRC also ranks departments according to diversity and student-valued metrics, and in these areas UNM typically is among the top 2-4 schools listed.

These various rankings suggest that while CCB may have a relatively good environment for students, UNM lags behind other flagships in the region with respect to the quality and 'profile' of its chemistry department. This is probably related to CCB's small faculty size relative to those departments and to issues resulting from poor retention of junior faculty.

Table 5. Size of Peer Group Chemistry Departments by Graduates and by Faculty

University	ACS BS	Non-ACS BA + BS	MS	PhD	Faculty	
U of Texas Austin	192	0	17	30	51	
Texas A&M	22	45	6	33	76	
U of Colorado - Boulder	5	79	4	24	55	
U of Utah	46	19	9	29	32	TT
Univ of Arizona	19	55	12	25	46	
Colorado State	18	8	9	16	35	
Arizona State	10	91	16	23	68	
U of California-Riverside	9	19	12	11	37	TT
U of Iowa	17	5	12	15	32	
U of Kansas	15	21	2	13	29	
U of Nebraska-Lincoln	0	9	6	5	26	TT
U of Tennessee-Knoxville	3	14	5	11	29	
Kansas State	6	4	2	9	21	
U of Houston	27	10	8	15	31	TT
U of Missouri-Columbia	8	19	3	6	21	TT
U of Oklahoma-Norman	7	54	12	16	25	TT
UNM	**0**	**37**	**4**	**11**	**20.5**	
Utah State	6	14	3	6	21	TT
Oklahoma State U	5	5	3	7	21	TT
Texas Tech	15	44	1	3	33	
NMSU	0	31	3	5	21	
U of Texas Arlington	12	2	4	6	21	
Florida International U	18	38	12	9	31	TT
U Colorado-Denver	8	6	4	-	15	TT
U of Nevada-Las Vegas	3	15	8	2	19	TT
U of Texas El Paso	12	0	7	0	21	

TT Tenured and tenure-track only (lecturers not counted)
Degrees awarded 2008-2009 from ACS CPT
Faculty numbers from recent (2013) website listings

Table 6. Rankings of Peer Group Graduate Chemistry Programs

University	USNews	S-Rank High	S-Rank Low	Research High	Research Low
U of Texas Austin	12	16	59	9	36
Texas A&M	19	41	97	30	106
U of Colorado - Boulder	26	19	67	13	63
U of Utah	36	18	61	21	88
Univ of Arizona	38	27	76	25	99
Colorado State	45	67	141	24	101
Arizona State	60	31	86	19	87
U of California-Riverside	60	51	113	39	109
U of Iowa	67	41	104	39	123
U of Kansas	67	43	105	48	137
U of Nebraska-Lincoln	78	109	162	104	163
U of Tennessee-Knoxville	78	80	139	74	140
Kansas State	83	52	117	44	123
U of Houston	83	55	119	45	121
U of Missouri-Columbia	83	92	150	80	150
U of Oklahoma-Norman	90	56	116	80	149
UNM	**94**	**50**	**129**	**72**	**157**
Utah State	94	91	152	97	166
Oklahoma State U	107	156	175	126	172
Texas Tech	107	102	159	110	168
NMSU	129	128	169	112	167
U of Texas Arlington	129	N/R			
Florida International U	not pub.	80	153	103	172
U Colorado-Denver	not pub.	N/R			
U of Nevada-Las Vegas	not pub.	N/R			
U of Texas El Paso	not pub.	N/R			

S = scholarly qualities
R = research metrics

USNews = rankings from US News and World Report in 2010.
grad-schools.usnews.rankingsandreviews.com/best-graduate-schools/top-science-schools/chemistry-rankings
Other rankings from the National Research Council (NRC) 2010 report.
http://chronicle.com/article/NRC-Rankings-Overview-/124713/

X. Future Directions for UNM CCB

Strengths- Principal assets for the program include a cadre of high-quality junior faculty and a complement of successful senior faculty mentors, proximity to two national laboratories and the attractive quality of life in New Mexico. Highly competitive searches allowed CCB to bring in 6 assistant professors over the last 6 years, now comprising over 1/3 of the tenure track faculty; these junior faculty bring expertise in synthesis, instrumentation and chemical biology which they are applying to photonic and electronic materials, and to biomedical research. Over this same time period, the department added three lecturers who are experimenting with active learning and on-line pedagogies. Sandia and Los Alamos National Laboratories are a potential source of ideas, collaborators and instrumentation; "outreach" labs like the Center for Integrated Nanotechnology (CINT) and the Advanced Materials Laboratory (AML) are specifically designed to attract and enhance university collaborations, and provide access to resources for analysis and fabrication with minimal cost to faculty researchers. The labs and the unique cultural life in the high desert are potent recruiting tools for additional faculty and students.

Weaknesses- Weak areas for CCB include internal factionalism, small faculty and graduate student numbers, badly aging facilities and equipment, and state-wide problems with K-12 education. The 2003 GRC noted that "*The Dept. of Chemistry appears to have a culture of individuals under one roof rather than a community."* Unfortunately, in many ways this behavior persists, even rising to the level of un-civil and unprofessional interactions among faculty. This works to CCB's disadvantage in many ways, including low retention levels of junior faculty, minimal participation in large-scale grant proposals, and a history of unsuccessful department-wide initiatives. In addition, the small size of the research-active faculty hampers graduate student recruitment in a competitive environment, and departmental F&A generation currently is too low to support necessary faculty hiring packages. Large sections of Clark Hall are unused or underused because the space is unsuitable for modern research. Labs which are in use are plagued by broken pipes, inadequate ventilation, and problematic power supply. In addition to the toll on research efforts; these facility problems significantly complicate faculty recruiting and retention. Finally, New Mexico consistently lags most of the nation in pre-college education metrics, and our incoming students are frequently poorly prepared for college-level science courses.

Opportunities- At the same time, ongoing events provide the department with several opportunities, some of which may not be repeated. Renovation of Clark Hall and moving the organic teaching labs into the SMLC initially will be disruptive, but will eventually greatly improve the square footage and quality of usable lab space. Not only will renovated space improve CCB recruiting and research, but it will enable new collaborations with other units which require access to modern lab space and CCB facilities. The approaching decrease in federal research funding opportunities should also help to create interdisciplinary collaborations by forcing faculty away from increasingly scarce single-PI grants. Finally, the informal experiments in pedagogy conducted by some of our lecturers and PTIs are providing the background for creation of a formal program in chemical education. UNM is the only flagship university that is both designated Carnegie High Research and an HSI (Hispanic Serving Institution). By partnering with the College of Education and other STEM departments, we have the possibility of establishing a graduate program in disciplinary-based educational research which could show us how to improve student learning in the UNM context- “A flagship university education for America’s emerging majority”.

Threats- CCB faces both internal and external threats, both immediate and over the next 10 years. Perhaps the most serious threat is the possibility that a combination of inadequate funding and/or departmental factionalism will decrease the research active faculty numbers below “critical mass”, leading to a spiraling decrease in research activity and graduate student numbers and further faculty loss. Avoiding this depends upon improving the departmental “culture”, increasing external research funding, and stabilizing departmental I&G (instructional and general funds from tuition and the state) budgets in some way that acknowledges the very significant teaching mission beyond historical budgeting. A longer term threat is the possibility that online courses, either MOOCs or more traditional on-line education being aggressively pursued by universities in neighboring states, will erode the student base on which UNM’s I&G funding depends.

Chemistry and Chemical Biology: 10-year goals (AY 22-23)
The central science at UNM

I. Departmental Assets

24 Tenure-track faculty
6 Lecturers (long-term)
Top-quality research space in renovated Clark Hall and shared labs (e.g., AML, PandA)
Access to state-of-the-art chemical instrumentation (NMR, MS, ESR, TEM, etc.)
Skilled staff to support administrative (6), teaching (6) and research (5) tasks

II. Undergraduate Teaching Mission

Widespread science literacy, especially for education majors, via introductory chemistry
Well-integrated support for BA and BS in other science and engineering programs
Popular and high-quality BA and BS chemistry programs
Online courses available for all of the above (except upper-division labs)

III. Graduate Teaching Mission

Active contributions to interdisciplinary graduate programs (NSMS, DBER, OSE, WRP)
Graduate student enrollment of 80-100 full-time students, ~75% on RA
25% PhD students receiving highly competitive positions (e.g. NRC or HHMI post-docs)

IV. Research and Recognition

Research publications and funding ranked in top 25 public universities
National awards (NSF CAREER, ACS, editorships, etc.) for over 1/3 of faculty

V. Outreach and Community Integration

Faculty, post-docs and graduate students better reflect NM population
Productive partnerships with local industry and national labs
Large and active departmental alumni group

Chemistry and Chemical Biology: 4-year goals (AY 16-17)

a. Maintaining, civil, professional and collaborative departmental environment

b. Reaching a level of 20 FTE tenure-track faculty

c. Successful renovations of Clark Hall

d. Graduate recruitment balanced with respect to sub-discipline and student diversity (>50% domestic students, >25% Hispanic and Native American)

e. Improving science literacy for UNM undergrads by offering "Chemistry in our Community"

f. Classes and programs developed for Chemical Education (secondary, and post-secondary)

g. Restructuring graduate program to reflect departmental strengths

h. Restructure undergraduate general/organic sequence to better serve biology and engineering students

i. Expanded online education to include all 1xx courses and organic lecture classes for non-majors

j. Productive research collaborations across campus and with LANL and SNL

k. Teaching collaborations across campus and across NM (branch campuses, other universities)

l. Constituting an external advisory board

m. Expanded industrial collaborations- internships, student placement, start-ups, etc.

n. Workshops and certificate programs for post-grads

o. All current assistant professors will have external funding, 50% will have "awards"

p. >75% of BS and >50% of BA graduates will have research experience

q. A revenue-neutral shared instrumentation facility for mass spectrometry and other methods

Appendices

Appendix A1. Former CCB Faculty (based upon W. Litchman's departmental history)

Fritz Schreyer Allen (PhD 1969, Univ of Illinois, Biophysical), (arrived 1970, became Acting Dean of the College of Arts and Sciences, retired 2002). Served as chair of chemistry. Among other work, Fritz was hired as a consultant for Mesa Diagnostics (Los Alamos) which became Acrogen. He then consulted for Chromex, Inc, which holds patents related to Raman spectrometers. Chromex became New Chromex, Inc, and was eventually sold to Bruker.

Thomas Bein (PhD 1984, University of Hamburg, Inorganic), (arrived 1987, left for Purdue University, 1991, from 1999 at the University of Munich, Germany). Tom is professor of chemistry at the University of Munich and has a strong interest in nanotechnology.

Carlos Bustamante (PhD 1981, University of California-Berkeley, Biophysics), (arrived 1982, left for Univ of Oregon, 1992). Now at the University of California-Berkeley. Awarded Alfred P Sloan Foundation Fellow (1985), Presidential Lecturer in Chemistry, University of New Mexico (1986) and State of New Mexico Eminent Scholar (1989). He has twice been a Howard Hughes Medical Institute Investigator (1994-98, 2000-present), and was elected Fellow of the American Physical Society (1995). Carlos' research efforts are primarily in the area of the structural characterization of nucleo-protein assemblies. He uses high resolution scanning force microscopy (SFM) to investigate the structure of chromatin and protein-nucleic acid complexes involved in the control of transcription in prokaryotes.

Roy Dudley Caton (PhD 1963, Oregon St Univ, Analytical), (arrived 1963, retired 1994). Roy is a Master Gardener and recognized expert in fertilizers, soils, and naturalizing bulbs.

Lorraine M DiStefano Deck (PhD 1989, Univ of New Mexico, Organic), (arrived 1969, still serving at UNM). Lorraine has extensive experience at UNM and is recognized for her work in molecular design, synthesis, and kinetic inhibition studies of biologically important compounds structurally related to natural products. She received the Camille and Henry Dreyfus Scholar award in 1997-1999 and the NSF Career Advancement award and NSFILI award in 1998-2000.

Mark Hampden-Smith (PhD 1984, London University, Inorganic) (arrived 1988, retired to enter business). Mark, with Toivo Kodas, founded Superior MicroPowders in 1997 and made such a success of the business that it was purchased by Cabot Corporation (Boston) in 2003 for $16M (see http://www.azom.com/news.asp?newsID=652). They continue to work with the new combination business as general managers for the company's local operations and have recently (2006) leased a large manufacturing space in Washington

Commerce Center here in Albuquerque. In addition, they have a location at Mechenbier's commerce center.

Ulrich Hollstein (PhD 1956, Univ of Amsterdam, Organic), (arrived 1967, retired 1993, deceased 2001).

William Morris Litchman (PhD 1965, Univ of Utah, Physical), (arrived 1967, University of Utah, retired 1994). Bill worked in the field of natural-abundance carbon-13 and nitrogen-15 nuclear magnetic resonance, particularly structural and solvent effects on chemical shifts. He was an Associated Western Universities scholar at LANL for five summers (1968-73) and a Senior Research Fellow at the University of London (Queen Mary College) (1974-75).

Donald Reed McLaughlin (PhD 1965, Univ of Utah, Physical-theoretical), (arrived 1964, retired 2002). Don was director of the Los Alamos Graduate Center from 1981-1986 and a visiting staff member at LANL (1970-1980). He is a visiting associate professor in the Department of Computer Science, UNM.

Cary Jacks Morrow (PhD 1970, Tulane Univ, Organic), (arrived 1972, retired 2008). Cary has twice been the chair of chemistry. Cary's research interests include applications of enzymes to problems in the synthesis and modification of polymers and optically active polymers. He has won an excellence in teaching award.

Thomas M Niemczyk (PhD 1972, Michigan St Univ, Analytical), (arrived 1973, retired 2006). Served as chair of chemistry. Tom is seriously involved in bicycling in New Mexico, serving as volunteer for races and other biking activities. At age 59, Tom was 7 minutes off the leader in a 54-mile “Tour de Los Alamos” race (10th place). Tom won a 1992 technical excellence award from Global Research Collaboration for his work on "Chemometrics for the Analysis of Dielectric films - Multivariate Analysis of FTIR Spectra for B and P Concentration and Thickness of BPSG Films." He shared that award with two co-authors. In 2005, Tom (along with UNM department chairs in Biology, Earth and Planetary Sciences, Physics, Anthropology, and Mathematics) took a stand against the adoption of “Rio Rancho Science Policy 401” which allowed non-scientific topics such as “intelligent design” and “evidence against evolution” into public school science classrooms.

Peter Remsen Ogilby (PhD 1981, University of California-Los Angeles, Organic), (arrived 1983, left for Aarhus University, Denmark). Peter is professor of chemistry and director of the Center for Oxygen Microscopy and Imaging at Aarhus. See http://www.chem.au.dk/~comi/.

Mark R Ondrias (PhD 1979, Michigan State University, Biophysical), (arrived 1982, became Assistant Dean of University College 2000, still serving at UNM). Mark is very much interested in rock climbing and is noted for his office furniture.

Joseph Vincent Ortiz (PhD 1981, University of Florida, Theoretical), (arrived 1983, left for Kansas State Univ, 1996). University Distinguished Professor at Kansas State Univ (9 yrs there). Named chair of Chemistry and Biochemistry and Ruth M Mollette Professor of Chemistry at Auburn University.

Eleftherios Paul Papadopoulos (PhD 1961, Univ of Kansas, Organic), (arrived 1969, retired 2000, deceased 2008). Paul's major research interest involved synthesis and characterization of heterocyclic compounds.

Su-Moon Park (PhD 1975, University of Texas-Austin, Electrochemistry), (arrived 1975, left for Pohang University of Science and Technology, Pohang, Gyeongbuk, South Korea, 1994). Su-Moon was elected a life-time member of the Korea Academy of Science and Technology (1997). In 1999 he received the Director's Award from the patent administration office of Korea, in 2000 he received T K Rhee's Award of Excellence (given to the Korean Chemical Society member with the highest achievement in chemistry), and in 2001 he received the Q Won Choi's Award in electrochemistry (similar to T K Rhee's award but in electrochemistry). He has also received the Khwarizmi International Award for outstanding contributions to basic science (Iranian Research Organization for Science and Technology, 2008).

James D Satterlee (PhD 1975, University of California-Davis, Biophysical), (arrived 1981, went to Washington State Univ, 1989). Jim was an Alfred P Sloan Foundation Fellow (1983-87) and was awarded a National Institutes of Health Research Career Development Award from 1988-92.

Riley Schaeffer (PhD 1949, University of Chicago, Inorganic), (arrived at UNM in 1981, retired 1994). Riley served as chair of chemistry from 1981-1987 . He was a Guggenheim Fellow in 1965. He was recently honored by the establishment of the Riley Schaeffer Endowed Lectureship in Chemistry (2008). He has served as faculty member at Iowa State University (1952-1957), Indiana University (1958-1976), University of Wyoming (1976-1981), and retired from UNM in 1992. He served as chemistry department chair at Indiana (1967-72) and UNM 1981-87). He was Dean of the College of Arts and Sciences at Wyoming (1976-81). His research interests included the synthesis and characterization of boranes and carboranes.

David L Vander Jagt (PhD 1967, Purdue Univ, Biochemistry), (arrived 1972, left for department of Biochemistry, UNM, 1994). Dave's research includes 1) the chemistry of diabetic complications including the role of endogenous aldehydes, oxidative stress and growth factors in endothelial cell dysfunction, 2) structure-based drug design including dehydrogenases (Rossmann fold), cholesterol esterase, protein disulfide isomerase, thioredoxin, BCLxl, urokinase, 3) biological properties of the natural product polyphenols and analogs: gossypol, curcumin, resveratrol, and 4) development of anti-inflammatorydrugs targeted at transcription factors NFkB & AP-1.

Edward A Walters (PhD 1966, Univ of Minn, Physical), (arrived 1968, retired 2004). Ed has served in several capacities for the International Conference on Technology and Education, as a member of the Planning and Advisory Board and on conference executive committees (1998-2001). He is an expert on the use of fire-retardant materials.

James R Brozik (PhD 1996, Washington State University, Physical) (arrived 1999, resigned to go to Washington State Univ, 2006).

Richard M Crooks (PhD 1987, University of Texas-Austin, Analytical) (arrived 1989, resigned in 1991 to go to Texas A & M University). Richard is now at the University of Texas-Austin where he serves as department chair and the William H Wade Endowed Professor in Chemistry. He is involved in electrochemistry, catalysis, nanomaterials, and biological and chemical microsensors. Richard has some interesting things to say about science and academia at: http://esi-topics.com/msa/interviews/RichardMCrooks.html

John Engen (PhD University of Nebraska, Analytical) John joined CCB in 2001, was tenured and promoted to Associate Professor in 2006 and resigned to move to Northeastern Univ. in 2007. Currently he is Professor of Bioanalytical Chemistry and Faculty Fellow in the Barnett Institute of Chemical and Biological Analysis at NEU. He is a Fellow of the European Molecular Biology Organization (EMBO), was recently recognized with the 2009 Arthur F. Findeis Award from the American Chemical Society, and has served on the Board of Directors for the American Society for Mass Spectrometry (ASMS). http://www.hxms.neu.edu/index.htm

Christie G Enke (PhD 1959, University of Illinois, Analytical) (arrived 1994, retired 2006). Chris is professor emeritus of chemistry at Michigan State University and the University of New Mexico. He has served as chair of the Analytical Division of the American Chemical Society, as President of the American Society for Mass Spectrometry, and chair of the Computers in Chemistry Division of the American Chemical Society. He received ACS awards for scientific instrumentation (1974), computers in chemistry (1989), the ASMS award for distinguished contribution to mass spectrometry (1993) and the J Calvin Giddings award for excellence in education from the ACS (2003).

Philip D Hampton (PhD 1989, Stanford University, Organic) (arrived 1991, left for California State University, Channel Islands). Philip is professor of chemistry and department chair at California State University-Channel Islands.

David L Tierney (PhD, University of Michigan, Inorganic) (arrived 2000, left in August 2009 for Miami University - Ohio). Dave is interested in electron-nuclear hyperfine interactions in paramagnetic states and bio-inorganic chemistry.

Ignacio Villegas (PhD 1991, University of Georgia, Analytical) (arrived 1996, resigned 1999).

Richard Watt (Ph.D. 1998, Univ. Wisconsin, Biochemistry) Arrived 2000, resigned 2006. Currently Asst. professor of Bioinorganic Chemistry at BYU.
http://www.chem.byu.edu/users/rwatt

Appendix A2. Departmental Handbook

Handbook for Faculty Members of the Department of Chemistry and Chemical Biology

Approved April 3, 2013

Table of Contents

I. Preface

This Handbook provides the faculty of the Department of Chemistry and Chemical Biology (CCB) with a written record of departmental procedures and policies. It has been constructed to be a continuation of University procedures and policies that are outlined in the UNM Faculty Handbook (http://handbook.unm.edu). The policies and procedures outlined herein are subject to revision as a result of careful consideration and 2/3 majority vote of the CCB faculty.

II. Authority

Article II, (College and Departmental Organization) in Section 4(a) of the Faculty Constitution (which appears as Policy A51 in the Faculty Handbook) states as follows:

Sec. 4(a) Departments: The Faculty of each Department shall, with the advice and consent of the Dean of the College, decide upon the organization and procedure for the efficient functioning of the Department.

The CCB bylaws and guidelines that follow amplify and complement parts of the UNM Faculty Handbook. Nothing in this document shall be interpreted as revising or contradicting the provisions of the UNM Faculty Handbook.

III. Voting Faculty

All faculty holding a ≥0.5 appointment in CCB shall be eligible to vote on department matters, consistent with Policy A51 in the Faculty Handbook, section 1.

Sec. 1(a) Membership: The University Faculty shall consist of the Professors, Associate Professors, Assistant Professors, Lecturers, and Instructors, including part-time and temporary appointees. The President of the University, Vice President for Academic Affairs, Vice President for Student Affairs, Vice President for Research, Vice President for Business and Finance, Associate Vice President for Computer and Information Resources and Technology, Director of the Medical Center, Deans of Colleges and Schools, Dean of Graduate Studies, Dean of Students, Dean of the University College, Dean of Admissions and Records, Registrar, Dean of Continuing Education and Community Services, Director of the Center for Graduate and Upper Division Programs Studies at Los Alamos, Director of the Center for Graduate Studies at Santa Fe, Dean of Library Services, Commanding Officers of the ROTC Units, and the Secretary of the University shall be ex-officio members of the Faculty whether or not they are actively engaged in teaching.

(b) Voting Faculty: Members of the University who are eligible to vote shall include all full-time members of the University Faculty holding professorial rank (instructors, assistant professors, associate professors, and professors) or lectureships. No person holding an interim or temporary appointment on the teaching staff shall be a member of the Voting Faculty unless he or she be a member ex officio or on an initial term appointment. The ex officio members of the University Faculty as listed in Sec.1(a) shall be ex officio members of the Voting Faculty.

After the University approved part-time tenured/tenure-track faculty appointments (1998), voting privileges at all organizational levels were extended to this group of faculty members.

Visiting and temporary faculty do not vote, nor do untenured faculty vote on tenure decisions, nor do faculty vote on promotion to ranks above their own.

IV. Guidelines for Meetings of the CCB Faculty

Schedule- Regular faculty meetings will be held once every four weeks at a minimum during the academic year. A regular one-hour time slot will be set aside for meetings during which no departmental courses are taught. The chair may call additional regular meetings as needed, using the same time slot when possible. Emergency meetings to deal with urgent items may be held in other time slots if necessary. All committee and faculty meetings will be conducted in a civil and professional manner in accordance with UNM policy (Respectful Campus Policy, University Business and Procedures manual #2240: http://www.unm.edu/~ubppm/ubppmanual/2240.htm).

Attendance- All CCB faculty are expected to attend assigned committee and departmental faculty meetings. As a courtesy, those unable to attend will inform the committee Chair or the Department Chair, in advance, of their absence.

Agenda- A meeting agenda will be distributed to all faculty 24 hours in advance of each regular meeting. Faculty wishing to place an item on the agenda should contact the departmental administrator at least 48 hours before the meeting. The agenda will indicate if an item may require a vote or is for discussion only. No item will be voted on at a regular meeting unless it has been discussed at a previous meeting. The text of proposed motions should be distributed to the entire faculty at least 48 hours before the meeting. The chair may add urgent, last-minute agenda items for emergencies only.

Conduct- Meetings will be conducted by the chair or, in the chair's absence, the associate chair. All regular meetings will contain a time for general comments, including requests for topics to discuss at the next meeting. Each faculty member will have an opportunity to speak to the topic in each discussion, although the chair may limit the time per speaker.

Voting- Decision by consensus is the general goal, but may not always be possible. Votes to modify this handbook, to change degree requirements or other substantial issues as designated by the chair must have a 2/3 majority (of those voting yes or no) for approval. Personnel decisions and other especially important decisions (as designated by the chair) will be made by confidential written ballot. Faculty may abstain from voting if they feel the matter is outside their interests or expertise.

Summaries- A meeting summary, containing the general topics of discussion and the decisions reached, will be posted by the departmental administrator within *one week* after the meeting. Faculty are expected to read the summary and send any corrections to the administrator within one week of receipt.

V. Guidelines for the Chair

Appointment The Dean of Arts and Sciences shall appoint a chair after consultation with departmental faculty, as outlined in Section C40 of the UNM Faculty Handbook (http://www.unm.edu/~handbook/C40.html).

Role of the Chair The department Chair has several overlapping roles
Administrator The Chair is responsible for the day to day operations of the department. This role includes, but is not limited to, personnel matters (faculty recruitment and hiring, evaluations, disciplinary actions, and delegation of responsibilities), teaching workloads (class scheduling, instructor assignments, peer evaluations), and budgetary oversight (resource allocation) as well as supervising departmental employees and implementing procedures in accordance with university requirements

Department Representative As the public face of the Department, the Chair represents the interests, expertise, needs, and opinions of the Department's entire faculty, staff, and students to other departments, other Chairs, the Dean and other relevant UNM administrators. The Chair also communicates the department's mission, strengths, and needs to the outside world as needed and as opportunities arise.

Facilitator It is the Chair's role to create a working environment in which faculty interactions and collaborations may flourish; in which faculty are provided the clerical, fiscal, and administrative support necessary to successfully attain both their own and institutional goals; and in which all students are afforded the opportunities to successfully complete their academic classes and programs.

Leader The Chair is expected to introduce and foster new ideas into departmental discussions, and fashion consensus among differing viewpoints. This includes leading the department as it reaches consensus about its mission. The Chair should foster innovation and creativity throughout the teaching, research, and service missions of the department.

Chair Behavior The Chair occupies a position of authority that carries with it expectations regarding modes of behavior. It is expected that the Chair will conduct all business of the department in an objective manner and that resources will be allocated fairly and proportionately to all areas and objectives. To that end, given that the research active faculty members are the sole contributors to the department overhead account, any financial decisions involving this account should be made in conjunction with at least the Advisory Committee. In addition, it is assumed that when faculty, staff and students request a confidential discussion with the Chair that the discussions will be kept confidential excepting for those situations that may require official reporting. The Chair will in all instances conduct himself or herself in a manner that precludes any perception of favoritism or targeted dislike or disdain.

Duties and responsibilities The faculty handbook and university regulations describe many of the responsibilities and duties of a department chair. This list is not intended to repeat or replace those documents. The CCB department chair-

Hires and supervises staff, directly or indirectly
Hires and supervises faculty
Provides annual evaluations of faculty and staff
Oversees tenure, promotion and re-appointment processes
Schedules classes and makes teaching assignments
Presides over faculty meetings
Appoints the associate chair and other faculty administrative positions as needed
Appoints chairs and members of standing committees
Allocates department-controlled space
Allocates the departmental budget
Represents the department within and outside the university

VI. Guidelines for the Advisory Committee
Purpose The Advisory Committee advises the chair on substantive policy, procedural and personnel decisions. As such, it is important that the committee enjoys the confidence of the faculty as a whole and is able to represent a variety of viewpoints in discussions with the chair.

Duties The committee will meet at least monthly during the academic year, meetings to be chaired by the department chair, associate chair or a designated member of the AC. The committee will be asked to provide advice on:

Membership on ad hoc committees
Faculty salary increments during years when merit raises are available
Substantial policy, procedure or curriculum proposals, whether originating from the chair or from other committees

The committee may also be asked to provide advice on other issues and to prepare or evaluate reports on subjects of broader import.

Composition The advisory committee will consist of four faculty members serving staggered 2-year terms. All departmental faculty are eligible to serve, but the department chair will not be a member of the committee.

Selection Two committee members will be elected each May to begin a 2-year term the following academic year. The date of election will be announced at least two weeks in advance, and candidates should be nominated (including self-nominated) at least one week in advance. A list of nominees who have agreed to be candidates will be distributed three days in advance of the election. Each faculty member may vote for two candidates. The two candidates receiving the most votes will become members of the advisory committee.

VII. Guidelines for Committees

In addition to the elected advisory committee, the department will have standing committees and *ad hoc* committees to carry out various functions.

Purpose Standing committees may exist for multiple years, and membership should change slowly to provide continuity. They typically have regular (annual) functions and special charges for certain years, and the committee chair may be required to report on these to the departmental faculty and chair. Typical standing committees might include an undergraduate studies committee, a graduate studies committee and a building/facilities committee. *Ad hoc* committees are formed for a special purpose and are discharged when that purpose is fulfilled. Examples of *ad hoc* committees include faculty search committees, tenure and promotion committees and special review committees.

Appointment The chair will appoint members of **s**tanding committees to three year terms, and will select one committee member as committee chair. The chair will consult with the advisory committee before appointing members and a chair for *ad hoc* committees, and the members will serve until the committee is discharged.

Charge and scope At the beginning of the academic year, the chair will provide each standing committee with a written charge or list of responsibilities. The charge is not intended to be an exhaustive list of required actions, but to avoid overlap or duplications with other committees or individuals. Similarly, the chair will provide each *ad hoc* committee with a written charge when it is formed.

VIII. Guidelines for Tenure Decisions

Awarding of tenure is one of the most important processes for the department, college and university. Rules which apply to all faculty members can be found in the faculty handbook **Policy on Academic Freedom and Tenure** where section B.4 discusses annual review, mid-probationary review and the tenure review (http://handbook.unm.edu/newhb.html), Additional information pertaining specifically to A&S can be found on the college guideline pages (http://www.unm.edu/~artsci/for-faculty/promotion-tenure.htm). Departmental guidelines cannot contradict or supersede those rules, and in case of apparent disagreement the university and college level rules must apply.

Expectations The general areas of evaluation for a successful tenure decision, set forth in the UNM faculty handbook policy on academic freedom and tenure, are:

"1.2 CATEGORIES FOR FACULTY PERFORMANCE EVALUATIONS
(a) The categories in which faculty performance will be evaluated are the following:
(1) Teaching, (2) Scholarly Work, (3) Service, (4) Personal Characteristics…
(b) In order to earn either tenure or promotion or both, faculty are required to be effective in all four areas. Excellence in either teaching or scholarly work constitutes the chief basis for tenure and promotion. Service and personal characteristics are important but normally round out and complement the faculty member's strengths in teaching and scholarly work."

CCB will evaluate candidates on an absolute basis; a tenure (or other personnel) decision about one candidate should be based only on the performance and promise of that candidate, not a comparison to a prior or subsequent candidate. Evaluations encompass both past performance and future promise.

In CCB, research-active faculty are expected to obtain external research funds, supervise graduate and undergraduate students and/or postdoctoral fellows, participate in departmental seminars and governance, and teach a normal load of approximately one three-unit course per semester.

Expectations for a successful tenure decision are:
(1) Teaching- The candidate has demonstrated effective classroom teaching through favorable peer and student reviews and through evidence of student learning. Student mentoring and development of course materials can also contribute to the evaluation.
(2) Research- The candidate has established an independent and internationally-recognized research program as evidenced by peer-reviewed publications, externally funded grants, presentations at inter/national scientific conferences and favorable evaluations from recognized scholars in the field. In the chemical sciences this constitutes what the Faculty Handbook calls "Scholarly Work."

(3) Service- The candidate has provided conscientious service to the department via committee memberships and minor administrative roles, and to the profession through manuscript, proposal reviewing, or other like activities.
(4) Personal characteristics- The candidate's interactions with faculty, staff and students have been collegial, professional and considerate.

Mentoring and evaluation of probationary faculty Normally, the department will evaluate assistant professors annually until the 6th year, when a tenure evaluation and vote will occur. The mid-probationary review and evaluation, typically conducted the 3rd year, requires a formal file submission, vote by the faculty, and further evaluation at the college and university level. The tenure evaluation also requires a formal file submission, vote by the faculty, and further evaluation at the college and university level; only the tenure evaluation requires the participation of external, non-UNM referees to evaluate the candidate's research program. Other written evaluations ('annual reviews') will be conducted by the chair in consultation with senior faculty. All evaluations will consider teaching, research and service components, and the candidate is expected to submit a file containing the relevant information for the evaluation period.

Mentoring committee Each probationary faculty member (candidate) will have a mentoring committee charged both with advising the candidate and with presenting the mid-probationary and tenure files to the tenured CCB faculty for discussion. The committee will have three members, two tenured CCB faculty and one tenured UNM faculty from outside of CCB. Once formed, the committee should meet with the candidate at least annually. The chair will appoint the committee members with input from the candidate. A member of the hiring committee, usually the chair, will be assigned temporary mentoring responsibilities once the new faculty member has accepted the department's offer. At least one regular mentor should be selected by the middle of candidate's first semester at UNM, and all three must be selected by end of the candidate's second year. Members of the mentoring committee may be replaced at the request of either the member or the candidate.

Candidate seminars The candidate will present a departmental seminar at the beginning of the Fall term of the 3rd (mid-pro) and 6th (tenure) years in the department. In each case, the seminar should be viewed as an opportunity to present the candidate's overall research program (not simply past results or a subset of overall research) to the CCB faculty and students. *In each case, the seminar should include specific plans for future research*. These seminars should help the faculty form opinions about the research program; it also provides an opportunity for constructive criticism and comments, especially after the 3rd year seminar.

Peer teaching evaluations The candidate's teaching should be observed each term by a tenured faculty member or senior/principal lecturer selected by the chair. A teaching report will be prepared by the observer, and may include comments on the teaching style and subject matter, student preparedness and response, course syllabus, assignments and tests, and other related topics. These reports will be provided immediately to the candidate, and then also included in the candidate's mid-pro and tenure evaluation files, and the CCB chair(s) should ensure that a cross-section of courses taught is represented by the end of year 5.

Annual reviews General information on the annual review process can be found in section 4.2 of the **Policy on Academic Freedom and tenure-**
The annual evaluation file should contain a cv, written materials (manuscripts published, abstracts of presented talks and proposals submitted) from the past year, and copies of peer and student teaching reviews from the past year. In addition to this, it should include a 1-page self-evaluation and a 1-paragraph set of goals for the coming year. The review meeting will be conducted in the Spring term, and the chair should send a written letter of evaluation to the candidate within two weeks of the review. If the candidate disagrees with the letter, he or she may also submit a reply. These annual review letters are to be included in the candidate's file for mid-probationary and tenure review.

Tenure and mid-probationary reviews Tenured CCB faculty are expected to meet to discuss each mid-probationary and tenure decision. The candidate's file should be made available to the faculty at least four weeks before the meeting, and should contain teaching evaluations (student and peer), copies of manuscripts published and funded proposals, a list of service activities, and self-evaluations of the candidate's teaching, research and service contributions; both short (2-page maximum) and longer (up to 15 pages) self-evaluations should be included. For tenure evaluation *only*, the file should include letters of evaluation from external referees, approximately half chosen by the candidate and half by the chair in consultation with senior faculty. The meeting date and time should be announced when the file is made available. Although an oral 'straw vote' may occur during the meeting, only written votes are considered official. These written votes using A&S recommendation forms should be submitted to the chair within two weeks of the meeting. The chair is responsible for submitting the file and all faculty votes to the Dean, along with the chair's letter of evaluation and recommendation.

IX. Guidelines for Promotion Decisions

Promotion in rank to associate or full professor is an important process described in some detail in the UNM faculty handbook (sections B.2.2.3, 4.8.1, 4.8.3, and 4.8.6). Evaluation for promotion generally considers the same performance categories as the tenure process: teaching, scholarship, service and personal characteristics. The specific CCB requirements for promotion to Associate Professor are the same as those for the awarding of tenure, as is usual at UNM.

Although technically these are separate decisions, they are almost always made at the same time using the same dossier and the same requirements (Faculty Handbook section B.4.8.2). Promotion to Full Professor is a separate process which typically emphasizes significant research accomplishments recognized on a national and international level.

Process: Promotion to the rank of full professor is conducted on an absolute basis within the department, not by comparison to past or present CCB faculty. The anticipated length of service as associate professor prior to consideration for promotion to the rank of professor is at least five years. Recommendations for promotion in less time, "early promotion", must demonstrate unusual accomplishment. The review for promotion to full professor should be requested by the candidate before the beginning of the Fall semester, and the chair will appoint a committee of three full professors to help the chair select external referees and to evaluate and present the case to departmental full professors for a vote. The vote should be completed by the end of the Fall semester and the candidate's application file, faculty votes, and chair's letter should be submitted to the college before the beginning of the following Spring semester (exact date determined by the college). Notification of the outcome of the review is made no later than June 30 of that year.

Expectations: According to the Faculty Handbook, **"***qualifications for promotion to the rank of professor include attainment of high standards in teaching, scholarly work, and service to the University or profession. Promotion indicates that the faculty member is of comparable stature with others in his or her field at the same rank in comparable universities. Service in a given rank for any number of years is not in itself a sufficient reason for promotion to professor*."

Appendix A3. ACS Guidelines and Evaluation Procedures for Bachelor's Degree Programs

Office of Professional Training
American Chemical Society
1155 Sixteenth Street, N.W.
Washington, DC 20036
202-872-4589
cpt@acs.org
www.acs.org/cpt

Undergraduate Professional Education in Chemistry

ACS Guidelines and Evaluation Procedures for Bachelor's Degree Programs

Spring 2008
American Chemical Society
Committee on Professional Training

Published by
American Chemical Society
1155 Sixteenth Street, N.W.
Washington, DC 20036

The cover graphic is the 600 MHz phase-sensitive double quantum filtered COSY spectrum of cholesterol.

Disclaimer
The evaluation and reevaluation of undergraduate chemistry programs by the American Chemical Society (ACS) and the ACS Committee on Professional Training are undertaken with the objective of improving the standards and quality of chemistry education in America. The following ACS guidelines for evaluating and reevaluating undergraduate chemistry programs have been developed from sources believed to be reliable and to represent the most knowledgeable viewpoints available with regard to chemistry education. No warranty, guarantee, or other form of representation is made by ACS or ACS's Committee on Professional Training or by any of its members with respect to any aspect of the evaluation, reevaluation, approval, or disapproval of any undergraduate chemistry program. ACS and the ACS Committee on Professional Training hereby expressly disclaim any and all responsibility and liability with respect to the use of these guidelines for any purposes. This disclaimer applies to any liability that is or may be incurred by or on behalf of the institutions that adopt these guidelines; the faculties, students, or prospective students of those institutions; and any member of the public at large; and includes, but is not limited to, a full disclaimer as to any liability that may be incurred with respect to possible inadequate safety procedures taken by any institution.

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I. GUIDELINES FOR PROGRAM APPROVAL AND STUDENT CERTIFICATION

1. Goals of Program Approval and Student Certification

Chemistry is central to intellectual and technological advances in many areas of science. The traditional boundaries between chemistry subdisciplines are blurring, and chemistry increasingly overlaps with other sciences. Unchanged, however, is the molecular perspective which is at the heart of chemistry. Chemistry programs have the responsibility to communicate this molecular outlook to their students and to teach the skills necessary for their students to apply this perspective.

The American Chemical Society (ACS) promotes excellence in chemistry education for undergraduate students through approval of baccalaureate chemistry programs. The ACS has charged the Committee on Professional Training (CPT) with the development and administration of guidelines for this purpose. ***ACS, through CPT, approves chemistry programs*** meeting the ACS guidelines. Approved programs offer their students a broad-based and rigorous chemistry education that provides them with the intellectual, experimental, and communication skills to participate effectively as scientific professionals. Offering such a rigorous program requires an energetic and accomplished faculty, a modern and well-maintained infrastructure, and a coherent chemistry curriculum that incorporates modern pedagogical approaches. ACS recognizes that the diversity of institutions and students is a strength in higher education. Thus, these guidelines provide approved programs with opportunities to develop chemistry degree tracks that are appropriate to the educational missions of their institutions.

ACS authorizes the chair of the ACS-approved program to certify graduating students who complete a bachelor's degree meeting the ACS guidelines. Graduates who attain a certified degree must often complete requirements that exceed those of the degree-granting institution, but this comprehensive undergraduate experience provides an excellent foundation for a career in the molecular sciences. A certified degree signifies that a student has completed an integrated, rigorous program which includes introductory and foundational course work in chemistry and in-depth course work in chemistry or chemistry-related fields. The certified degree also emphasizes laboratory experience and the development of professional skills needed to be an effective chemist. Certification gives a student an identity as a chemist and helps in the transition from undergraduate studies to professional studies or employment.

ACS approval publicly recognizes the excellent chemistry education opportunities provided by an institution to its students. It also provides standards for a chemistry curriculum based on broad community expectations that are useful for a department when designing its curriculum or acquiring resources. The approval process provides a mechanism for departments to evaluate their programs, identify areas of strength and opportunities for change, and leverage support from their institutions and external agencies. Faculty benefit from the commitment to professional development required of approved programs. Students benefit from taking chemistry courses from a department that meets the high standards of ACS approval, and ACS-certified graduates benefit from their broad, rigorous education in chemistry and the recognition associated with their degree.

2. Institutional Environment

An approved program in chemistry requires a substantial institutional commitment to an environment that supports long-term excellence. Because the approved program exists in the context of the institutional mission, it must support the needs, career goals, and interests of the institution's students. Similarly, in order to support a viable and sustainable chemistry program, the institutional environment must provide the following attributes.

2.1 Institutional Accreditation. The institution must be accredited by the regional accrediting body. Such accreditation ensures broad institutional support in areas such as mathematics, related sciences, and the humanities.

2.2 Program Organization. The administration of the approved program should rest in a chemistry department organized as an independent unit with control over an adequate budget, faculty selection and promotion, curriculum development, and assignment of teaching responsibilities. If the program is part of a larger unit, the chemistry faculty must have reasonable autonomy over these functions.

2.3 Program Budget. An approved undergraduate program in chemistry requires continuing and stable financial support. The institution must have the ability and will to make such a commitment at a reasonable level that is consistent with the resources of the institution and its educational mission. Adequate support enables a program to have

- a chemistry faculty with the scientific breadth to offer the educational experiences described in these guidelines,
- nonacademic staff and resources for administrative support services, stockroom administration, and instrument and equipment maintenance,
- a physical plant that meets modern safety standards with adequate waste-handling and disposal facilities,
- resources for capital equipment acquisition and replacement along with the expendable supplies required for high-quality laboratory instruction,
- modern chemical information resources,
- research resources for faculty and students,
- support for faculty and student travel to professional meetings, and
- opportunities for professional development and scholarly growth by the faculty, including sabbatical leaves.

2.4 Minimum Number of Graduates. Initial and continuing approval requires that the program award an average of at least two chemistry degrees per year during any five-year period. There is no required minimum number of certified graduates.

3. Faculty and Staff

An energetic and accomplished faculty is essential to an excellent undergraduate program. Faculty members are responsible for defining the overall goals of the undergraduate program. The faculty facilitates student learning of content knowledge and development of professional skills that constitute an undergraduate chemistry education. An approved program, therefore, has mechanisms in place to maintain the professional competence of its faculty, to provide faculty development and mentoring opportunities, and to provide regular feedback regarding faculty performance.

3.1 Faculty. The faculty of an approved program should have the range of educational backgrounds and expertise to provide a sustainable, robust, and engaging environment in which they educate students. The faculty of an approved program has the following attributes:

- There must be at least four full-time, permanent faculty members wholly committed to the chemistry program. Most vigorous and sustainable approved programs have a larger number.
- At least three-fourths of the chemistry faculty must hold the Ph.D. or an equivalent research degree.
- The collective expertise of the faculty should reflect the breadth of the major areas of modern chemistry.
- Because faculty members serve as important professional role models, a program should have a faculty that is diverse in gender, race, and ethnic background.

3.2 Adjunct, Temporary, and Part-Time Faculty. Full-time, permanent faculty should teach the courses leading to student certification in an approved chemistry program. Programs may occasionally engage highly qualified individuals outside the regular faculty when permanent faculty members are on sabbatical leaves or to deliver special courses. The Committee strongly discourages, however, excessive reliance on temporary, adjunct, or part-time faculty in an ACS-approved program and will review such situations carefully.

3.3 Teaching Contact Hours. Contact hours are the actual time spent in the direct supervision of students in a classroom or laboratory by faculty and instructional staff. The institution's policies about teaching contact hours should provide all faculty and instructional staff adequate time for professional development, regular curriculum assessment and improvement, contact with students outside of class, and supervision of research. The number of contact hours in classroom and in laboratory instruction for faculty and instructional staff *must not exceed 15 total hours per week*. To accommodate occasional fluctuations in instructional responsibilities, up to two individuals may have as many as 17 contact hours in one semester or quarter, provided that the average for each individual during the academic year does not exceed 15 contact hours per week. Fifteen contact hours is an upper limit, and a significantly smaller number should be the normal teaching obligation. Faculty and instructional staff in the most effective programs usually have substantially fewer contact hours, particularly when they supervise undergraduate research.

3.4 Professional Development. Sound policies regarding salaries, duties, promotions, sabbatical leaves, and tenure are essential. Institutional policies and practices should provide opportunity and resources for scholarly activities that allow faculty and instructional staff to stay current in both their specialties and modern pedagogy in order to teach effectively.

- The institution should provide opportunities for renewal and professional development through sabbaticals, participation in professional meetings, and other professional activities. Faculty and instructional staff should use these opportunities for improvement of instructional and research programs. Institutions should provide resources to ensure program continuity during sabbaticals and other leaves.
- The program should provide formal mechanisms by which senior faculty mentor junior faculty. Proper mentoring integrates all members of the instructional staff into the culture of their particular academic unit, institution, and the chemistry profession, ensuring the stability and vitality of the program.

3.5 Support Staff. A sustainable and robust program requires an adequate number of administrative personnel, stockroom staff, and technical staff, such as instrument technicians, machinists, and chemical hygiene officers. The number of support staff should be sufficient to allow faculty members to devote their time and effort to academic responsibilities and scholarly activities.

3.6 Student Teaching Assistants. The participation of upper-class chemistry undergraduates and graduate students in the instructional program as teaching assistants both helps them reinforce their knowledge of chemistry and provides a greater level of educational support to students in classes. If graduate or undergraduate students serve as teaching assistants, they should be properly trained for and supervised in their roles in the instructional program.

4. Infrastructure

A modern and comprehensive infrastructure is essential to a vigorous undergraduate program in chemistry. Program infrastructure must receive strong institutional support in order to provide sustainability through inevitable changes in faculty, leadership, and funding levels.

4.1 Physical Plant. An approved program should have classroom, teaching laboratory, research, office, and common space that is safe, well-equipped, modern, and properly maintained.

- Chemistry classrooms and chemistry faculty offices should be reasonably close to instructional and research laboratories. Classrooms should adhere to modern standards for lighting, ventilation, and comfort and have proper demonstration facilities, projection capabilities, and internet access.
- Laboratories should be suitable for instruction in the chemical sciences and must meet applicable government regulations. Properly functioning fume hoods, safety showers, eyewashes, first aid kits, and fire extinguishers must be readily available. Construction or renovation of laboratory facilities must conform to the regulations of the Occupational Safety and Health Administration (OSHA) and national norms. The number of students supervised by a faculty member or by a teaching assistant should not exceed 25. Many laboratories require smaller numbers for safe and effective instruction.
- Faculty and student research laboratories should have facilities appropriate for the type of work conducted in them. These facilities should permit maintaining experimental arrangements for extended periods of time during ongoing research projects.
- The program should have access to support facilities such as machine, electronic, and glass fabrication shops to support both teaching and research.

4.2 Instrumentation. The characterization and analysis of chemical systems requires an appropriate suite of modern chemical instrumentation and specialized laboratory apparatus to support undergraduate instructional and research missions.

- Instrumentation should be modern, high quality, and properly maintained.
- Approved programs must have a functioning NMR spectrometer that undergraduates use in instruction and research. The Committee strongly recommends an FT-NMR spectrometer.
- Throughout their curriculum, undergraduates must use additional instrumentation and specialized laboratory apparatus from most of the broad categories listed below, chosen as appropriate to the teaching and research needs of the program:

  - Optical spectroscopy (e.g., UV-vis, FT-IR, fluorescence, atomic absorption and emission, Raman, laser)
  - Mass spectrometry (e.g., MS, GC-MS)
  - Structure determination methods (e.g., NMR, X-ray diffraction)
  - Chromatography and separations (e.g., HPLC, GC, electrophoresis)
  - Electrochemistry (e.g., potentiometry, voltammetry)
  - Vacuum and inert-atmosphere systems (e.g., Schlenk line, dry box)
  - Thermal analysis (e.g., DSC, TGA)
  - Imaging and microscopy methods (e.g., electron microscopy, scanning probe microscopy)
- The program should have resources for maintenance and upkeep of this instrumentation, including knowledgeable support staff.

4.3 Computational Capabilities and Software. The ability to compute chemical properties and phenomena complements experimental work by providing understanding and predictive power. Students should use computing facilities and computational chemistry software in their course work and research.

4.4 Chemical Information Resources. The vast peer-reviewed chemical literature must be readily accessible to both faculty and students. Historically such access came through a good library providing monographs, periodicals, and facilities for database searches. Electronic access has changed the function of libraries as physical repositories. An approved program must provide students with the following minimum chemical information resources:

- An approved program must provide access to no fewer than 14 current journals chosen from the CPT recommended journal list (available from the CPT Web site) in either print or electronic form. At least three must come from the general content list, and at least one must come from each area of analytical chemistry, biochemistry, inorganic chemistry, organic chemistry, physical chemistry, and chemistry education. In addition, the library should provide access to journal articles that are not readily available by a mechanism such as interlibrary loan or document delivery services. If primary student access is electronic, cost or impractical times for access should not limit it unduly.
- Students must have print or electronic access to *Chemical Abstracts*, including the ability to search and access full abstracts.

4.5 Chemical Safety Resources. The program must be conducted in a safe environment that includes

- adherence to federal and state regulations regarding hazardous waste management and laboratory safety including, but not limited to, development of a written chemical hygiene plan and maintenance of proper facilities and personnel for chemical waste disposal,
- safety information and reference materials, such as material safety data sheets (MSDS), and
- personal protective equipment readily available to all students and faculty.

5. Curriculum

The curriculum of an approved program provides both a broad background in chemical principles and in-depth study of chemistry or chemistry-related areas that build on this background. These guidelines divide the chemistry curriculum for the certified major into three categories: the *introductory* chemistry experience, *foundation* course work that provides breadth, and rigorous *in-depth* course work that builds on the foundation. Because chemistry is an experimental science, substantial laboratory work must be part of these experiences. Programs have the opportunity to design innovative curricula that meet the needs and interests of their particular students by defining degree tracks or concentrations requiring specified in-depth course work. The curriculum must also include experiences that develop student skills essential for their effective performance as scientific professionals.

5.1 Pedagogy. An approved program should use effective pedagogy in classroom and laboratory course work. Programs should teach their courses in a challenging, engaging, and inclusive manner that accommodates a variety of learning styles. Additionally, a program should provide opportunities for faculty to maintain their knowledge of best practices in chemistry education and modern theories of learning and cognition in science. An approved program should regularly review its pedagogical approaches to ensure that it provides excellent content and builds skills that students need to be effective professionals.

Faculty should incorporate pedagogies that have been shown to be effective in undergraduate chemistry education. Examples include problem- or inquiry-based learning, peer-led instruction, group learning, learning communities or

networks, writing throughout the curriculum, and technology-aided instruction. Laboratory work provides a particularly attractive opportunity for inquiry-driven and open-ended investigations that promote independent thinking, critical thinking and reasoning, and a perspective of chemistry as a scientific process of discovery.

5.2 Introductory or General Chemistry. The introductory or general chemistry experience plays a vital role in educating all students. An introductory course provides a common background for students with a wide range of high school experiences. It also allows a maturation period for students, both in chemical topics and in mathematical and laboratory skills.

The purpose of introductory chemistry course work for those students pursuing a degree in chemistry is preparation for the foundation course work. This introduction ensures that students know basic chemical concepts such as stoichiometry, states of matter, atomic structure, molecular structure and bonding, thermodynamics, equilibria, and kinetics. Students need to be competent in basic laboratory skills such as safe practices, keeping a notebook, use of electronic balances and volumetric glassware, preparation of solutions, chemical measurements using pH electrodes and spectrophotometers, data analysis, and report writing.

The diversity of institutions and students requires a variety of approaches for teaching general or introductory chemistry. Offerings range from a full-year course to a one-semester course to waiving the introductory course requirement for very well-prepared students. To accommodate all these situations, these guidelines only describe the requirements and characteristics of experiences beyond the introductory level.

5.3 Foundation Course Work. Foundation course work provides breadth and lays the groundwork for the in-depth course work. Certified majors must have instruction *equivalent* to a one-semester course of at least three semester credit hours in each of the five major areas of chemistry: analytical chemistry, biochemistry, inorganic chemistry, organic chemistry, and physical chemistry. Programs operating on the quarter system can achieve this breadth with at least eight three-credit one-quarter courses that include the equivalent of at least one quarter of coverage of each of the five areas.

Foundation course work typically builds on the introductory chemistry experience. Textbooks for foundation course work are specialized books that serve as an introduction to each field, rather than a general chemistry textbook. Exam questions should cover concepts in greater detail than is typical in an introductory or general chemistry course. At the conclusion of a foundation course, a student should have mastered the vocabulary, concepts, and skills required to pursue in-depth study in that area.

Some areas, particularly organic and physical chemistry, have traditionally been taught as year-long courses. This practice may continue, using the first-semester course in the sequence as a foundation course and the second-semester course as an in-depth course. Integrated foundation course work may provide exposure to multiple foundation areas of chemistry or a group of topics organized by overarching themes (for example, synthesis, characterization, and reactivity) rather than by the traditional organization of chemistry subdisciplines.

Foundation courses can also be used to introduce topics that span multiple areas of chemistry. For example, the synthesis, analysis, and physical properties of small molecules give an incomplete picture of the higher order interactions in macromolecules and supramolecular systems (e.g., the physical properties of synthetic polymers, information storage and transfer by biopolymers, or aggregate properties of self-assembled systems). Students should be exposed to the principles of macromolecules across foundation areas, which could then serve as the basis for deeper exploration through in-depth course work or degree tracks.

5.4 In-Depth Course Work. The curriculum for the certified major must also include at a minimum the equivalent of four one-semester courses or six one-quarter courses (corresponding to at least 12 semester or 18 quarter credit hours) of in-depth course work. An in-depth course builds on prerequisite foundation course work. The goals of in-depth course work are both to integrate topics introduced in the foundation courses and to investigate these topics more thoroughly. Exams and other assignments associated with in-depth courses should require critical thinking and problem-solving skills.

The in-depth course work could be additional study in chemistry that increases a student's understanding of a traditional chemistry subdiscipline. For example, in a two-semester course sequence, the first semester could be a foundation course in a traditional chemistry subdiscipline (analytical, biochemistry, inorganic, organic, or physical) and the second an in-depth course. In-depth course work could also integrate multiple chemistry

foundation areas and therefore have those foundation courses as prerequisites.

Alternatively, in-depth course work could be a collection that supports a specialized, department-defined degree track (see Section 5.6). Although another department might teach some of these courses, they still must contain significant chemistry or chemistry-related content at a level beyond foundation course work to count as an in-depth course. The collection of in-depth course work required for a specialized degree track should provide a coherent experience in that area. Programs should be able to provide the rationale for each degree track and its requirements.

5.5 Laboratory Experience. The certified major must have 400 hours of laboratory experience beyond the introductory chemistry laboratory. Laboratory course work must cover at least 4 of the 5 foundation areas of chemistry and may be distributed between the foundation and in-depth levels. The laboratory experience must include synthesis of molecules; measurement of chemical properties, structures, and phenomena; hands-on experience with modern instrumentation; and computational data analysis and modeling. Students should understand the operation and theory of modern instruments and use them to solve chemical problems as part of their laboratory experience. They must have hands-on experience with a variety of instruments, including spectrometers (such as those for NMR, FT-IR, and UV-visible spectroscopy), chemical separations instruments (such as those for GC, GC-MS, and HPLC), and electrochemical instruments. Undergraduate research can serve as part of the laboratory hours and the in-depth course work if accompanied by a comprehensive written report.

5.6 Degree Tracks or Concentrations. A degree track used to certify graduates is a specialized, department-designed curriculum meeting the foundation, in-depth, and laboratory requirements that focuses on

- chemistry,
- a specific chemistry subdiscipline, or
- a chemistry-related multidisciplinary area.

Degree tracks offer the opportunity to incorporate emerging areas of chemistry, take advantage of faculty and local expertise, and match departmental and institutional missions. The faculty is responsible for defining these degree tracks for its program. The responsibility for student learning, consequently, resides with those who can best implement and assess it. While the ACS approves chemistry programs, it does not approve specific degree tracks developed by individual chemistry programs.

A chemistry degree track might require the second semesters of organic and physical chemistry, along with two semesters of in-depth electives or research. More specialized tracks might provide greater depth of instruction focused on a chemistry subdiscipline such as advanced organic synthesis, computational chemistry, polymer chemistry, or chemical measurement science. Examples of cross-disciplinary tracks are focused study in bioanalytical chemistry, biochemistry, biophysical chemistry, chemical education, chemical physics, environmental chemistry, forensic chemistry, green chemistry, materials science, medicinal chemistry, or other specialties.

Degree tracks might also include additional requirements determined by the department that do not count as in-depth courses. For example, a forensic chemistry degree track might require a course in the criminal justice system, although such a course would not qualify as an in-depth course because it would not have sufficient chemistry content which builds on the foundation courses.

5.7 Cognate Courses. Certified graduates must complete course work equivalent to two semesters of calculus and two semesters of physics with laboratory. The Committee strongly recommends a calculus-based physics curriculum and study of multivariable calculus, linear algebra, and differential equations.

5.8 Frequency and Location of Course Offerings. In all but the most exceptional cases, the program must teach all foundation courses annually. In rare cases, it may be possible to teach some foundation courses on a regular biennial schedule that enables all students to complete them in a planned way. Because in-depth courses determine the rigor of the undergraduate experience, the program must teach at least four semester-long or six quarter-long in-depth courses annually, exclusive of research. The frequency of the foundation and in-depth courses must allow students to complete the requirements for a chemistry degree in four years. While permanent, full-time chemistry faculty usually teach the courses in the chemistry curriculum, in some cases it may be appropriate to include courses taught by faculty outside the chemistry department. For example, a student

might obtain a foundation biochemistry experience through a course taught in a biochemistry or biology department.

5.9 Transfer Students. With students increasingly transferring among institutions during their undergraduate education, approved programs should be aware of the educational background of their students. Programs should provide transfer students with orientation and academic advising to assist with a successful transition to their new institution. Departments should regularly communicate with chemistry programs that are a significant source of transfer students to ensure that their chemistry curricula are coordinated.

6. Undergraduate Research

Undergraduate research allows students to integrate and reinforce chemistry knowledge from their formal course work, develop their scientific and professional skills, and create new scientific knowledge. A vigorous research program is also an effective means of keeping faculty current in their fields and provides a basis for acquiring modern instrumentation. Original research culminating in a comprehensive written report provides an effective means for integrating undergraduate learning experiences, and allows students to participate directly in the process of science.

Conducting undergraduate research with a faculty advisor allows the student to draw on faculty expertise and encourages a student-faculty mentor relationship. The research project should be envisioned as a component of a publication in a peer-reviewed journal. It should be well-defined, stand a reasonable chance of completion in the available time, apply and develop an understanding of in-depth concepts, use a variety of instrumentation, promote awareness of advanced safety practices, and be grounded in the primary chemical literature.

Research can satisfy up to four semester credit hours or six quarter credit hours of the in-depth course requirement for student certification and can account for up to 180 of the required 400 laboratory hours. A student using research to meet the ACS certification requirements must prepare a well-written, comprehensive, and well-documented research report including safety considerations. Although oral presentations, poster presentations, and journal article coauthorship are valuable, they do not substitute for the student writing a comprehensive report.

Research performed during the summer or performed off-campus, even though it might not receive academic credit, may count toward student certification. In such cases, the student must prepare a comprehensive written report that a faculty member of the home institution evaluates and approves.

7. Development of Student Skills

While formal course work provides students with an education in chemical concepts and training in laboratory practices, students should go beyond course content alone to be effective and productive scientists. They need to master a variety of skills that will allow them to become successful professionals.

7.1 Problem-Solving Skills. The ultimate goal of chemistry education is to provide students with the tools to solve problems. Students should be able to define problems clearly, develop testable hypotheses, design and execute experiments, analyze data using appropriate statistical methods, and draw appropriate conclusions. In this process, students should apply their understanding of all chemistry subdisciplines. Students should use appropriate laboratory skills and instrumentation to solve problems, while understanding the fundamental uncertainties in experimental measurements.

7.2 Chemical Literature Skills. Students should be able to use the peer-reviewed scientific literature effectively and evaluate technical articles critically. They should learn how to retrieve specific information from the chemical literature, including the use of *Chemical Abstracts* and other compilations, with online, interactive database-searching tools. Approved programs must provide instruction on the effective retrieval and use of the chemical literature. A specific course is an excellent means of imparting information-retrieval skills, though such a course usually would not qualify as an in-depth course. Integrating the use of these skills into several individual courses is also an effective approach. Both library and online exercises should be a part of such instruction on information retrieval.

7.3 Laboratory Safety Skills. Approved programs should promote a safety-conscious culture in which students understand the concepts of safe

laboratory practices and how to apply them. Programs should train students in the aspects of modern chemical safety appropriate to their educational level and scientific needs. A high degree of safety awareness should begin during the first laboratory course, and both classroom and laboratory discussions must stress safe practices. Students should understand responsible disposal techniques, understand and comply with safety regulations, understand and use material safety data sheets (MSDS), recognize and minimize potential chemical and physical hazards in the laboratory, and know how to handle laboratory emergencies effectively.

7.4 Communication Skills. Effective communication is vital to a scientist. Speech and English composition courses alone rarely give students sufficient experience in oral and written communication of technical information. The chemistry curriculum should include writing and speaking opportunities, and the chemistry faculty should evaluate them critically. Students should be able to present information in a clear and organized manner, write well-organized and concise reports in a scientifically appropriate style, and use technology such as poster preparation software, word-processing, chemical structure drawing programs, and computerized presentations in their communication.

Knowledge of one or more foreign languages is another component of communication. Even though English is the international language of science, chemistry is worldwide in scope. The study of a foreign language adds greatly to a student's education, although ACS certification does not require it.

7.5 Team Skills. Solving scientific problems often involves multidisciplinary teams. The ability to work in such teams is essential for a well-educated scientist. Students should be able to work effectively in a group to solve scientific problems, be effective leaders as well as effective team members, and interact productively with a diverse group of peers. Programs should incorporate team experiences in classroom and laboratory components of the chemistry curriculum.

7.6 Ethics. Ethics should be an intentional part of the instruction in a chemistry program. Students should conduct themselves responsibly and be aware of the role of chemistry in contemporary societal and global issues. As role models, faculty should exemplify responsible conduct in their teaching, research, and all other professional activities.

7.7 Assessment of Student Skills. Both dedicated courses and integration of learning opportunities throughout the curriculum can be used to develop student skills and provide a means of assessing them. Examples of the former approach are a course emphasizing technical writing and presentation, such as a senior capstone experience or a chemical literature course. The latter approach could include the conscious introduction of team projects into courses or having students make presentations related to the current literature. Undergraduate research is a highly effective means for imparting, integrating, and assessing these skills. Approved programs should have an established process by which they assess the development of student skills.

7.8 Student Mentoring and Advising. Effective advising and mentoring of undergraduates are central to student achievement. Successful mentors provide guidance for a student's development, networking, confidence building, and career planning. Mentoring can ease the transition for students who transfer into the chemistry major. Faculty should advise students about the many career options available to chemistry graduates and should encourage those with a strong interest in teaching or research to pursue advanced study in chemistry or related sciences. It is particularly important to encourage members of underrepresented groups to pursue chemistry as a career. Undergraduate research is an exceptional opportunity for mentoring students, especially when it is started early and maintained throughout the course of study.

8. Program Self-Evaluation

An approved chemistry program should regularly evaluate its curriculum and pedagogy, faculty development opportunities, and infrastructure needs relative to the program's teaching and research mission. Self-evaluation is a process for continual improvement of a program, not a static end product. The result of an effective self-evaluation is a vibrant, sustainable, and resilient program that produces a steady stream of dedicated and accomplished students, supports continual professional development and scholarly activities

of faculty, and provides a strong infrastructure to support the educational and scientific missions of the program.

9. Certification of Graduates

The chair of an approved program certifies those chemistry majors receiving a baccalaureate degree consistent with the guidelines described here. Students usually receive certification when they complete the baccalaureate degree. It is also possible to certify students who initially obtain a noncertified baccalaureate degree from an approved program and subsequently complete additional study in an ACS-approved undergraduate program to qualify for certification. The Office of Professional Training provides certificates for certified graduates upon request.

II. APPROVAL PROCESS AND REVIEW PROCEDURES

1. Membership of the Committee

The CPT has 17 members. The ACS Board of Directors and the president of the Society with the advice of the ACS Committee on Committees jointly appoint 16 voting members. One member serves as an appointed chair and one serves as an elected vice chair. There is also one nonvoting staff secretary. The secretary communicates the results of all reviews conducted by CPT and consults with faculty and administrators about guidelines and procedures related to ACS approval. Initial appointments are usually for a three-year term, and reappointment for up to a total of nine years of service is possible. The Committee occasionally retains one or more former members or appoints individuals with special expertise as nonvoting consultants. Members of the CPT are experienced educators and scientists from all areas of the country, chosen to represent different fields of chemistry, possess different points of view, come from different types of academic and nonacademic institutions, and reflect the breadth of the chemical community.

2. Costs Associated with the Approval Program

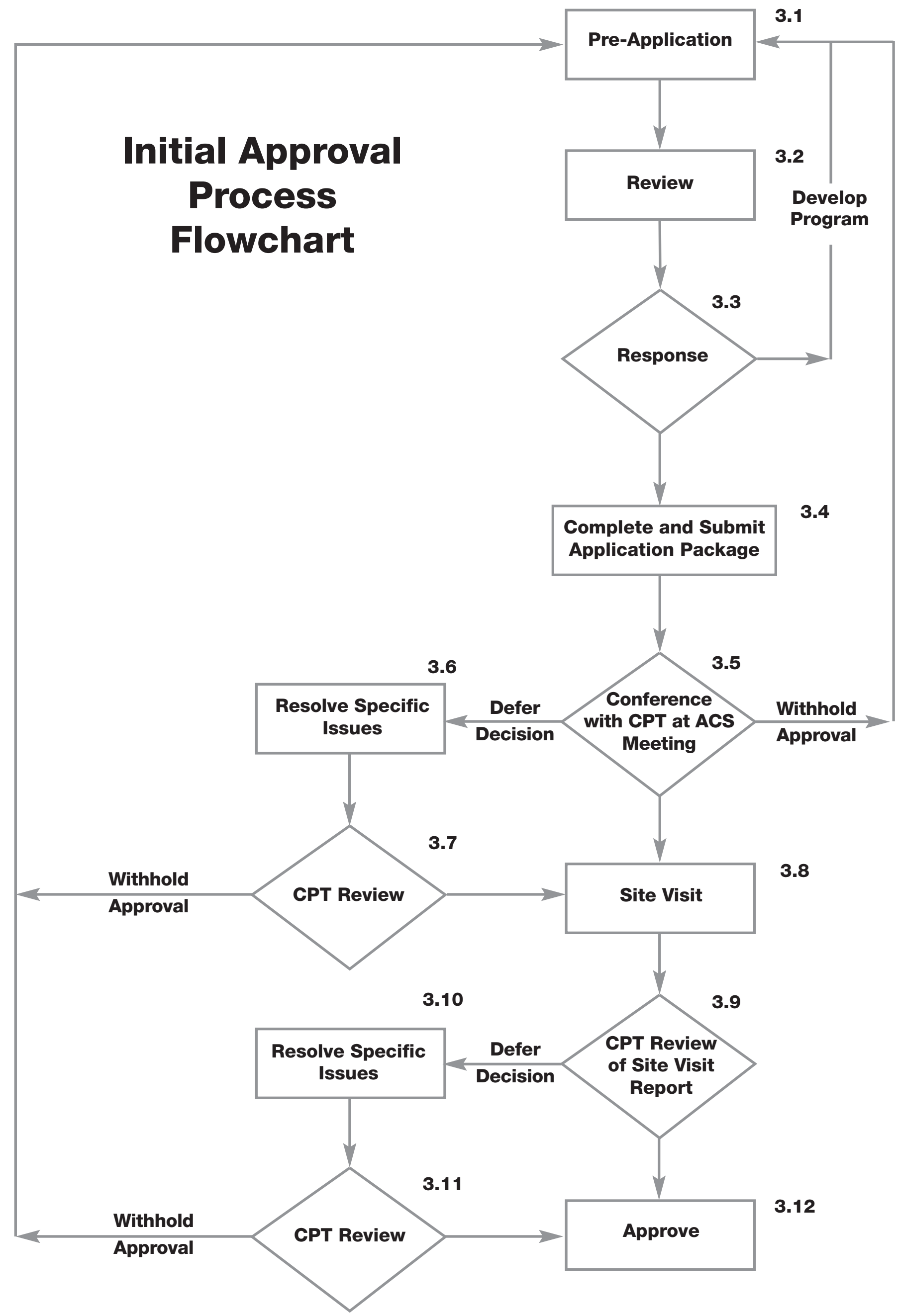
The Society does not charge academic institutions for the evaluation of the chemistry program, including site visits by Visiting Associates of CPT (Section 8).

3. Initial Approval Process

The ACS, through CPT, establishes the recommendations and requirements for approval of bachelor's degree programs in chemistry and policies for administering the approval process. The chemistry faculty should conduct a self-study to determine the program's readiness to begin the approval process. The following flowchart summarizes the steps of the initial approval process, and the accompanying text describes each of the steps in the flowchart.

3.1 Pre-Application. The chemistry department completes a pre-application form, which is available at the CPT Web site, and submits it by the deadline given on the pre-application Web page.

Initial Approval Process Flowchart



3.2 Review. The Committee reviews the pre-application form within two months of the submission deadline.

3.3 Response. The Secretary of the Committee reports the outcome of the review to the department chair by letter. Two outcomes are possible.

1) *The applicant does not meet* the requirements for ACS approval that are covered in the pre-application form. The letter identifies the deficiencies and instructs the department to develop the program further and submit a new pre-application form after addressing the areas identified.
2) *The applicant meets* the requirements for ACS approval that are covered in the pre-application form. The Committee invites the department to submit a full application package.

3.4 Complete and Submit Application Package. Departments complete an extensive self-study questionnaire and provide supporting documentation including course syllabi, examinations, and student research reports. ACS staff reviews the package for completeness and assigns the applications for review by the Committee at the fall or spring ACS National Meeting following the deadline for submission of the application.

3.5 Conference with CPT. The chair of the chemistry program and other faculty members or administrators meet with the Committee at the fall or spring ACS National Meeting. During this conference, CPT members discuss the chemistry program and may inquire about certain aspects of the application package. The Secretary of CPT communicates the outcome of CPT's review to the chair of the department that administers the chemistry program. Three outcomes are possible.

1) *The applicant and Committee arrange a site visit* (Section 3.8) by a Visiting Associate. (Section 8)
2) *The Committee defers a decision* pending submission of additional information. (Sections 3.6, 3.7)
3) *The Committee withholds approval of the program.* The letter from the Secretary of CPT describes the areas of noncompliance. After addressing these concerns, the applicant must start the application process again with the submission of the pre-application form.

3.6 Resolve Specific Issues. The department must resolve the specific issues identified in the letter from the Secretary of CPT and submit a response by the deadline given in the letter.

3.7 CPT Review. ACS staff verifies that the information submitted by the applicant is complete and schedules the application for review at the next regular CPT meeting. Two outcomes are possible.

1) *The Committee decides to proceed with a site visit* (Section 3.8) by a Visiting Associate. (Section 8)
2) *The Committee decides to withhold approval of the program.* The Secretary of CPT reports the outcome of this review via letter to the applicant following the CPT meeting.

3.8 Site Visit. The Secretary of CPT reports the decision to proceed with a site visit by letter to the chair of the department that administers the chemistry program. The president (or chief administrative officer of the institution) must then invite ACS to make a site visit. One Visiting Associate (Section 8) will make the site visit, which typically lasts one to two days. The ACS pays all expenses of the site visitor. ACS staff provides the site visitor with a copy of the applicant's self-study questionnaire, background information on the chemistry faculty, and the college catalog pages for the chemistry program. The site visitor submits a written report on the site visit to the Secretary of CPT within six weeks following the visit.

3.9 CPT Review of Site Visit Report. CPT reviews the written report of the site visitor at the next regular meeting after it is received. Two decisions are possible.

1) *The Committee approves the chemistry program.* (Section 3.12)
2) *The Committee identifies specific issues needing resolution.* (Sections 3.10, 3.11)

3.10 Resolve Specific Issues. The department must resolve the specific issues identified in the letter from the Secretary of CPT and submit a response by the deadline given in the letter. This is not an iterative step and occurs only once following the site visit.

3.11 CPT Review. CPT reviews the department's report describing the resolution of the specific issues. Two decisions are possible after this review.

1) *The Committee approves the chemistry program.* (Section 3.12)
2) *The Committee withholds approval of the program.* The letter from the Secretary of CPT will describe the areas of noncompliance. After addressing these concerns, the applicant starts the application process again with the submission of the pre-application form.

3.12 Approve. The Secretary of CPT writes to the president of the institution and the chair of the department that administers the chemistry program to report this decision. The Committee will post the name of the institution on the list of ACS-approved chemistry programs on its Web site. An approved institution must satisfy the reporting requirements described in Sections 4 and 5. Failure to comply with the annual and periodic review requirements will lead to probationary action (Section 6).

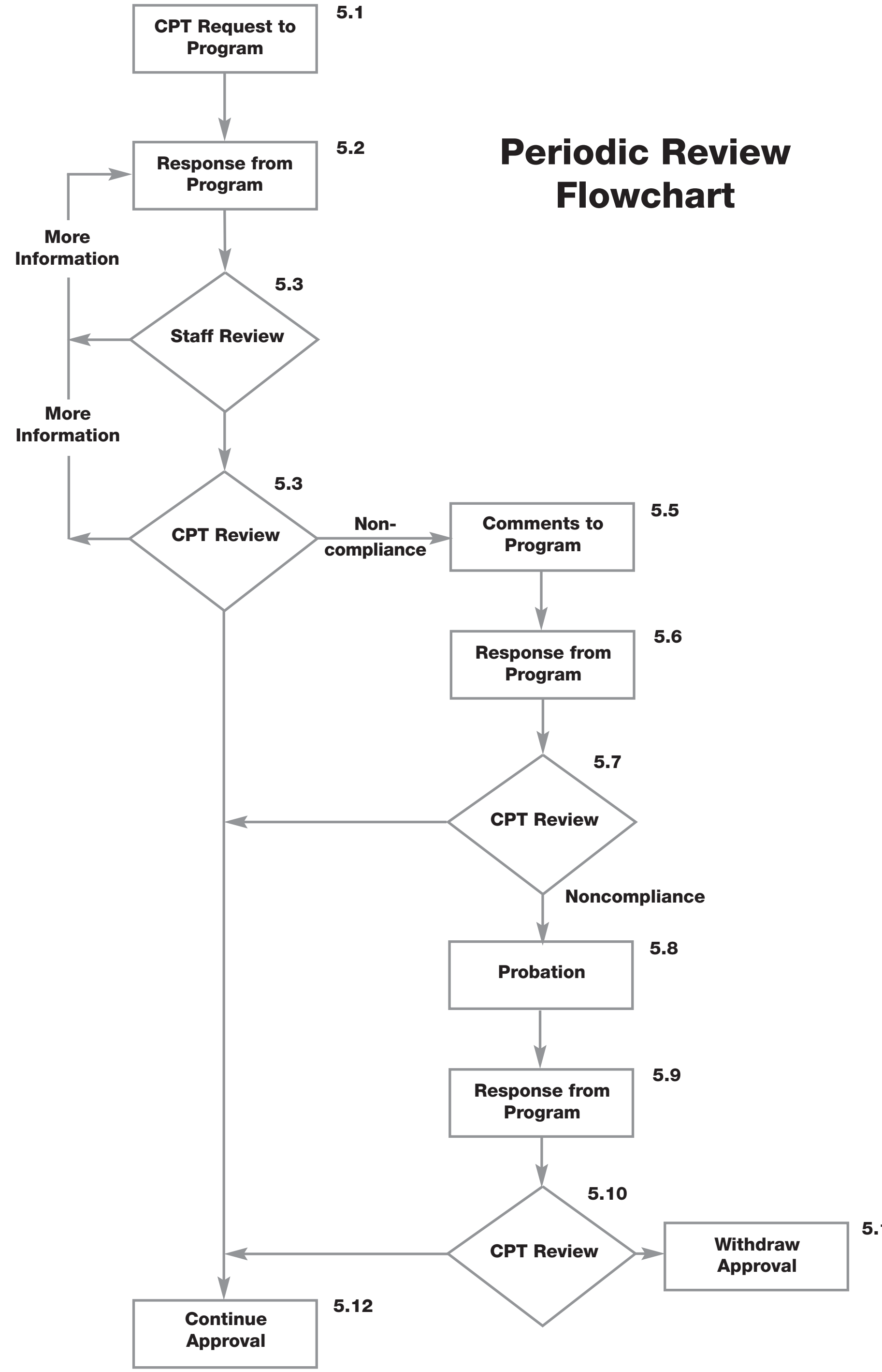
4. Annual Review

Approved institutions must report annually to the Committee on the number of degrees granted by the chemistry program, all graduates and the certification status of the baccalaureate graduates, and supplemental information on the curriculum and faculty. The Committee reviews the report for completeness and consistency with the guidelines and may request additional information from the program. The Committee summarizes and publishes the statistical information about the numbers of graduates at the various degree levels each year.

5. Periodic Review

To ensure compliance with the ACS guidelines, approved programs must submit a periodic report about their program using a form provided by CPT. The following flowchart summarizes the steps of the review process, and the accompanying text describes each of the steps in the flowchart.

Periodic Review Flowchart



5.1 Request for Periodic Report. The Secretary of CPT contacts the chair of the department that administers the ACS-approved chemistry program with instructions for completing the periodic report. The Secretary of CPT sends a report form that includes questions on all components of the ACS guidelines for approval and a copy of the letter reporting the final outcome of the previous review. The Committee also may ask departments to provide copies of specific course syllabi, examinations, and student research reports. Departments must submit a periodic report every five years.

5.2 Response from Program. The department must respond by the deadline provided in the letter from the Secretary.

5.3 Staff Review. An ACS staff member reviews the periodic report package for completeness and corresponds with the department chair to obtain any missing information.

5.4 CPT Review. The Committee reviews the periodic report at one of its three yearly meetings. Three outcomes are possible.

1) *The Committee requests more information.* The CPT members may find that essential information is missing from the report package despite the staff review step and ask a staff member to obtain this information from the department.
2) *The Committee determines that the chemistry program is not in compliance* with the requirements specified in the guidelines or has not adequately addressed the recommendations in the previous periodic review. (Section 5.5)
3) *The Committee continues approval.* (Section 5.12)

5.5 Comments to Program. The Secretary of CPT identifies the area(s) of noncompliance in a letter to the chair of the department. The Committee establishes a reasonable time frame for response that is appropriate to the nature of the issues.

5.6 Response from Program. The department must report to CPT on the measures taken to address the deficiencies identified by the deadline provided in the letter from the Secretary.

5.7 CPT Review. The Committee reviews the department's response at the first possible meeting after receiving it. Two outcomes are possible.

1) *Continue approval.* (Section 5.12)
2) *Probation.* (Section 5.8)

5.8 Probation. If the department has not corrected the deficiencies identified in the correspondence from the Secretary, CPT will place the department on probation. The Secretary of CPT communicates this decision and the areas of noncompliance in a letter to the president (or chief administrative officer) of the institution and the chair of the department that administers the chemistry program. The probation decision is confidential between CPT and the institution. During probation, the institution remains on the list of ACS-approved schools, and the department chair may continue to certify graduates who have satisfied the requirements as specified in the guidelines.

5.9 Response from Program. The probationary period normally lasts from 12 to 18 months. The institution must provide a written report that describes how it has corrected all of the areas of noncompliance, including supporting documentation as appropriate. Either the department chair or a member of the administration may prepare the response, which must be submitted to the Secretary of CPT before the end of the probationary period.

5.10 CPT Review. The Committee reviews the department's response at the first possible meeting after receiving it. In some circumstances, CPT may request a site visit by a Visiting Associate (Section 8). Two outcomes are possible.

1) *Continue approval.* (Section 5.12)
2) *Withdraw approval.* (Section 5.11)

5.11 Withdraw Approval. If the department does not meet all of the requirements for ACS approval by the end of the probationary period, CPT withdraws approval of the chemistry program. The Secretary of CPT reports this outcome in a letter to the president of the institution (or chief administrative officer) and the chair of the department responsible for administering the chemistry program. The institution will be removed from the published list of ACS-approved schools, and the chair may no longer certify graduates. The institution may appeal this decision as described in Section 7.

5.12 Continue Approval. If CPT determines that the chemistry program meets all of the requirements for ACS approval and the spirit of the guidelines, the Committee continues approval of the program. The Secretary of CPT reports this outcome in a letter to the chair of the department responsible for administering the ACS-approved chemistry program with a copy to the president of the institution (or chief administrative officer). The letter may contain CPT's recommendations and suggestions for strengthening and further development of the chemistry program. The department must adequately address these recommendations as part of the next periodic review. Failure to do so may lead to a determination of noncompliance in the future. Under certain circumstances, CPT may request a shorter review cycle.

6. Administrative Probation

The Committee may place an ACS-approved chemistry program on probation if it does not comply with the following administrative requirements for maintaining approval:

- Submission of the periodic review report by the deadline.
- Submission of additional information requested following CPT review of a periodic report.
- Completion of an annual report by the deadline.

The chair of the department responsible for administering the chemistry program receives two warnings that the program has missed the deadline before the Secretary of CPT contacts the president (or chief administrative officer) of the institution. The Secretary of CPT notifies the president that the department does not comply with the requirements for maintaining approval and allows 30 days to correct the situation before placing the program on administrative probation. Administrative probation lasts no longer than 60 days. During administrative probation, programs retain approval and may certify graduates. The Committee withdraws approval of any program that fails to submit the required report or information within the 60-day period.

7. Appeal of an Adverse Decision

An institution may petition for review of an adverse decision (withholding or withdrawal of approval) if it believes that the Committee has not adhered to its own established policies and procedures or has failed to consider all of the evidence and documentation presented during the evaluation. The petition must reach the Committee within 60 days following the date of the letter advising the institution of the adverse decision. Within four months of submitting the petition, the institution must provide any additional information and documents in support of the petition. After receiving the petition and supporting information, the Committee reviews the matter at its next regular meeting, which may include a conference with representatives of the institution if desired by either the institution or the Committee. After the meeting and deliberation, the Committee reports its findings to the institution.

Every institution has the right to appeal the Committee's decision to an independent Appeals Board convened for that purpose. The Society's president and the chair of its Board of Directors will appoint an Appeals Board, consisting of three individuals who are not members of the Committee, to hear the appeal.

Any action of any Society unit is always subject to review by the Society's Board of Directors, which has full legal responsibility for all Society activities.

8. Visiting Associates

Visiting Associates of the Committee are experienced educators and scientists familiar with the ACS guidelines and the administrative and technical aspects of conducting a successful undergraduate program in chemistry. The Committee periodically holds meetings with Visiting Associates to brief them on guidelines policy and evaluation procedures. The Visiting Associate receives comprehensive and detailed instructions on CPT's expectations for the site visit that also are sent to the chair of the department to aid in preparation for the visit. In addition, the Associate receives confidential comments from CPT that describe aspects of the program that should receive careful attention during the site visit and in the visitor's report. Visiting Associates serve as fact-finders for CPT and do not fill the role of an external consultant who might advise the faculty on the development of the chemistry program.

In the selection of a Visiting Associate, the Committee makes every effort to eliminate any possibility of bias or conflict of interest. For example, a graduate of the institution under review or a person with a close and continuing relationship to the institution or members of the faculty would not be chosen to make a site visit. The Committee would not select an Associate who is a faculty member at an institution in the immediate geographical area.

9. Confidentiality

The information provided to the Committee and all related discussions and correspondence between the Committee and an institution are solely for the confidential use of the Committee. In the event that an institution appeals a Committee decision, the Committee provides the information necessary for the proper conduct of the appeal to the Appeals Board.

The Committee communicates all decisions to the department chair. In the case of approval, continued approval, report on a site visit, probation, or withdrawal of approval, the Committee also informs the principal administrative officer of the institution. These communications summarize the reasons for the decisions made by the Committee.

In its annual published reports, the Committee identifies those institutions whose programs are currently approved as meeting the ACS guidelines for undergraduate professional education in chemistry. These annual reports also summarize statistical information provided by each institution about its chemistry graduates. Otherwise, the Committee does not publish any additional information about a particular program or evaluation.

APPENDIXES

A. The Formal Mandate of the Committee on Professional Training

A resolution of the ACS Council established the Committee on Professional Training in 1936, and the Committee published the first edition of the guidelines for approval of undergraduate programs in 1939. In 1968, the Committee became a Joint Committee of the ACS Board and Council, reporting to both. In 1979, the Society codified the responsibilities of the CPT in ACS Bylaw III,3,(h):

(1) The SOCIETY shall sponsor an activity for the approval of undergraduate professional programs in chemistry. The Committee on Professional Training, constituted as an Other Joint Board-Council Committee under this Bylaw, shall act for the Board and Council in the formulation and implementation of the approval program with published criteria and/or guidelines, as well as published evaluation policies and procedures.

(2) The goals of the approval program shall be *inter alia*:

   a. promoting and assisting in the development of high standards of excellence in all aspects of postsecondary chemical education, and undertaking studies important to their maintenance,
   b. collecting and making available information concerning trends and developments in modern chemical education, and
   c. cooperating with SOCIETY and other professional and educational groups having mutual interests and concerns.

(3) Institutions may petition for review of adverse evaluation decisions to an established Appeals Board consisting of three members of the SOCIETY, not members of the Committee, appointed jointly by the President and the Chair of the Board.

B. Members of the Committee on Professional Training

CPT Members – 2008

Ruma Banerjee, *University of Michigan*
Robert A. Copeland, *GlaxoSmithKline*
Ron W. Darbeau, *McNeese State University*
Ron C. Estler, *Fort Lewis College*
Joseph S. Francisco, *Purdue University*
Cornelia D. Gillyard, *Spelman College*
Carlos G. Gutierrez, *California State University, Los Angeles (Consultant)*
Suzanne Harris, *University of Wyoming*
Scott C. Hartsel, *University of Wisconsin-Eau Claire*
John W. Kozarich, *ActivX Biosciences (Consultant)*
Cynthia K. Larive, *University of California, Riverside, Vice Chair 2007-08*
Anne B. McCoy, *Ohio State University*
Nancy S. Mills, *Trinity University*
George R. Negrete, *University of Texas at San Antonio*
Lee Y. Park, *Williams College*
Jeanne E. Pemberton, *University of Arizona, Chair 2000-02 (Consultant)*
William F. Polik, *Hope College, Chair 2006-08*
Barbara A. Sawrey, *University of California, San Diego (Consultant)*
Joel I. Shulman, *University of Cincinnati*
George S. Wilson, *University of Kansas*
Cathy A. Nelson, *American Chemical Society, Committee Secretary*

Former CPT Members Who Participated in the Development of the Guidelines

Robert J. Angelici, *Iowa State University*
Diane M. Bunce, *Catholic University of America (Consultant)*
Charles E. Carraher, Jr., *Florida Atlantic University*
Sally Chapman, *Barnard College, Chair 1994-96*
Norman C. Craig, *Oberlin College*
F. Fleming Crim, *University of Wisconsin-Madison, Chair 2003-05*
Royce C. Engstom, *University of Montana*
Edward N. Kresge, *Exxonmobil Chemical Company (Retired)*
Margaret V. Merritt, *Wellesley College*
Jerry R. Mohrig, *Carleton College, Chair 1997-99*
C. Dale Poulter, *University of Utah, Vice Chair 2003-04*
Erik J. Sorensen, *Princeton University*
Elizabeth C. Theil, *Children's Hospital Oakland Research Institute*

Appendix A4. Report of the 2003 Graduate Review Committee

Report of the Graduate Review Committee

Department of Chemistry
University of New Mexico

Albuquerque, NM

March, 2003

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Executive Summary

Because or the role molecular science plays in nearly all aspects of our modern world, chemistry is vital to the educational process of all strong research universities. The University of New Mexico is no exception.

Given the focus of the Chemistry Department over the past decade, there are distinct recruiting advantages in changing the name of the department. Perhaps the appropriate name would be the **Department of Chemistry and Chemical Biology**.

With the proximity of the University to several key US Government laboratories, the UNM Mission plays well into the manifold opportunities these laboratories provide for collaboration and synergy with chemical education and research. This effort appears to be producing an excellent model for building bridges to the significant resources of the state's national laboratories.

A key to future success of the Chemistry Department is significant improvement in faculty governance.

Unfortunately little progress appears to have been made since the last graduate review in 1993 on the issues of research space and facilities. Short term space needs for research appear to be adequate but not optimally organized. In the long term, new facilities are essential.

The lack of proper facilities maintenance protocols has raised serious issues of health and safety within the Chemistry Department. The Chair, in consultation with other chairs and Administrators, should establish a protocol and communication network that will allow discussion of any physical plant maintenance that will disrupt electricity, water, or hoods CONSIDERABLY BEFORE such work is undertaken, so that researchers can plan their activities around these job actions.

The support staff organization appears to have been developed nicely under good leadership. A positive morale has been created that appears to have overcome problems that existed in 1993. Even so, the standard of staff support for the Chemistry Department is far below that of peer institutions, particularly as research active faculty numbers increase.

The hiring of many excellent junior faculty and four well established senior faculty, all supporting the departmental thrust areas, has been a significant positive development. However, retention of junior faculty is one of the most important roles needed to be done by the senior faculty and administration.

The Chemistry Department is to be commended for its policy on post tenure review. This is really a model for other institutions.

The departmental web page should be professionally produced, be up to date, and have links to the faculty web pages, which should list research interests and publications.

The Chemistry Department must find a mechanism to increase graduate student stipends. The current stipend for graduate students in chemistry at UNM ($15,400) is well below the stipends in the peer schools, and in research universities in the west. The Chemistry Department must strengthen its recruitment of quality domestic students and especially Hispanics, Native Americans, and other minorities.

Procedures for early identification of outstanding undergraduate students who may later be approached as potential undergraduate assistants (and potential graduate assistants) must be implemented.

The graduate students in the chemistry department seem to be satisfied with the program although the number of graduate students is well below the desirable number for the size of the faculty.

A core set of courses should be required of all students in each discipline that ensures the students to obtain the requisite knowledge. This means that core courses must be given regularly.

The Chemistry Department must aggressively pursue funding to upgrade departmental facilities and equipment.

The committee recommends that an instrumentation committee be established to coordinate efforts in the Chemistry Department to submit proposals annually .

Introduction

This is the report of the Review Committee of the Graduate Program of the Chemistry Department at the University of New Mexico. The review was conducted during February 2426, 2003. The review was made at the request of the Senate Graduate Committee in conjunction with the leadership of the office of Graduate Studies. The Review Committee included John P. Fackler, Jr.(chair), Texas A&M University; Gary Molander, U. of Pennsylvania; Ignacio Tinoco, U. California, Berkeley; Kathryn Vogel, Dept. of Biology, U. of New Mexico; Isiah Warner, Louisiana State University. This report follows the Chemistry Departments self study report which was developed in the "Fall of 2002".

The review began at 9 AM on February 25, 2003, with an entrance interview with Teresita Aquilar, Dean of Graduate Studies. The committee was picked up from the hotel by Thomas Niemczyk, the Chemistry Department chair. Discussions followed with Jack McIver, Deputy Vice Provost for Research, Nancy Uscher, Associate Provost for Academic Affairs, and Reed Dasenbrock, the Dean of the College of Arts and Sciences. These were followed by separate discussions over the three days with faculty, the Graduate Recruitment Committee, Jackie Shane from the library, graduate students, and the Graduate Studies Committee. The formal process was completed by an oral presentation of the committee findings and discussion with a group of faculty and the above mentioned administrators.

The sections of this document present the best thinking of the review committee directed toward guiding the Chemistry Department to strengthening its graduate program. Chemistry, because of the role molecular science plays in all aspect of modern science and technology, is vital to the educational process of all strong research universities. The University of New Mexico is no exception.

Special developments since the last review

The 1993 review team was chaired by the current Associate Director for Strategic Planning for the Los Alamos National Laboratory and included among its membership the President-Elect of the American Chemical Society. The report it created emphasized support for a departmental focus in its graduate efforts on two areas, materials science and biological chemistry. It pointed out that the Chemistry Department "now has the opportunity for further growth to a higher echelon of research-oriented chemistry departments." In the list of the "most pressing issues confronting the department" there has been considerable progress since 1993 in faculty teaching loads and the strengthening of the program by faculty hires in biological chemistry. Unfortunately in many other areas discussed in the 1993 report, either no progress has been made or the Chemistry Department has lost ground.

It is not surprising therefore that departmental cynicism for the review process exists. *Perhaps this fact even contributed to the failure of the department to produce a meaningful self-examination document consistent with the Mission of the University*. It appears that very little department debate and discussion occurred as part of the creation of the self study document. The document contains few concrete suggestions for mechanisms by which the department can successfully address issues brought forth in the 1993 review and even fails to identify clearly its mission as a Chemistry Department for the University and the State.

Where has progress been achieved? Clearly the hiring of many excellent junior faculty and four well established senior faculty, all supporting the departmental thrust areas, has been a significant positive development. Creative ways were identified to find the necessary start-up funds for some of these people. Thus, in spite of the significant loss of faculty in the materials science area since 1993, research funding income appears to be near a department historical high. Indirect cost return is 12% higher than it has ever been previously in the Chemistry Department. One of these new senior hires is jointly funded by Sandia National Laboratory. This effort appears to be producing an excellent model for building bridges to the significant resources of the State's national laboratories. It is also an effort directly related to a strategic advantage recognized in the Strategic Plan of the University. These are significant achievements for which the Chemistry Department and University are to be complimented.

The department also appears to have made considerable progress toward solving faculty work load problems although some additional effort still is needed (see p.15 below). Research education with graduate students must be viewed appropriately in the workload assessment of faculty. (The management, support and guidance of 3 or 4 graduate students in chemistry is considered fully equivalent to teaching a three credit hour course at the best research universities.) Considerable progress appears to have been made toward "nurturing and rewarding successful junior faculty". The support staff organization appears to have been developed nicely under good leadership. A positive morale has been created that appears to have overcome problems that existed in 1993. Even so, the staff support for the Chemistry Department is far below that of peer institutions, particularly for a department with research active faculty (see p. 16).

Unfortunately little progress appears to have been made since 1993 on the issues of research space and facilities. Short term space needs for research appear to be adequate but not optimally organized. In the long term, new facilities are essential. Undergraduate and research laboratories for chemistry may already be out of National Code for safety and environment. This issue must be addressed in University planning.

A key to future success of the Chemistry Department depends upon the development of significant improvement in departmental faculty governance. Clearly what is being done now needs to be re-examined.

By failing to utilize this self study effort to bring the faculty together to address important issues of departmental development, the committee believes that the department may have lost an important opportunity to gain administrative support for its goals and ambitions.

University Environment for Graduate Research in the Context of the UNM Mission

The University has recently developed a Strategic Plan presumably with input from all university programs including chemistry. The mission of the University to engage students, faculty and staff in its comprehensive educational, research and service programs is clear. Chemistry is the central molecular science that bridges biology, and medical and engineering technologies. Hence it plays a vital role in the University development. ***Every effort should be made by the University to insure that the Chemistry Department functions effectively and in a manner consistent with the teaching and research mission of the University.***

With the proximity of the University to several key US Government laboratories, the UNM Mission plays well into the manifold opportunities these laboratories provide for collaboration and synergy with chemical education and research. This report addresses some aspects of the effort being made by the Chemistry Department in this regard.

Faculty Structure, Culture and Governance

The departmental focus on biological chemistry suggests that there are distinct graduate recruiting advantages in changing the name of the department. Perhaps the appropriate name would be the **Department of Chemistry and Chemical Biology**. This, or an equivalent name reflecting the departmental mission in both biochemistry and materials chemistry, would more appropriately reflect the focus of the departmental research organization and structure.

Leadership and Departmental Administration

The Dept. of Chemistry appears to have a culture of individuals under one roof rather than a community. This culture is damaging to the department in two ways. First, it does not promote effective mentoring of new faculty, with the result that over the last 20 years a high proportion of expensive hires into the department have not stayed at UNM or, if they stay at UNM, have moved away from their departmental and research roles. The second cost is that the department has not taken advantage of the national funding resources now available for departmental equipment and building remodeling, as well as for undergraduate and graduate training. Effective departmental leadership must deal with both of these problems head on.

Leadership from the chairman with help from the Dean is needed for the Chemistry Department to take advantage of the extraordinary national funding now available for departmental equipment and building remodeling, as well as for student training. Faculty members who become involved in writing proposals for departmental equipment or programs must be shown the benefits (salary, reduced teaching) and gratitude of the rest of the department. An undergraduate research program might be just what is needed to capture and hold more students in the chemistry major. However, this must be a group effort. A graduate training program (such as is already demonstrated with the optics IGERT) will enhance research interactions across campus and enhance the pool of applicants for graduate school. The chairman can take a lead in starting this process by developing and submitting proposals in this area, with the help of other interested faculty.

Faculty Development and Retention

Faculty recruiting and retention in the Chemistry Department at the University of New Mexico is such a critical element to its success that even the graduate students listed it as their number one priority for improvement in the department. There appears no question that there are too few permanent faculty in the department to meet its commitment of quality education in both the undergraduate and graduate programs. Given the limited resources, the department has laudably chosen to focus in two research areas: biological chemistry and materials related research.

Most recently, the Chemistry Department has been successful in identifying candidates for faculty positions in biologically related areas and convincing them to come to the University of New Mexico. Over the past ten years, both senior and junior hires in this area have significantly enhanced the quality and prestige of the faculty. This success is owed to competitive start-up packages and salaries, in addition to imaginative means of financing these hires.

Less success has been achieved in materials science. Indeed, efforts in the latter area appear to be dormant at this time. The Chemistry Department appears strongly committed to this focus area, but it needs to move aggressively to hire new faculty in this area in order to take advantage of opportunities to connect with other programs on campus as well as with the national laboratories that are moving forward with their own initiatives. Incredible opportunities will be lost if action is not taken immediately.

A formal faculty mentoring program should be instituted. One option (but see below) is to assign each new faculty member at least two tenured faculty members as "mentors". One of these should be from a division other than that to which the new person belongs in order to increase interactions throughout the Chemistry Department. The chairman should meet with each new faculty member each semester to ask about how things are going, give feedback and deal with any questions. The mentors should visit the classroom and be willing to read proposals before they are sent out. The new faculty member should feel free to allow a mentor to see incomplete and undeveloped proposals and manuscripts in order to receive useful criticism, without fear that they will later be judged harshly for it.

All members of the tenured faculty need to see retention of junior faculty as one of their most important roles because it is in their own best interest to do so. Even an intellectual loner must admit that retaining new faculty members improves the intellectual environment of the department, reduces the teaching and committee load on everybody, and reserves IDC funds to do things in the department other than set up yet another new faculty member. The Chemistry Department now has an excellent group of young faculty members; it must take vigorous steps to allow them to succeed and want to stay at UNM.

The mentoring of junior faculty is very important. Although the inorganic division appears to be doing a good job of providing advice and counsel to junior faculty, mentoring across the other divisions appears ad hoc. In addition to the mandatory annual meetings with the chair, each junior faculty member should be assigned a tenure and promotion committee that meets at least annually on a formal basis. This committee should be willing to read grant proposals and manuscripts. They should also provide advice on publication (when to publish and in which journals), grant submissions (where to submit and how much to ask for, special funding opportunities), as well as on which scientific meetings to attend. If the junior faculty cannot get enough graduate students in their groups to carry out the research, the committee could aid in seeking good postdoctoral researchers to fill positions. The committee should be the point persons in promoting junior faculty. For example, the committee should be responsible for nominating the junior faculty for national awards, and in helping junior faculty become invited to present seminars at peer research institutions and Gordon Research Conferences where the junior faculty gain visibility. Funds must be identified for sending junior faculty to Washington D.C. to meet with program directors of their funding agencies. They must learn grantsmanship first hand, and there is no better way than to discuss issues and opportunities directly with the individuals who are handling the evaluation and funding of their proposals.

The Chair and other key faculty may also benefit by an excursion to Washington, particularly to be informed of funding available for infrastructure development (e.g., EPSCOR) and in minority programs.

Although covered elsewhere in this document, one of the highest and most critical resource concerns for faculty is access to adequate numbers of high quality graduate students to carry out the research effort in the Chemistry Department. Both the recruitment of graduate students and their equitable and effective distribution among the active research groups are problems the department must resolve.

The faculty must discuss and reach some consensus concerning resource allocation in Colloquia versus more specialized seminars. Few faculty seem genuinely pleased with the status quo, and some compromise must be reached wherein the majority of faculty believe the balance offered is of benefit to their development and that of their students.

The Chemistry Department is to be commended for its policy on post tenure review. This is really a model for other institutions. It provides a clear outline of the expectations of senior faculty and outlines procedures for continued faculty development and evaluation. Virtually all contingencies appear to be covered in this comprehensive document, which should reduce conflicts that inevitably arise in many other departments around the country.

The administration should support the development of all faculty by providing them with travel grants to subsidize attendance at scientific meetings to present their work and to interact with peers. (A similar program should be made available for graduate students.) The retention of faculty is a major concern. Salary increases have been virtually nonexistent over the past few years, and this, combined with salaries already far below peer institutions, has discouraged the faculty. During the past 20 years, 16 faculty members that have been hired have either left or become administrators at the university. This is an atrocious track record that has sapped resources from the Chemistry Department and the University. With its limited resources, the University simply cannot afford this level of hemorrhage. The Administration must recognize that competitive salaries and retention packages must be assembled in order to retain outstanding faculty. To try and save money in this arena is simply a false economy that ends up costing more money in the long run, and sabotages the department's efforts to build a stable, nationally recognized, research active unit.

Graduate Student Recruiting and Diversity

Recruiting graduate students

The Chemistry Department at the University of New Mexico (UNM), consistently indicated that one of their highest priority is recruiting and retaining better graduate students. However, with few exceptions, it appears that the department has elected not to participate in the graduate recruiting competition.

In spite of what is said the recruiting of graduate students does not appear to be a high priority of the department; it is definitely not effective. Some faculty seem to think that obtaining more students is impossible, and thus a waste of their time. Other faculty recruit students vigorously, but only for their research groups. A concerted effort should be made to obtain more students, and more U.S.-born students, while keeping the quality of the students high. It will require more time from the faculty, and more state and federal funding.

The recruitment of chemistry graduate students has become a highly competitive business in almost every chemistry department across the entire nation. The competition has accelerated to the point that graduate assistant (GA) stipends in the mid twenties are not uncommon. In addition, many departments have developed highly innovative schemes which will give them a recruitment edge over their peers/competitors. These schemes include. but are not limited to 1) coordinated campus visitations for potential recruits, 2) coordinated visitations to schools with potential recruits, 3) extensive web-based recruiting materials, 4) summer Research Experiences for Undergraduate (REU) programs, 4) extensive personal contact during recruitment. and 5) even signing bonuses.

Students should be brought to UNM during the summer before their senior year to do research. They could be supported from faculty research grants, from federal programs to increase minority students, and from campus-wide competitive fellowships. The national laboratories supported by DOE have summer internship programs, so UNM may be able to collaborate with LANL to have students do collaborative research during the summer. A productive summer experience should produce a strong attraction to the graduate program.

It appears that the organic division at UNM is the most aggressive in their recruitment efforts in that they have implemented some of the strategies outlined above. In fact, the organic division has a major fraction of the current graduate student population. However, the negative side of this effort is that their recruitment appears to have focused mainly on the recruitment of students from mainland China such that this group is a significant fraction of the overall graduate population. While it is much easier to recruit students from mainland China than domestic students, the long-term strategy of this group as well as the overall department must be to focus on the recruitment of domestic students. This is the only way that the university can make a convincing argument to state legislators for investing more heavily into graduate education efforts at UNM. It should also be noted that this problem was cited in the last review, almost ten years ago. Instead of improving the situation, the Chemistry Department has gone in the opposite direction with an increase in its dependence on foreign students.

The recruitment efforts of the Chemistry Department as a whole are dismal and far less aggressive than that of the organic division. Other divisions should follow the lead of the organic division in their aggressive recruiting. It is counter-productive to believe that domestic graduate students will come to UNM without some components of the aggressive recruiting efforts outlined in the first paragraph above. In particular, it is incumbent on junior and mid-career faculty to take the lead in this process since their careers will depend more heavily on the quality of graduate students that can be attracted to the department. It is quite apparent that very-good to excellent graduate students can be recruited to UNM since it appears that other programs are having demonstrable success in this area. Some additional funds should be sought from the Dean of Graduate Studies to assist in implementing a more aggressive recruiting effort which includes visitation to neighboring schools as potential sources of future graduate students.

Despite the lack of aggressive graduate student recruitment by UNM chemistry faculty, the visiting committee found signs of hope among the graduate students that were interviewed during the site-visit. Aside from the usual complaints, many of these students appeared to be happy with their decision to matriculate at UNM. One disconcerting complaint was that some of the chemistry faculty appear to give the students the opinion that they are " ... second-rate students in a second-rate graduate program." If this is true, it is not a healthy attitude for the students. nor for future recruiting since current graduate students can be your best recruiters or your worst enemies for future recruiting.

The Chemistry Department must find a mechanism to increase graduate student stipends. The department should develop a clearly focused strategic plan for requesting funding in order to keep the number of stipends at a level consistent with the teaching needs, department growth, and at a competitive stipend level. The plan should allow the department to have funds for increased numbers of graduate students as its recruiting effort succeeds. (It is common for from 25-40% of the graduate students in chemistry departments with large service teaching roles to be supported totally or partly as teaching assistants.) The department must find a mechanism to implement many of the aggressive recruiting efforts outlined in the first paragraph above.

Diversity in the Graduate Program

The state of New Mexico has one of the highest percentage of Hispanics (-43%) and Native Americans (-7%) in the country. In light of these demographics, it is puzzling that the graduate program at UNM has very few Hispanic and apparently no Native American graduate students. The Chemistry Department must develop a more aggressive plan for recruitment of Hispanics, Native Americans, and other minorities into its graduate program. Serving the entire state population should be a goal of the flagship institution of all states. In addition, as a "minority-serving" institution, there are many government programs, particularly at NIH, which can be sought to help in this effort. Examples of these programs include BRIDGE for interfacing with community colleges and Research Centers in Minority Institutions (RCMI) which provides large amounts (-2 million dollars/ year) of long-term funding for departments or programs. The department should aggressively look into these programs as a possible solution to some of their graduate recruiting and infrastructure needs. It is very alarming that the department was not aware of these programs, nor do they participate to any significant extent in those that are already on campus, e.g. MBRS (RISE). Finally, the department should explore funding options which exploit their EPSCOR designation for this and other goals in the department.

Graduate Program including Instruction, Research Opportunities and Student Development

The Graduate Program

The graduate students in the Chemistry Department seem to be mainly satisfied. The ones we talked to-a self-selected group- said they would recommend UNM to their friends. They thought that a small department had the advantage that most of the faculty knew them and that they knew many of their fellow students. They recommended more social occasions. and admitted that they could probably have more, if they organized them. Once the students enter the program, most can benefit and acquire the skills to succeed in science. The key problem is to recruit more, high quality, students. This will, in turn, make it easier to hire and retain excellent faculty.

In the spring semester 2003 the Chemistry Department listed 21 faculty and about 55 graduate students. The low number of graduate students in the chemistry program is a very significant obstacle to the improvement, and growth of the department. The lack of graduate students makes it difficult to hire and retain the best faculty. Many of the faculty have federal funding to support research assistants, but none are available. Without students to help on research projects, the faculty will not be able to renew grants or to compete effectively for new grants. A vigorous effort must be made to attract more students, and to ensure an equitable distribution of the ones that enter the program. The students should have a basic understanding of chemistry on entering the program; any deficiencies in this knowledge can be corrected by course work in the first year. On finishing the program, each student should have acquired advanced knowledge in one of the four main subdivisions of chemistry, usually considered to be analytical biochemistry, inorganic, organic, and physical, although the borders between divisions are blurring nationally and biological chemistry crosses over each of these traditional areas. A core program of required courses in each area is the usual method for accomplishing this. Each student should obtain experience in teaching, and in presenting their work orally and in writing. Finally, each student who receives a Ph. D. should be able to do independent, original research as demonstrated by writing a thesis, and usually by publishing their results in a peer-reviewed journal.

The first year

The first year of graduate school requires the students to demonstrate a basic knowledge of chemistry, to take graduate courses, to serve as teaching assistants, and to choose a research director. It is a stressful period. The Chemistry Department provides guidance in all these areas, but the students and faculty have strong opinions on how to improve the process. ***The goal is to have clearly stated requirements that are applied consistently and uniformly to all students. It is important to treat all graduate students equally and uniformly across divisions.*** The students should be instructed in becoming effective teaching assistants, and should be guided to choose a research director that is consistent with their interests, but also provide an equitable distribution of research assistants.

Each division should commit to offering at least one graduate course each semester, and first year students should enroll in these courses, even if the courses are not directly related to each student's research plans. The process for assigning specific teaching roles was not clear. This appears to be left entirely to the divisions. At what point does the chairman step in to assure coverage across the department and fairness among divisions and among junior and senior faculty?

A core set of courses should be required of all students in each discipline that ensures the students do obtain the requisite knowledge. This means that core courses must be given regularly, which is not done at present because of the demands of undergraduate teaching. Possible solutions include using sabbatical visitors, lecturers or postdoctorals to teach some undergraduate courses, and having scientists from LANL and Sandia teach some graduate courses. The LANL teachers could give some lectures by video. The optimum, long range solution is to have enough faculty to teach all the required courses.

1. Entering students should be given a clear description of requirements, duties, and available services. This should be on the web, in printed form, and discussed in an early meeting.

2. Students who do not have proficiency in a fundamental area of chemistry should be required to pass a course in the subject with a B-or-better grade. At present students show a basic proficiency in chemistry by passing standardized American Chemical Society exams. Students who do not pass have the option of passing a course, or retaking the same exam. The committee (and some faculty) think that retaking the exam does not test the student's knowledge adequately and should not be allowed.

3. Students should be instructed, before the course starts, in being an effective teaching assistant for each course they supervise. The Chemistry Department seems to concentrate on teaching assistants in the beginning chemistry course, and on pairing one new teaching assistant with an experienced one in advanced courses. This is helpful, but some teaching assistants have had no training before teaching a course for the first time. The campus should also provide lectures to help graduate students become better teachers before the beginning of each semester.

4. The chairman of the Chemistry Department in consultation with the faculty should approve each student's choice of research director. The appropriate distribution of students among research groups is a difficult problem, because there are many competing desires among the students, faculty, and administration. Of course the interest of the student should be dominant, so they should have ample opportunity to learn about the faculty research programs. In addition to attending the present mandatory course where faculty talk about their research, each student should be required to interview at least three to five faculty members. The students should then submit to the chairman's office a list of their three top choices. Although every effort should be made to have the student's first choice ratified, the approval among the listed choices should rest on the following criteria: Assistant professors need to establish programs and an effort should be made to get at least one graduate student each year to these people for their first four or five years. Tenured professors without funding generally should be allowed no more than one departmentally supported research assistant in their group unless special circumstances exist (such as a recent loss in funding with new proposals submitted, a new research direction with

proposals pending, etc.). It is a waste of departmental resources to support students in senior faculty groups that cannot get funding, and it is probably not good research training for the students. Faculty members also must be consulted regarding acceptance of a student listing them as the first choice.

Advanced graduate education and research

In the second year and succeeding years each student learns the core knowledge that makes them a professional chemist, and does original, independent research resulting in a Ph. D. thesis. The students demonstrate their knowledge by their course grades and by passing a minimum number of cumulative exams in chemistry. Before being advanced to candidacy each student writes a research proposal, presents it orally to a public audience, then defends it before a faculty committee.

The departmental core courses for graduate students should be tied to both the proficiency and cumulative exam process and therefore taught regularly. The cumulative exams should not only serve to test knowledge, but they should help the students learn chemistry. To accomplish this each cumulative exam should be the responsibility of two faculty members; this should improve the relevance and uniformity of the questions. Written answers to all the questions should be available soon after each exam.

The student's public presentation of the research proposal should be separated from its defense by at least one week. The research proposal, its presentation, and its defense has multiple goals, and requires different skills. Separating the presentation from the defense gives all students the best opportunity to learn from their presentation, and to demonstrate their abilities.

When the student is advanced to candidacy, a thesis committee should be assigned to meet with the student once a year to discuss progress. The committee may help avoid trouble when the student is not making progress, or the faculty member is being too demanding, or other problems arise.

Teaching Loads for Faculty

The Chemistry Department has an unusual teaching structure, but one rather normal for chemistry in research universities, in that it teaches vital service courses to many campus programs but has very few students who choose to major in Chemistry. There are more graduate than undergraduate students majoring in Chemistry, and more graduate than undergraduate degrees awarded by the department. As a result, the department must put more energy into its graduate academic program.

The teaching loads did not appear to be a major issue in the Chemistry Department. For research-active faculty the load of one full course each semester is the norm, in addition to mentoring and meeting with graduate students. This is in line with the practice in chemistry departments around the country. It is also reasonable that faculty members who are no longer research active will take on greater teaching responsibility, as currently appears to be happening in Chemistry. Faculty members with partial administrative assignments at UNM are also major contributors to the undergraduate teaching mission. This is helpful. There could be some additional benefit if more lecturers were to hired to take on teaching in the freshman and non-major programs, although we recommend against turning this over entirely to non-tenure track faculty because of the importance of getting students interested in chemistry early on. The department is to be congratulated for having its research faculty involved in the undergraduate courses and it seems likely that the number of undergraduate majors could be increased as a result.

In the context of this program review it is clear that if the overall faculty time assigned to freshman courses could be reduced, this time would be available to offer more graduate-level instruction. The organization of graduate instruction needs careful thought.

Facilities, Resources and Infrastructure

Some of the individual/divisional instrumentation facilities in the Chemistry Department are superb - matching the best in the nation. The spectroscopic center housed in the inorganic division and the mass spectrometry instruments in the biological group are examples. On the other hand, with the exception of the chemical stockroom, many of the shared departmental facilities are significantly less state of the art and/or create other concerns.

The Chemistry Department is in the luxurious position of having staffing of the NMR facility as a line item in the University budget. Still, the Chair must be sensitive to funding the upkeep and maintenance of the facility. At this point in time, the burden for these costs falls on a very limited number of faculty. Until junior faculty users of the facility acquire outside funding to help support the NMR center, the facility may have to be subsidized. Fortunately, the number and quality of the instruments in place appear adequate for the time being.

The same cannot be said for the X-ray facility. Here, the instrumentation is badly outdated (>20 years old), and as a result many faculty are sending samples outside. Consequently, funds that might remain in the department for upkeep and maintenance of this facility are being drained away. For this reason, as well as for educational purposes, the department must write a proposal for a modern CCD X-ray diffractometer.

Shared mass spectrometry in the Chemistry Department is also woefully inadequate (virtually non-existent). It is our understanding that the department has tried to raise federal funding for a high-resolution mass spectrometer, and has thus far been unsuccessful. This is not uncommon for any department, and must not prevent them from trying again. Additionally, the department might consider writing proposals for routine, walk-on GC/MS and LC/MS instruments. This would not only facilitate research in small molecule chemistry, but is also absolutely necessary for educational purposes (both graduate and advanced undergraduate).

The Chemistry Department must aggressively pursue funding to upgrade departmental facilities. The case must be made for modern instrumentation, not only for the research mission of the individual groups, but also for the educational mission of the department. Both graduate students and undergraduates alike must be exposed to modern, state of the art instrumentation in order to be considered well-trained for future careers in the sciences. The committee recommends that an instrumentation committee be established to coordinate efforts in the department to submit proposals annually to NIH, NSF, and perhaps other agencies to acquire funding to upgrade these and any other instrumentation needs of the department.

Staffing must also be found to assist faculty in their computational/networking needs. This may be a talented undergraduate or graduate student from the computer science department or a full time staff person perhaps shared with other departments on campus. Along these lines, systems for computational modeling must be developed/enhanced.

In order to maintain first class electronic and machine shops, the Chemistry Department should actively discuss the possibility of establishing shared facilities with other units on campus as equal partners.

The lack of proper facilities maintenance protocols has raised serious issues of health and safety within the Chemistry Department. The Chair, in consultation with other chairs and Administrators, should establish a protocol and communication network that will allow discussion of any physical plant maintenance that will disrupt electricity, water, or hoods CONSIDERABLY BEFORE such work is undertaken, so that researchers can plan their activities around these job actions. All measures must be taken to inform faculty, graduate students, undergraduate researchers, and postdoctoral research associates of the contacts that should be made in the event of physical plant breakdowns (e.g., power outage, leaks, hood malfunctions, etc.).

Although perhaps little of the space in chemistry is ideal by modern standards, the committee does find that there is adequate space for the immediate future. Thus, the building appears to have the capacity to house about 100 graduate student and postdoctoral researchers. At present, there are only 70 researchers in the department. However, if the junior faculty are to develop as hoped, and if further faculty hires are imminent, this small cushion wi11 rapidly evaporate. It is inevitable that if the department is successful, modem, safe new space must be created. The department should take the initiative in this by writing proposals to the NIH and/or NSF to acquire funds for building renovation/construction that will provide seed money for enhancing the possibilities of more substantial funding from the Administration/State. The Administration must continue to press for funding construction of a new chemistry building as a top priority.

Within the framework of current space, there are some critical needs as well. Space must be assigned to incoming graduate students so that they feel a part of their new environment. Whether this is in an assigned room or located within (random) individual laboratories, this should be a priority. Upgraded, modern classroom space for small graduate and undergraduate classes, group meetings, T A office hours, and committee meetings must be found and properly equipped.

Faculty in the Chemistry Department are fortunate to have what appears to be first rate resources in the library. In particular, the library Web design and access to electronic databases are very impressive. The library staff appears enthusiastic and well informed, and both their training facility and training program are first rate. The department should take every advantage to interact with the library staff to enhance interactions and keep the lines of communication open for further development and enhancement of this valuable resource.

The departmental Web page, by contrast, is outdated and poorly maintained. Some of the links are over two years out of date and/or no longer work. This is a highly critical resource for any department these days, particularly for graduate recruiting. The Chemistry Department must find a way to make this an attractive and useful source of information. One highlight of the departmental Web page as it exists is the free, online graduate program application. This appears to be a marvelous success.

As in the report of the previous graduate review committee, secretarial support appears virtually non-existent. The standard for the Chemistry Department is far below that of its peers, particularly for research active faculty. The Administration must recognize that its most valuable resource is the faculty, and the time the faculty must spend doing photocopying and running simple errands is simply a waste of this valuable resource. Similarly, the organic chemistry faculty must be offered teaching assistant aid in grading examinations and quizzes to free up their time for more valuable pursuits (e.g., course development, research proposal writing, etc.).

Finally, the result of discussion and negotiations between the Chemistry Department and the Administration concerning this external review should lead to a contract for improvement between the units that must be honored. It is evident that, in the past. these program reviews have simply been ignored. This has led to a cynical view on the part of the department that the review is simply a useless exercise that must be undertaken every ten years. The department should be willing to indicate to the Administration what plans it will implement and resources it will provide to improve its standing, and at the same time the Administration must be willing to do the same. This should result in a blueprint for success that should be consulted on a regular basis so that both the department and the Administration are working effectively toward a common goal.

Relationship of Graduate Program to the Undergraduate Program

As in most doctoral granting institutions, there is a clear interplay between the chemistry graduate program and the undergraduate program at UNM. This relationship stems largely from the use of graduate students to teach chemistry laboratory courses. Clearly, the extensive use of foreign graduate students, whose first language is not English, in this role can be detrimental to the education of undergraduates. This concern is yet another reason for the Chemistry Department to more aggressively recruit domestic students. In addition, while some programs are outlined for training foreign students to teach in the undergraduate laboratory, it was not clear that these programs are effective or aggressively enforced .

Another interplay between graduate and undergraduate students at UNM involves the use of senior-level undergraduates to perform graduate student teaching functions, i.e. teaching chemistry laboratories. While this effort appears to be having success, it is suggested that a more formal process (written rules) for selection of these students be implemented. This process could include the use of graduate students for early identification of outstanding undergraduate students who may later be approached as potential undergraduate assistants.

Finally, discussions with graduate students suggest that equipment in undergraduate laboratories is completely outdated. If this is true, the department should begin an aggressive effort to replace this outdated equipment. For example, the department should approach the upper administration about increasing laboratory fees to provide funding for this effort. In addition, NSF has potential funding to assist in this endeavor. There was no evidence that the Chemistry Department is pursuing such efforts.

Appendix A5. University of New Mexico Mission Statement

Mission of The University of New Mexico

The mission of The University of New Mexico is to serve the educational needs of the citizens of the state, and those of the nation and world. This mission involves four (4) interrelated dimensions:

(1) The University develops and offers comprehensive educational programs at the associate, baccalaureate, master, and doctoral levels in a wide range of academic, professional, and occupational fields.

(2) The University, a designated Carnegie I research university, conducts research and engages in scholarly and other creative activities to support undergraduate, graduate, and professional educational programs, and to create, interpret, apply, and accumulate knowledge.

(3) The University contributes to the quality of life in New Mexico by providing selected services to the public that are part of, contribute to, or originate from the University's teaching and scholarly activity programs.

(4) The University Health Sciences Center is a valuable resource to New Mexico. Added value is provided to health care through leadership in providing innovative, collaborative education; advancing the frontiers of science through research critical to the future of health care; delivering health care services that are at the forefront of science; and facilitating partnerships with public and private biomedical and health enterprises.

Appendix A6. Academic Program Plans for Assessment of Student Learning Outcomes

Academic Program
Plan for Assessment of Student Learning Outcomes
The University of New Mexico

A. College, Department and Date

1. College: Arts and Sciences: Main Campus
2. Department: Chemistry and Chemical Biology
3. Date: 1/13/09

B. Academic Program of Study

B.A. Chemistry

C. Contact Person(s) for the Assessment Plan

Alisha Ray, Lecturer II, adray@unm.edu

D. Broad Program Goals & Measurable Student Learning Outcomes

Undergraduate Program Learning Goals and SLOs

Students graduating from this program will:

1. Understand major chemical concepts, theoretical principles and experimental findings in the field of chemistry
   a. Apply their understanding of atomic theory, molecular structure and bonding, thermodynamics, kinetics, chemical reactions, spectroscopy and synthesis on examinations and laboratory exercises
2. Be able to employ critical thinking and hypothesis-driven methods of scientific inquiry
   a. Solve problems using multiple layers of data analysis
   b. Use statistics to evaluate quantitative hypotheses
   c. Critically evaluate experimental data
   d. Be able to extract chemical information from available resources

3. Convincingly present scientific data and arguments in an oral and written format
   a. Organize and represent experimental data using appropriate methods (spreadsheets, etc)
   b. Be able to write coherent scientific reports
   c. Present scientific ideas and arguments in a professional setting

4. Be prepared for entry into graduate school or professional school (e.g. medical, dental, pharmacy, etc) or the chemical industry or government service.
   a. Apply general knowledge of chemical concepts to solve novel problems
   b. Develop an awareness of the opportunities and applications of chemical knowledge to the world
   c. Obtain a working knowledge of basic chemical concepts, laboratory skills and safety

d. Develop scientific literacy and be familiar with the status of current research in the field of chemistry
e. Acquire general skills to work in small groups to accomplish scientific projects

E. <u>Assessment of Student Learning Three-Year Plan</u>

All programs are expected to measure some outcomes annually and to measure all priority program outcomes at least once over two consecutive three-year review cycles. Describe below the plan for the next three years of assessment of program-level student learning outcomes.

1. Student Learning Outcomes

<u>Relationship to UNM Student Learning Goals</u> (insert the program SLOs and check all that apply):

University of New Mexico Student Learning Goals				
Program SLOs	Knowledge	Skills	Responsibility	Program SLO is conceptually different from university goals.
1a. Apply their understanding of atomic theory, molecular structure and bonding, thermodynamics, kinetics, chemical reactions, spectroscopy and synthesis on examinations and laboratory exercises.	X	X		
2a. Solve problems using multiple layers of data analysis.	X	X		
4a. Apply general knowledge of chemical concepts to solve novel problems	X	X		

2. How will learning outcomes be assessed?

A. <u>What</u>:

i. Each SLO will be measured using samples of evidence of learning from courses required by the B.A. program. For the 2008-2009 academic year, samples of evidence of learning will be gathered for program SLO 2a in Dr. Lisa Whalen's CHEM 302 course. Professor Debi Evans will collect data related to SLO 1a in her CHEM 315. Depending on course enrollment numbers for chemistry majors, Dr. Joe Ho will use evidence from CHEM 253 to measure SLO 4a. Each will provide at least one direct measurement using graded material (exams, homework, or quizzes). The same SLOs and samples of learning will be gathered for the following two years unless the feedback obtained for the pilot study suggests major changes.

ii. Each SLO measured in the 2008-2009 academic year will be a direct measure. If no major changes are made to the proposed program assessment plan then all measures over the next three years will be direct.

iii. The program's assessment target is to have 60% of the students in the B.A. program to perform satisfactory or better. Scoring rubrics will be used for some measures, but they are not currently available.

B. Who:

Less than half the students in each undergraduate program will take part in the pilot assessment during the next academic year. Because both B.A. and B.S. programs are undergoing major curriculum changes in the next few years there will be difficulties in efficiently assessing all the students in the program each year. However over the next three years it is expected that 80% of students in the program will be assessed using at least one direct measure. A sample representing more than three quarters of the students in the program will be valid since it reflects the majority of students.

3. When will learning outcomes be assessed? When and in what forum will the results of the assessment be discussed?

Each fall (2008, 2009 and 2010) semester a minimum of one and maximum of three "priority" SLOs (1a, 2a, and 4a) will be assessed. The results of the outcomes measured the previous fall will be discussed each February (2009, 2010 and 2011) by a group of faculty including, but not limited to, Dr. Evans, Dr. Ho, Dr. Whalen, and Ms. Ray. All department faculty will be notified via email and invited to the meeting no less than 3 weeks before the scheduled meeting.

4. What is the unit's process to analyze/interpret assessment data and use results to improve student learning?

1. The faculty collecting evidence during that academic year and the chair of the Assessment Committee will meet each February to analyze and interpret the assessment data. All faculty will be invited to participate in the meeting. For the 2008-2009 academic year each faculty member who collected data will present how they carried out the assessment (the tools/techniques used), how they analyzed the data, and what will be done to improve student learning. Finally, plans will then be made for the following year so that only one or two SLOs are tested using one or more direct measures and the analysis is done by everyone attending the meeting using a "calibrated" rubric rather than just the faculty member who collected the data.
2. The implications of the assessment will be discussed at a meeting in February each year.
3. Recommendations will be compiled at the February meeting by the assessment committee chair and communicated in writing to the department chair with the signatures of all members of the assessment committee by May 15th each year. Copies of the document will be provided and discussed in the annual faculty retreat each August.

Academic Program
Plan for Assessment of Student Learning Outcomes
The University of New Mexico

A. College, Department and Date

1. College: Arts and Sciences: Main Campus
2. Department: Chemistry and Chemical Biology
3. Date: 1/14/09

B. Academic Program of Study
B.S. Chemistry

C. Contact Person(s) for the Assessment Plan
Alisha Ray, Lecturer II, adray@unm.edu

D. Broad Program Goals & Measurable Student Learning Outcomes
Undergraduate Program Learning Goals and SLOs

Students graduating from this program will:

1. Understand major chemical concepts, theoretical principles and experimental findings in the field of chemistry
   a. Apply their understanding of atomic theory, molecular structure and bonding, thermodynamics, kinetics, chemical reactions, spectroscopy and synthesis on examinations and laboratory exercises
2. Be able to employ critical thinking and hypothesis-driven methods of scientific inquiry
   a. Solve problems using multiple layers of data analysis
   b. Use statistics to evaluate quantitative hypotheses
   c. Critically evaluate experimental data
   d. Extract chemical information from available resources

3. Demonstrate the ability to construct and test hypotheses using modern laboratory equipment and appropriate quantitative methods
   a. Construct and test hypotheses
   b. Design experiments
   c. Use instrumentation to collect data
   d. Process data using a computer and use statistics to evaluate data
   e. Recognize, generate and analyze alternative explanations and models for experimental data
   f. Interpret experimental results and draw conclusions

4. Convincingly present scientific data and arguments in an oral and written format
   a. Organize and represent experimental data using appropriate methods (spreadsheets, etc)

b. Write coherent scientific reports
c. Present scientific ideas and arguments in a professional setting

5. Be prepared for entry into graduate school or professional school (e.g. medical, dental, pharmacy, etc) or the chemical industry or government service.
   a. Apply general knowledge of chemical concepts to solve novel problems
   b. List and explain some of the opportunities and applications of chemical knowledge to the world
   c. Have a working knowledge of basic chemical concepts, laboratory skills and safety
   d. Demonstrate scientific literacy and be familiar with the status of current research in the field of chemistry
   e. Have general skills to work in small groups to accomplish scientific projects

E. Assessment of Student Learning Three-Year Plan

All programs are expected to measure some outcomes annually and to measure all priority program outcomes at least once over two consecutive three-year review cycles. Describe below the plan for the next three years of assessment of program-level student learning outcomes.

1. Student Learning Outcomes

Relationship to UNM Student Learning Goals (insert the program SLOs and check all that apply):

University of New Mexico Student Learning Goals				
Program SLOs	Knowledge	Skills	Responsibility	Program SLO is conceptually different from university goals.
1a. Apply their understanding of atomic theory, molecular structure and bonding, thermodynamics, kinetics, chemical reactions, spectroscopy and synthesis on examinations and laboratory exercises.	X	X		
2a. Solve problems using multiple layers of data analysis.	X	X		
3f. Interpret experimental results and draw conclusions	X	X		
5a. Apply general knowledge of chemical concepts to solve novel problems	X	X		

attending the meeting using a "calibrated" rubric rather than just the faculty member who collected the data.

2. The implications of the assessment will be discussed at a meeting in February each year.
3. Recommendations will be compiled at the February meeting by the assessment committee chair and communicated in writing to the department chair with the signatures of all members of the assessment committee by May 15th each year. Copies of the document will be provided and discussed in the annual faculty retreat each August.

Academic Program
Plan for Assessment of Student Learning Outcomes
The University of New Mexico

A. College, Department and Date

1. College: *Arts and Sciences: Main Campus*
2. Department: *Chemistry and Chemical Biology*
3. Date: 1/15/09

B. Academic Program of Study

M.S. Chemistry

C. Contact Person(s) for the Assessment Plan

Alisha Ray, Lecturer II, adray@unm.edu

D. Broad Program Goals & Measurable Student Learning Outcomes

Graduate Program Goals and Student Learning Outcomes

Upon graduating from the graduate program, students will:

1. Develop a broad understanding of the major areas of chemistry with an understanding and awareness of the professional, ethical and safe applications of their knowledge.
    a. Possess broad factual knowledge at an advanced level in multiple areas of chemistry
    b. Actively participate in the weekly departmental seminars
2. Acquire a significant and deep-rooted knowledge in their chosen sub-discipline in chemistry.
    a. Learn subject specific content such as synthesis and characterization, reaction mechanisms, thermodynamics, quantum mechanics, kinetics, spectroscopy, equilibrium and quantitative methods
    b. Attend divisional student seminars in their chosen area of chemistry
3. Report, present and/or publish the results of their research and independently solve research problems.
    a. Present independently researched topics in their divisional seminar
    b. Publish their research findings in peer reviewed scientific journals with their research advisor(s)
    c. Write a coherent masters thesis or written final project covering their specific contributions to the discipline of chemistry
4. Be prepared for entry into academe or industry.
    a. Be members of at least one professional scientific organization
    b. Engage in collaborative research with other scientists in their field
    c. Solve research problems independently or as a small team

Future goal to be developed: Students will have the knowledge, skills and ability to define and study a specific research project and apply appropriate scientific methods to it.

E. Assessment of Student Learning Three-Year Plan

All programs are expected to measure some outcomes annually and to measure all priority program outcomes at least once over two consecutive three-year review cycles. Describe below the plan for the next three years of assessment of program-level student learning outcomes.

1. Student Learning Outcomes

Relationship to UNM Student Learning Goals (insert the program SLOs and check all that apply):

University of New Mexico Student Learning Goals				
Program SLOs	Knowledge	Skills	Responsibility	Program SLO is conceptually different from university goals.
2a. Learn subject specific content such as synthesis and characterization, reaction mechanisms, thermodynamics, kinetics, spectroscopy, equilibrium and quantitative methods.	X			
3b. Publish their research findings in peer reviewed scientific journals with their research advisor(s).	X	X	X	
3c. Write a coherent masters thesis or written final project covering their specific contributions to the discipline of chemistry	X	X	X	

2. How will learning outcomes be assessed?

A. What:

i. SLO 2a will be measured using one or two questions from the cumulative examinations (written by faculty) given eight times each academic year. M.S. degree students must pass three exams within fourteen attempts.
SLO 3b will be measured by having graduate advisors submit a list of the work published each year involving their graduate students.
Evidence for SLO 3c will be gathered from final project committee members using the Report on Thesis or Dissertation provided by the Office of Graduate Studies (see attachment).

ii. SLO 2a will be measured ~~using~~ directly and SLOs 3b, and 3c will be measured indirectly.

iii. The program's performance target for SLO 2a is for one-third of the students required to take the exam to perform acceptably on the chosen cumulative exam question(s). The target for SLO 3b is to have 50% of the students in the program have their research published in a peer reviewed journal each year. The expected target for SLO 3c is that 75% of students giving a final project defense each year pass without needing extensive written revisions.

B. Who: Evidence from each student in the M.S. program will be sampled over a three year cycle.

3. When will learning outcomes be assessed? When and in what forum will the results of the assessment be discussed?

Data collected for SLOs 2a, 3b, and 3c in fall 2008 and spring of 2009 will be included in the program pilot assessment. Interpretation and discussion of the same SLOs will be completed by mid June 2009. Data collected in the summer of 2009, fall 2009 and spring 2010 over the same SLOs will be interpreted and discussed at the fall faculty retreat in August 2010. A similar pattern will follow for the next academic year.

4. What is the unit's process to analyze/interpret assessment data and use results to improve student learning?

1. The chair of the assessment committee will be the faculty member responsible for collecting evidence during the academic year and the committee will include one or two other faculty members to analyze and interpret the assessment data.
2. The implications of the assessment will be discussed at a meeting in April each year.
3. Recommendations will be compiled by the assessment committee chair and communicated in writing to the department Chair by May 15th each year. Copies of the document will be provided and discussed in the annual faculty retreat each August.

Appendix A7. Undergraduate degree requirements and example 4-year schedules

UNM Core Curriculum (2012-2013 catalog)

The University adopted a revised Core Curriculum as of Fall 2003 which all undergraduate students must complete as part of their baccalaureate program. The Core consists of several groups of courses designed to enhance each student's academic capabilities. Its goal is to give all students at the University a grounding in the broad knowledge and intellectual values obtained in a liberal arts education and to assure that graduates have a shared academic experience. The required courses encourage intellectual development in seven areas of study: writing and communication, social and behavioral sciences, mathematical reasoning, scientific methods in the physical and natural sciences, the humanities, the fine arts, and languages. The Core consists of lower-division courses which develop these skills and abilities, and students are strongly encouraged to complete the Core early in their college careers. Individual student substitutions should be minimal and are discouraged. Except where noted (see "Alternative Credit Options" in the Undergraduate Admissions section of the Catalog), students may apply AP or CLEP credit to the Core requirements.

Departments and colleges may restrict student choices within the Core to meet departmental and college degree requirements. A grade of C (not C-) is required in all courses used to fulfill the requirements of the Core Curriculum. Courses taken CR/NC can be applied to the core, subject to general University and individual college and department regulations on the number of credits that can be taken CR/NC and the applicability of courses taken CR/NC to the individual degree.

The University recognizes, however, that the highly structured nature of many degree programs and the presence of numerous transfer and non-traditional students requires flexibility on its part. Transfer and re-entering students will receive advising in the college and department to which they are admitted in order to establish an appropriate program which will meet their needs and the aims of the Core. Where degree program requirements are so structured that a student's total academic program credits would be increased by taking a Core course in a particular Core area, a department may approve a blanket substitution of a course in a particular Core area for all students pursuing an undergraduate degree in that particular program. Approval of substitutions or exceptions is handled on a department and college basis.

The basic Core Curriculum requires approximately 37 hours of courses in seven areas of study.

Writing and Speaking (9 hours): English 101 and 102 plus an additional course chosen from English 219, 220; Communication and Journalism 130; Philosophy 156. Students with ACT English scores of 29 and higher or SAT Critical Reading scores of 650 or higher have satisfied the University Writing Requirement and should enroll for courses of their choice in the Writing and Speaking Core. Students with ACT English scores of 26, 27, 28 or SAT Critical Reading scores of 610 or higher may enroll directly in English 102 and, upon passing, meet the University Writing Requirement. Students with ACT English scores of 25 or lower or SAT Critical Reading scores below 610 should enroll in English 101. Students who have taken an Advanced Placement examination in English Language or Literature should refer to "Advanced Placement" for placement and credit information.

Mathematics: One course chosen from MATH 121, 129, 150, 162, 163, 180, 181, 215, Stat 145.

Physical and Natural Sciences: Two courses, one of which must include a laboratory, chosen from Anthropology 150 and 151L, 120 (lab required), 160 and 161L; Astronomy 101 and 101L; Biology 110 and 112L, 123 and 124L; Chemistry 111 (lab required), 121 and 123L or 131L (lab required), 122L and 124L or 132L (lab required); Earth and Planetary Sciences 101 and 105L, 201L (lab required); Environmental Science 101 and 102L; Geography 101 and 105L; Natural Sciences 261L (lab required), 262L (lab required), 263L (lab required); Physics 102 and 102L, 105, 151 and 151L, 152 and 152L, 160 and 160L, 161 and 161L.

Social and Behavioral Sciences (minimum 6 hours): Two courses chosen from American Studies 182, 185; Anthropology 101, 130; Community and Regional Planning 181; Economics 105, 106; Engineering-F 200; Geography 102; Linguistics 101 (AOA Anthropology 110); Political Science 110, 200, 220, 240; Psychology 105; Sociology 101.

Humanities (6 hours): Two courses chosen from American Studies 186; Classics 107, 204, 205; Comparative Literature and Cultural Studies 222, 224; English 150, 292, 293; Foreign Languages (MLNG) 101; Geography 140; History 101, 102, 140, 161, 162, 181, 182; Honors Legacy Seminars at the 100- and 200-level; Philosophy 101, 201, 202; Religious Studies 107, 263, 264.

Foreign Language (non-English language; minimum 3 hours): One course chosen from any of the lower-division non-English language offerings of the Departments of Linguistics (including Sign Language), Spanish and Portuguese, Foreign Languages and Literatures, and foreign languages in other departments and programs.

Fine Arts (minimum of 3 hours): One course chosen from Architecture 121; Art History 101, 201, 202; Dance 105; Fine Arts 284; Media Arts 210; Music 139, 142; Theatre 122. Students may elect to take one 3-hour studio course offered by the Departments of Art and Art History, Music, Theatre and Dance, and Media Arts to fulfill this requirement.

Undergraduate Programs (in CCB, 2012-2013 catalog)

Major Study Requirements

The Bachelor of Arts degree has two options each of which requires a minimum of 24 credit hours earned in chemistry courses beyond CHEM 121, 123L, 122, 124L. The B.A. must also include the following: 253L, 301, 302, 303L, and 304L.

For the degree of Bachelor of Arts: CHEM 121, 123L, 122, 124L, 253L, 301, 302, 303L, 304L, 315, and sufficient hours of electives to bring the total to 31 hours (see approved electives below). Electives must be selected from the following courses: CHEM 421, 422, 424L, 425, 431, 471, 495-496 (no more then 2 credit hours in 495-496). The B.A. program must also include PHYC 151, 151L, 152, 152L and MATH 162 and 163. Those students who previously majored in a field requiring MATH 180 and 181 and then switched to the B.A. program in Chemistry, may substitute that sequence for MATH 162 and 163 with the permission of the Department of Chemistry and Chemical Biology Chairperson. If the substitution is approved, the student must also take an additional 3 hours of Mathematics in a course approved by the Chemistry and Chemical Biology Department Chairperson.

For the degree of Bachelor of Science: CHEM 121, 123L, 122, 124L, 253L, 301, 302, 303L, 304L, 311, 312, 411L, 431, 453L, and at least 7 additional hours selected from courses numbered CHEM 325-498 (at least 3 of the 7 credits must be a laboratory course). The program must also include PHYC 160, 160L, 161, 161L, mathematics equivalent to MATH 264 and one course from MATH 311-316. Up to 3 credits of CHEM 495-498 or 2 credits of 495-498 and 1 credit of 325-326 may be counted toward the B.S. degree.

NOTE: CHEM 131L may be substituted for CHEM 121 and 123L and 132L may be substituted for CHEM 122 and 124L.

NOTE: Physics and mathematics courses required for the B.S. or B.A. degree may not be taken on the credit/no credit grade option.

NOTE: If changing from a B.A. to a B.S., students will be required to complete MATH 162 and MATH 163 and PHYC 160, 160L, 161, 161L. Students wishing to have their B.S. degree certified by the American Chemical Society (ACS) must include CHEM 421 and 432L.

NOTE: Physics and mathematics courses required for the B.S. or B.A. degree may not be taken on the CR/NC grade option.

Students wishing to have their B.S. degree certified by the American Chemical Society (ACS) must include CHEM 421 and 3 hours of research in their 6 hours of electives.

No distributed minors are allowed for B.A. majors.

In lieu of a specific minor, a student in the B.S. program may obtain the following distributed minor:

Distributed Minor

Completion of the Chemistry B.S. requirements in addition to taking one additional course from MATH 311, 314 or 316 and ENGL 219.

Minor Study Requirements

Twenty hours in Chemistry to include: CHEM 121, 122, 123L, 124L, 253L, 301, 302, 303L, 304L.

Departmental Honors

The student enters the program at the beginning of the junior year. At this time the student's grade point average must be at least 3.20 overall and 3.50 in chemistry. This minimum must be maintained throughout the junior and senior years. Course requirements for graduation with honors are as follows: 121, 122, 123L, 124L, or (131L, 132L), 253L, 301, 302, 303L, 304L, 311, 312, 411L, 421, 431, 432L, 453L, and 7 hours of additional courses from 325-498, including at least 3 hours of 497-498. A senior honors thesis will be written based on the senior honors research and submitted to the faculty. An oral presentation will also be made in a departmental or divisional seminar. Honors students will also take the Graduate Record Examination Advanced Test in Chemistry in their senior year and must obtain a satisfactory score.

Any deviation from the requirements prescribed above must be approved in writing.

Example Schedule for the Chemistry BA Degree

First Year

Fall	CH	Spring	CH
CHEM 121 General Chemistry I	3	CHEM 122 General Chemistry II	3
CHEM 123L General Chem Lab I	1	CHEM 124L General Chem Lab II	1
MATH 162 Calculus I	4	MATH 163 Calculus II	4
Foreign Language core course[a]	3	BIOL 201 Molecular and Cell Biology	4
ENGL 101 Composition I	3	ENG 102 Composition II	3
Humanities or Social Science core[b]	3	Humanities or Social Science core[b]	3
Total	**17**		**18**

Second Year

Fall	CH	Spring	CH
CHEM 301 Organic Chemistry I	3	CHEM 302 Organic Chemistry II	3
CHEM 303L Organic Chem Lab	1	CHEM 304L Organic Chem Lab II	1
BIOL 202 Genetics	4	BIOL 203L Ecology and Evolution	4
PHYC 151 General Physics I	3	PHYC 152 General Physics II	3
PHYC 151L Physics Lab I	1	PHYC 152L Physics Lab II	1
Humanities or Social Science core[b]	3	Humanities or Social Science core[b]	3
Total	**15**		**15**

Third Year

Fall	CH	Spring	CH
CHEM 315 Physical Chemistry	4	CHEM 253L Quantitative Analysis	4
CHEM 421 Biological Chemistry	3	CHEM 425 Biological Pathways	3
BIOL 204L Plant and Animal Form	4	Biology elective[d]	3
Fine Arts core[c]	3	CHEM 496 Research/Problems	1
Elective	3	Electives	6
Total	**17**		**17**

Fourth Year

Fall	CH	Spring	CH
CHEM 4xx elective	3		
Biology elective[d]	3	CHEM elective	3
CHEM 495 Research/Problems	1	CHEM 496 Research/Problems	1
Electives	9	Electives	12
Total	**16**		**16**

This example schedule would satisfy the UNM requirements for a BA Chemistry with a minor in Biology, and would be a good background for medical or pharmacy school.

a. The university core requires one 3-hour lower division foreign language course.
b. The university core require 6 CH (two courses) of Social and Behavioral Sciences and 6 CH (two courses) of Humanities. In general, these can be taken in any order.
c. The university core requires 3 CH (one course) in Fine Arts.
d. The minor in Biology requires 6 CH beyond BIOL 204

Example Schedule for the Chemistry BS Degree

First Year

Fall	CH	Spring	CH
CHEM 121 General Chemistry I	3	CHEM 122 General Chemistry II	3
CHEM 123L General Chem Lab I	1	CHEM 124L General Chem Lab II	1
MATH 162 Calculus I	4	MATH 163 Calculus II	4
Foreign Language core course[a]	3	CS 151L Intro to Programming	3
ENGL 101 Composition I	3	ENG 102 Composition II	3
Humanities or Social Science core[b]	3	Humanities or Social Science core[b]	3
Total	**17**		**17**

Second Year

Fall	CH	Spring	CH
CHEM 301 Organic Chemistry I	3	CHEM 302 Organic Chemistry II	3
CHEM 303L Organic Chem Lab	1	CHEM 304L Organic Chem Lab II	1
MATH 264 Calculus III	4	MATH 316 Differential Equations[c]	3
PHYC 160 General Physics I	3	PHYC 161 General Physics II	3
PHYC 160L Physics Lab I	1	PHYC 161L Physics Lab II	1
ENGL 219 Technical Writing	3	Humanities or Social Science core[b]	3
		CHEM 326 Research/Problems	1
Total	**15**		**15**

Third Year

Fall	CH	Spring	CH
CHEM 311 Physical Chemistry I	3	CHEM 312 Physical Chemistry II	3
CHEM 253L Quantitative Analysis	4	CHEM 453L Instrumentation Lab	4
MATH 314 Linear Algebra[c]	3	CHEM 421 Biological Chemistry	3
Humanities or Social Science core[b]	3	Fine Arts core[d]	3
CHEM 495 Research/Problems	1	CHEM 496 Research/Problems	1
Elective	3	Elective	3
Total	**17**		**17**

Fourth Year

Fall	CH	Spring	CH
CHEM 431 Adv Inorganic Chem	3	CHEM 432L Synthesis Laboratory	3
CHEM 411L Physical Chem Lab	3	CHEM elective	3
CHEM 495 Research/Problems	1	CHEM 496 Research/Problems	1
Electives	9	Electives	9
Total	**16**		**16**

This example schedule would satisfy the UNM requirements for a BS Chemistry with a distributed minor and the American Chemical Society requirements for a certification.

a. The university core requires one 3-hour lower division foreign language course.
b. The university core require 6 CH (two courses) of Social and Behavioral Sciences and 6 CH (two courses) of Humanities. In general, these can be taken in any order.
c. two of MATH 311, 314 and 316 needed to fulfill the distributed minor.
d. The university core requires 3 CH (one course) in Fine Arts.

Appendix A8. Graduate Handbook from December 2010

University of New Mexico

Department of Chemistry & Chemical Biology

Graduate Handbook

Effective 12/1/10

The following is a detailed description of graduate degree requirements in the Department of Chemistry & Chemical Biology at the University of New Mexico. University requirements may be found in the current UNM Catalog at http://registrar.unm.edu/catalog/. Students are responsible for knowing and understanding these requirements, and for making satisfactory progress toward fulfilling them. If you have any questions please contact either the Graduate Coordinator or Chair of the Graduate Studies Committee.

Course Work & Academic Performance:

The Chemistry & Chemical Biology Graduate Studies Committee recommends which courses students will take during their first year. Following the end of both the first and second semesters of graduate work, student records are reviewed by the Graduate Studies Committee. This review is based on student performance with regards to grades and comments solicited from faculty members. Students are expected to earn a "B" or better (not B-) in Chemistry core requirements. Students are also required to maintain above a cumulative 3.0 GPA during their graduate studies at the University of New Mexico. Students failing to meet these minimum expectations will lose financial aid, may be limited to earning a Master's degree, or may be dismissed from the graduate program, depending on the faculty's evaluation of their overall ability and potential. The decision by the Graduate Studies Committee and faculty concerning student academic performance is final.

Minimum coursework hour requirements for graduate degrees are established by the Office of Graduate Studies (see UNM Catalog). The Department of Chemistry & Chemical Biology has additional requirements that must be met, including taking core courses.

All Chemistry & Chemical Biology graduate students are expected to maintain the highest standards of honesty and integrity in academic and professional matters. Academic issues such as cheating, plagiarism, failure to maintain a cumulative 3.0 GPA or greater or failure to make sufficient progress in courses and research can carry severe penalties, up to and including dismissal from the Chemistry & Chemical Biology graduate program. All students are responsible for knowing and complying with all academic regulations. Ignorance of a rule or policy will not be accepted as an excuse for non-compliance.

The Department of Chemistry and Chemical Biology graduate program is a four-to-six-year curriculum that prepares students for scientific careers in academia, research institutes, national laboratories, and industry. The first year of study consists primarily of coursework, seminars and undergraduate laboratory teaching. Students also investigate the research programs of departmental faculty, and choose a laboratory in which to carry out their dissertation research. In consultation with their Research Advisors, students choose the members of their Committee on Studies (COS). During the first year, student progress assessment consists primarily of course exams and student teaching evaluations.

During the second year of graduate studies, students focus on developing a theoretical and conceptual framework in their chosen areas of research through advanced courses, readings, group meetings and divisional seminars. In addition, the students begin to plan a dissertation research project and to accrue a collection of experimental techniques and protocols necessary to carry out the dissertation research. The students also learn how to read, understand, evaluate and critique the literature relevant to the dissertation research. During this period, it is important for the COS to begin to monitor and evaluate student progress toward synthesizing background material and experimental approaches relevant to the dissertation project, and to provide the student with constructive feedback.

PhD:

48 total hours including the following plus 18 hours of Dissertation (699):
18 hours of graded (A, B, …) coursework at the 500 level or above

Required core courses:
CHEM 511
CHEM 521
CHEM 536
CHEM 501
CHEM 545-002
3 - 6 hours of CHEM 625 (Divisional Seminar)
Enough hours of graduate credit (CHEM 650 or 623) to meet the total of 48 hours (no more than 24 hours of CHEM 650)

Plan I--Thesis Masters:

24 total hours including the following plus 6 hours of Thesis (599):
18 hours of graded (A, B, …) coursework
12 of the 18 hours of graded (A, B, …) coursework must be at the 500 level or above
Required core courses:
CHEM 511
CHEM 521
CHEM 536
CHEM 501
CHEM 545-002
2 - 4 hours of CHEM 625 (Divisional Seminar)
Up to 4 hours of CHEM 650

Plan II--Coursework Masters:

32 total hours including the following:
24 hours of graded (A, B, …) coursework
18 of the 24 hours of graded (A, B, …) coursework must be at the 500 level or above
Required core courses:
CHEM 511
CHEM 521
CHEM 536
CHEM 501
CHEM 545-002
2 - 4 hours of CHEM 625

Credit Hours (per semester):

All assistantship contracts allow a tuition waiver of 12 hours for each fall and spring semester (and up to 3 hours in the summer depending on your advisor). All graduate students are responsible for tuition costs incurred from enrolling in more credits then are allowed by the department for the semester. Students are not required to enroll in coursework during summer sessions unless the student will be graduating during the summer session. In this case, the student must enroll in at least 1 credit hour of CHEM 699 for Dissertation or 599 for Master's Thesis. Research Assistants should consult with their Research Advisor before enrolling for summer coursework. All students are expected to enroll full time each semester (at least 6 credit hours is considered full time). After completing formal coursework requirements, students need to enroll in CHEM 650 (Research/Readings) until they Advance to Candidacy and then they must enroll for either CHEM 699 (Dissertation) or CHEM 599 (Master's Thesis). A Student should consult his/her Research Advisor before taking any non-chemistry courses.

Lab Rotation (CHEM 499):

During the students' first year they will be required to sign up for CHEM 499 for the first semester, but the actual rotations may be spread out over two semesters. This is a lab rotation course where students will be actively involved in three separate research labs in the Department of Chemistry and Chemical

Biology. Students contact the research directors of three research groups and get permission to carry out rotations. Only research programs that are certified by the Department to train Chemistry and Chemical Biology graduate students can participate in the rotation course. During the rotation, the student is expected to discuss research projects with the Principal Investigator and other members of the group, read selected papers associated with the group's research, and attend group meetings. Upon completion of each rotation, the student will be required to write a single page synopsis of the group's research program, which will be evaluated by the Principal Investigator. These reports will be the basis for the grade of the class (credit/no credit) by the Graduate Studies Committee.

Selecting a Research Director:

Upon completion of the three rotations, students will be expected to choose a Research Advisor from the three groups in which the student rotated. The final decision will be based upon mutual agreement between the student and the Research Advisor. To finalize the agreement, the student and mentor will complete the "Mentor Agreement Form", which can be obtained from the Graduate Advisement Coordinator. This form must be on file by the end of the student's second semester in the Graduate Program.

Dissertation Committee:

Following the selection of a Research Advisor, a PhD student must select a Committee on Studies (COS). The composition of this committee is outlined in the University of New Mexico catalog under “Graduate Program Composition of the Dissertation Committee.” Students are expected to meet yearly with their Dissertation Committee to review progress on research problems and appropriate degree requirements. Depending on the field of research, the Committee on Studies may require the student to exhibit competence in additional skills such as mathematics, physics, computer programming, or electronics.

CRIK Assessments:

During the second year of the graduate program, students will take a set of 4 progressive assessments designed help the COS accurately evaluate the graduate students’ ability to read, understand, evaluate and critique the literature essential for his/her research, and to communicate this understanding through a timed short answer exam.

These CRitical Integration of Knowledge (CRIK) assessments will progress in difficulty and complexity throughout the year and culminate in the writing and oral defense of the research proposal (RP). In general, the exams will be administered on the first Friday of each month (November, December, February and March). Approximately three weeks prior to the exam, the research advisor will select a review article and/or a foundational paper that is related to the paper that will be selected for the exam. The student will use the review or seminal paper to study for exam. Seven days prior to the exam, the research advisor will provide the student with the paper on which the exam will focus. The student may discuss the paper with other students or postdoctoral fellows, but not faculty, including his/her own research advisor. The two-hour exam will consist of approximately 5-7 questions that must be answered without any notes. The questions will focus on hypotheses, questions, experimental approaches, data interpretation, results and conclusions. In addition, questions may focus on a critique of the paper. A copy of the paper will be made available at the exam. The answers will be reviewed by the members of the COS and returned to the student no later than one week after the exam was administered. The research advisor will summarize the comments of the COS in writing and will provide feedback to the student about the strengths and weaknesses of his/her performance on the assessment.

End of Second Year Assessment:

At the end of the second year, the COS will conduct a review of the student's performance to date (coursework, results of the CRIK assessments, results of the RP defense, and the performance in the laboratory). The COS will submit a report and a recommendation to the Department's Graduate Committee. The Departmental Graduate Studies Committee will make one of the following recommendations: (1) Advancement to PhD Candidacy; (2) completion of a Terminal Masters Degree (with or without an option to reapply to the PhD program); or (3) immediate dismissal.

Research Proposal:

The Research Proposal must be completed by the last day of the student's fourth semester in the program (not including summer), unless an extension is approved by the COS and the Graduate Studies Committee. If a student fails the defense, they may be allowed one additional attempt. This attempt must be completed no later than the end of the fifth semester. The COS may require students to repeat any or all parts of the research proposal. A second failure on any part of the requirement will prevent the student from progressing to PhD candidacy.

All students must submit a signed Announcement of Exam form to the Chemistry & Chemical Biology Department Advisement Coordinator at least two weeks prior to the scheduled RP. See the Advisement Coordinator for a copy of this form.

Rules and Guidelines:

The Research Proposal represents a thoroughly documented summary of the research that students expect to perform prior to writing their Dissertation. The written version of the proposal should consist of a long narrative (approximately 8-10 pages including references) describing the intended doctoral research project. The written proposal should be fully documented, with appropriate references to the primary chemical literature. It should state clearly and concisely the objective(s) of the research and provide sufficient background to convey the rationale for undertaking the research. Finally, key aspects of the planned method should be described briefly and their viability documented. A fully referenced abstract should be distributed to the students' Research Proposal Committee two weeks prior to the defense.

Research Proposal Guidelines:

These are only guidelines - it will ultimately be between you and your committee how the RP will be written and orally presented.

Abstract - approximately 400 words which states your objectives and goals
Introduction - approximately 1½ - 2 pages of a brief literature overview
Statement of Research Problem - not more than ½ page long
Statement of Goals and Objectives - not more than ½ page long
Research Plan - approximately 3 - 4 pages
Conclusion - approximately ½ page long
References

The total length should not exceed 10 pages, including references, figures, schemes, and equations. The style should be 12 pt. Times or Times Roman font, single spaced with 1" margins all around. A cover page should be included which has the title of the RP, the student's name, and the names of the committee members listed.

Oral RP Presentation Guidelines:

The organization of the oral RP should be similar to the written presentation, and should include the same sub-headings.

The oral presentation should be approximately 40-45 minutes in length, excluding a question period.

Seminars:

The Department of Chemistry & Chemical Biology has divisional and departmental seminars:

All graduate students are expected to register for and attend departmental and divisional seminars for as long as they are enrolled in the graduate program. Missing more than two Departmental Seminars in one semester will result in a "NC" being given.

Teaching Assistant Performance:

All graduate students who hold Teaching Assistantships are required to work the week before the fall and spring semester classes begin. Work during this week will involve preparation for the upcoming semester. Attendance during this week is mandatory for all TA's. Graduate TA attendance during the week of Final Exams is also mandatory. Violation of this will lead to serious penalties, including possible dismissal from the program. Do not plan travel, especially foreign travel, during these times.

The performance of all Teaching Assistant's will be reviewed every semester. When TA's have performed inadequately an evaluation and recommendations for improvement will be reported to the Graduate Committee by the TA's supervisor and a copy of the evaluation filed in the student's record. Students are expected to carry out research during the summer under the guidance of their research advisors. Students should discuss and coordinate plans for vacation or leave with their research advisors.

Limitations on Financial Aid:

The Department of Chemistry & Chemical Biology restricts departmental financial aid in the form of Research and Teaching Assistantships to a maximum of six calendar years from the date of entrance. At the end of fifth year, students' overall progress will be evaluated to determine their eligibility for a sixth year of support.

If, in the opinion of the Department faculty, a student shows little promise of completing the degree program, the Department will notify the student and the Graduate School in writing that the student is suspended from further work in the program.

Appendix A9. General Chemistry Parachute course

Description of CHEM 120, "The Parachute Course"

CHEM 121 is the first semester of the two-semester sequence of general chemistry for science majors. It has been listed by the University as a "killer course" due to its high failure rate (35 – 50%). To address this problem, we need to identify at-risk students and implement remediation to prepare them to retake the course for a passing grade. From the experience of other schools, it is crucial to offer remediation to the right group of students who are indeed at-risk as failing students do not often identify themselves as being at risk. As such we decided to use mid-term exams as a predictor to help students whose score are below a certain cut-off, and help convince them they need additional support. We offer these students a direct transfer from CHEM 121 into the remediation course, CHEM 120. CHEM 121 is erased from their transcript and replaced with CHEM 120. This is important as a lot of students need to maintain a certain number of credit hours to keep their scholarships. CHEM 120 meets at the same time as the CHEM 121, so students do not have to change their schedule.

In CHEM 120, we provide more in-depth discussion of chemistry material that was covered in the first part of CHEM 121. Through working in small groups, students can freely discuss and explore their misconceptions and learn from their peers. Students have more in-class practice applying the harder concepts and mathematics involved in these small gropus. In addition, students have regular short reflective writing assignments on aspects of their learning process, and these reflections are discussed in class to develop better learning strategies. The instructors take the role of learning facilitators, helping students identify the best learning strategies for themselves. The metacognitive skills they learn in this course will enable them to take charge of their own learning when they return to CHEM 121.

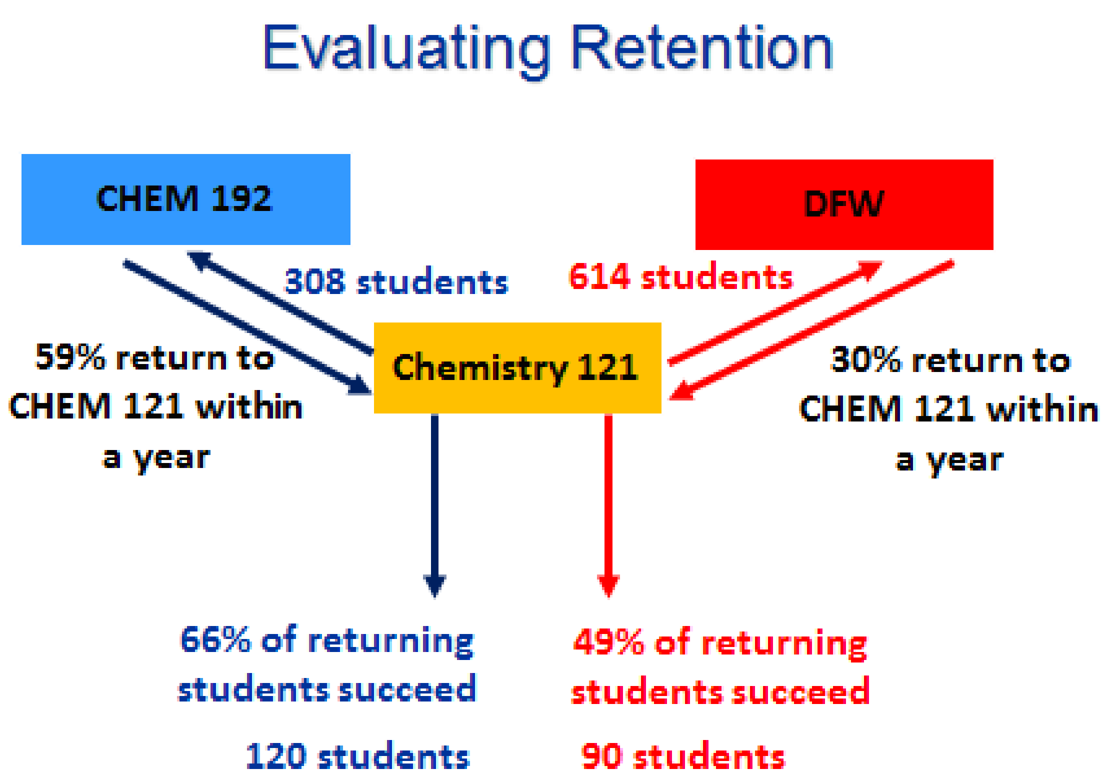
Preliminary analysis of data collected from the fall of 2010 to the fall of 2012 shows that 59% of the CHEM 120 students returned to CHEM 121 within a year versus 30% returned from students who did not take the parachute course and proceeded to withdraw from or fail CHEM 121. Among these students, 66% of parachuted students successfully passed the CHEM 121, but only 49% passed from the returned students who did not parachute. The passing students from parachute course also earned more A's and B's than the passing students who did not take the parachute course. We are collecting data to do a longitude study to compare student performance in the subsequent courses between the parachute and non-parachute students.

After two years of implementation, the parachute course for CHEM 121 has shown promising results for the main goal of the course – improving retention and success of students in this gateway course. While we will continue monitoring the progress of the students in this course and their performance when they return to CHEM 121, we will be working on a permanent protocol for the recruitment and transfer process, and set up a content standard for the course.

Bicentennial Conference on Chemical Education, 2012

Can a parachute class prepare students to succeed?
S. Knottenbelt and K. J. Ho

General Chemistry is a required course for many STEM disciplines. In many cases, students are unable to proceed with the sequence of classes until they have passed General Chemistry, and failing (sometimes repeatedly) at the first hurdle can discourage them from pursuing a career in the STEM fields. Helping at-risk students in general chemistry courses get on the right path to succeed has been a critical area of concern. From Fall 2010, students identified as failing General Chemistry at UNM during the semester have been offered the chance to 'parachute' into a preparatory class to maximize their chances of succeeding in General Chemistry when they return. We present initial data on the effectiveness of the parachute class in improving retention of students returning to General Chemistry. We also discuss some characteristics of students taking the parachute class, as well as introduce ideas of integrating learning skills with basic chemical concepts to maximize student success in General Chemistry.



Appendix A10. General Chemistry II course redesign

A. Student learning outcomes for CHEM 122, General Chemistry II

1. Explain the intermolecular attractive forces that determine physical properties and phase transitions; apply this knowledge to qualitatively evaluate these forces from structure and to predict the physical properties that result. (Related to HED Core Competencies Area III no. 2)

2. Calculate solution concentrations in various units and explain the effects of temperature, pressure and structure on solubility. (Related to HED Core Competencies Area III no. 2)

3. Describe the colligative properties of solutions and explain them using intermolecular forces. Determine solution concentrations using colligative property values and vice versa. (Related to HED Core Competencies Area III no. 2 and 4)

4. Explain rates, rate laws, and half-life; determine the rate, rate law and rate constant of a reaction and calculate concentration as a function of time and vice versa. (Related to HED Core Competencies Area III nos. 2 and 4 and Area II nos. 1 and 2)

5. Explain the collision model of reaction dynamics, including activation energy, catalysts and temperature; derive a rate law from a reaction mechanism and evaluate the consistency of a mechanism with a given rate law. (Related to HED Core Competencies Area III no. 2 and 4)

6. Describe the dynamic nature of chemical equilibrium and its relation to reaction rates; apply Le Chatelier's Principle to predict the effect of concentration, pressure and temperature changes on equilibrium mixtures. (Related to HED Core Competencies Area III no. 2)

7. Describe the equilibrium constant and use it to determine whether equilibrium has been established; calculate equilibrium constants from equilibrium concentrations and vice versa. (Related to HED Core Competencies Area III no. 2 and 4 and Area II no. 2)

8. Describe the different models of acids and base behavior, and the molecular basis for acid strength. (Related to HED Core Competencies Area III no. 2)

9. Apply equilibrium principles to aqueous solutions, including acid-base and solubility reactions; calculate pH and species concentrations in buffered and unbuffered solutions. (Related to HED Core Competencies Area III no. 2 and 4 and Area II no. 2)

10. Explain titration curves and speciation diagrams; calculate concentrations of reactants from the former and determine dominant species as a function of pH from the latter. (Related to HED Core Competencies Area III no. 2 and 4 and Area II nos. 1 and 2)

11. Explain and calculate the thermodynamic functions enthalpy, entropy and Gibbs free energy for a chemical system; relate these to equilibrium constants and reaction spontaneity. (Related to HED Core Competencies Area III no. 2 and 4)

12. Balance redox equations, express them as two half reactions and evaluate the potential, free energy and equilibrium K for the reaction, as well as predict the spontaneous direction. (Related to HED Core Competencies Area III no. 2 and 4)

13. Construct a galvanic or electrolytic cell; determine the standard (and non-standard) cell-potential of the former and relate current to electron transfer rates in the latter. (Related to HED Core Competencies Area III no. 2 and 4).

B: Proposed Elements of the Reformed Course

General Chemistry II (CHEM 122) is a gateway course for majors in science and engineering. For reasons outlined on the first page of this proposal, it suffers from high W/D/F rates and prevents many students from continuing with their chosen STEM major. We propose to improve student motivation, learning and retention in CHEM 122 by a course re-design emphasizing active learning, interdisciplinary exercises and multi-component assessment. Success will be gauged by a reduction in the W/D/F rate, improved student learning as measured by internal assessments, and measures of student satisfaction. Themes of this re-design will be

1. Revising learning outcomes to coordinate with skills and competencies needed in STEM majors requiring CHEM 122.

2. Converting traditionally taught lecture courses into learner-centered environments by incorporating active learning in the classroom.

3. Developing interdisciplinary exercises pitched at higher cognitive levels to provide a strong basis for student engagement and deeper learning.

4. Assessing student, class and re-design performance via multi-component measures of student learning and student opinions on how the class structure facilitates their own learning.

Of the 900 students who take CHEM 122 each year at UNM, less than 5% go on to become chemistry majors; of the remaining 95%, nearly half become biology and pre-health science majors, while about a quarter become engineering majors. Incorporating the needs and expectations of these departments into the course learning outcomes is essential if CHEM 122 is to remain relevant as a gateway STEM course. At the same time, outcomes must be related to subsequent chemistry courses to keep students up to date in chemistry and prepare them for advanced topics.

Extensive research points to improved student learning when using active learning pedagogies in the classroom. A significant study suggests that using these methodologies in the classroom can make more difference to student learning than the choice of instructor to teach them. In order to make time in the classroom to engage in such activities, we plan to use an 'inverted classroom ' approach, where the acquisition of the basic facts and concepts becomes the responsibility of the students before class, via structured reading assignments or online resources. Class time will then be focused on more difficult concepts, applications and synthesis in which the instructor and peer-learning facilitators help students engage with exercises designed to explore the outcomes. Clicker questions will be used to assess learning in these exercises, but also as a tool to promote student participation and engagement.

Interdisciplinary exercises can motivate students by the area of application and the level of conceptual integration, and engage higher-order reasoning skills. We plan to develop examples in engineering, health sciences and geochemistry since a major goal will be to show students how CHEM 122 principles can be applied in different STEM fields. Exercises will combine pre-class reading with in-class problem solving and optional post-class follow-up reading to see how the problem is solved in the 'real world' of application. In addition, these exercises will target known misconceptions and student difficulties and will aim for Bloom's taxonomy levels above simple knowledge and comprehension to application and above. Use of open source educational resources including the Journal of Chemical Education will allow the exercises to be textbook independent. Peer learning facilitators will be employed in larger sections to ensure that student groups remain 'on track' during in-class exercises.

Timetable for redesign:

Summer 2012: The redesign plan is finalized with OSET guidance by June 1st. The team will collaborate to develop materials for implementation, starting Fall 2012. Initial implementation of concept tests to use as pre- and post-course assessment will be piloted in CHEM 122 during Summer 2012. By the start of Fall 2012 we will have:

1. Established course learning outcomes that align with HED competencies and STEM major requirements.

2. Developed structured pre-class reading assignments and formative assessments to enable students and instructors to monitor acquisition of basic facts and concepts before class.

3. Created in-class, interdisciplinary exercises which require higher-order thinking with optional follow-up references.

4. Created a detailed multicomponent assessment plan for the initial implementation.

5. Developed subject-specific training materials for learning facilitators (TAs, SI and PLFs in the classroom)

Fall 2012: One section of CHEM 122 at UNM (Yang) and one section of CHEM 1810 at CNM (Sorensen-Unruh) will be taught using the initial redesign plan. CHEM 1810 will be taught as a hybrid class. A control section will be established, and a pre- and post concept test administered to ALL students taking CHEM 122. Assessment data will be collected during the semester (see detailed assessment plan following) and evaluated over Winter Break to inform the Spring implementation and assessment plan. We plan to evaluate the data incrementally over the semester, and meet before 12/24/2012 to make recommendations for adaptations in the Spring.

Spring 2013: 4 sections of CHEM 122 at UNM will apply the improved redesign plan taught by at least 3 different instructors (Yang, Cabaniss and Knottenbelt) and 2 at CNM (Sorensen-Unruh). Assessment data will be collected.

Summer 2013: 1 section of CHEM 122 at UNM (Ho). The course redesign team will evaluate assessment data collected over the year, and present the results and make recommendations for future implementations to the Chemistry Faculty at the annual Faculty retreat.

Fall 2013 and beyond: Assuming positive redesign results, the implementation will be extended to all sections of 122 in Fall 2013 and Spring 2014. To enable longer term assessment of the impact of the redesign, the Chair of the Department of Chemistry and Chemical Biology at UNM has committed to providing 1 month of compensation for Drs Ho and Knottenbelt to continue the analysis of assessment data in the summers of 2014 and 2015.

Additional resources:

In order to enable active learning in the classroom, we request at least 2 years of support for Peer-Learning-Facilitators in all CHEM 122 classes at UNM that implement the course redesign. We request 1 PLF for every 50 students above a base of 50 students. We anticipate needing 3 PLFs for Fall 2010 and 9 PLFs for Spring 2011. Personnel and Experience: All team members currently meet weekly as part of the General Chemistry subcommittee.

As Director of Chemical Education, Dr. Ho provides the leadership and continuity needed for an ambitious redesign. He has twenty two years of teaching experience in undergraduate chemistry courses and labs. He coordinates the labs associated with CHEM 121 and CHEM 122 and has recently redesigned them both to replace 'cookbook' labs with ones fostering the scientific method. He is currently developing the Chemical Concept Inventory that we intend to use for pre- and post- assessment and has implemented active learning techniques in his CHEM 122 summer section since 2010.

Dr Knottenbelt has implemented much of the methodology proposed herein in her Chem 121 sections in Fall 2010 and Spring 2010 and 2011, with the support of OSET and the Walmart Foundation. The redesigned course has achieved increased student retention and learning, as well as very positive student evaluations. She is currently using collaborative learning techniques to teach a section of CHEM 122 targeted at pre-health sciences.

Dr Cabaniss has previously taught General Chemistry II 7 times (4 at Kent State U, 3 at UNM) and is also testing an inverted classroom approach in his CHEM 122 section this semester. He brings expertise in Environmental Chemistry – a critical area to develop student interest and understanding for the 21st century.

Dr Yang started teaching during his graduate years at UNM and has been a part-time lecturer at CNM for two years and at UNM since Summer 2011. He is considered one of our regular part-time instructors. He strives to improve student learning by encouraging them taking a leading role and employing creative instructional techniques enhanced by technology. He is an active member in our General Chemistry committee, contributing much to our discussions.

Ms Sorensen-Unruh is full-time faculty at CNM teaching the full range of chemistry classes offered there. She teaches these classes in multiple environments, including interactive lecture (with group work), hybrid and blended. She is currently teaching a section of Chem 121 at UNM, transferring the structure developed by Dr Knottenbelt, in order to strengthen ties with UNM colleagues. She has always engaged her students in active learning, and has added this semester the on-time assessment (pre-class reading quizzes, muddy points, and clickers) in Chem 121 and all her classes at CNM.

Assessment plan

Our assessment plan seeks to answer the following questions:

1. Does the redesigned course improve student learning?

2. Which elements of the developed course materials are effective for students' learning?

3. Are gains from the redesigned course transferrable to different instructors, and to the different students served at UNM and CNM?

4. Does the redesigned course result in reduced D/W/F rates?

1. Improved Student Performance: To monitor improvements in understanding of chemistry concepts, we will administer a pre-test and post-test adapted from an established Chemical Concepts Inventory. This test (CI) has been largely developed and was implemented in the spring of 2012. Based on the statistics of student responses, the questions in the CI are currently being reviewed for validation and the final version of the test will be determined by the team members before June 4, 2012 when the summer semester starts. The pre- and post-tests will be given to all students taking CHEM 122 starting from the summer of 2012. The data from the summer will help establish a measure of student performance prior to the implementation of the active learning approach. In fall of 2012, we will select a control group and a test group as different sections of CHEM 122. Both groups will take the pre-test and post-test, but only the test group will experience the redesigned course. The performance gain between the pre- and post-

test from both groups will be used as the measure for a variety of analyses of students' performance.

2. Effective Elements of Redesigned Course: We will collect and scan relevant individual student responses to exam, assignment and in-class questions based on the learning outcomes of the course for the purpose of item analysis. Online student surveys will be administered to monitor the students' perception of their learning and their satisfaction with it at least twice during the semester. We will also conduct interviews with students in the test groups for more in-depth feedback. Data from the exercises and surveys will be analyzed by Dr. Ho and discussed by the design team members for further refinement during and after each semester. The expected outcome of this process is to identify specific areas where we need improve student learning by modifying resources available before class, after class, modifying exercises or a combination of the above.

3. Potential for Successful Transfer: Given the number of sections offered per year and the turnover in instructors teaching them, ability to transfer the redesigned course between instructors is critical. Following our initial implementation of one section each at UNM and CNM, we will select different team members to teach the test groups in the spring and summer semesters. This way, within the first year, we will have at least four different instructors teaching the new, developed approach from two institutions with different student demographics. We will analyze the performance gains from all the four instructors against the performance gains from the control groups, and look for statistical differences. We will also include in our analysis instructors' comments about the new approach. We aim to develop an adoption plan of the redesigned course by all sections of CHEM 122 in the future which will establish the resources and training needed for instructors who are interested in taking on the new teaching method.

4. Reduction of the D/F/W Rate: The ultimate success of the redesign will be measured in terms of improved student success that can be sustained over an extended time period. The D/F/W rate provides an important measure of this. Given the variability of this metric from semester to semester, we recognize that this is inherently a means of longer term assessment that will add to our more immediate measures detailed above.

Cited References

1. Improved learning in a large enrollment physics class, Louis Deslauriers , Ellen Schelew, and Carl Wieman, Science, 332, 862-864 (2011)

2. Peer Instruction: Ten Years of Experience and Results Catherine H. Crouch and Eric Mazur, Am. J. Phys., 69, 970-977 (2001).

3. Trochim, William M. The Research Methods Knowledge Base, 2nd Edition. Internet WWW page, at URL: <http://www.socialresearchmethods.net/kb/>

4. “Measuring What Students Know about How to Learn Chemistry”, Proceedings of the National STEM Assessment Conference, October 19–21, 2006, Hosted by the National Science Foundation and Drury University, Chief Editors: Donald Deeds and Bruce Callen, Drury University.

5. “Knowing what Students Know: The Science and Design of Educational Assessment”, Committee on the Foundations of Assessment, James W. Pellegrino, Naomi Chudowsky, and Robert Glaser, editors, Board on Testing and Assessment Center for Education Division of Behavioral and Social Sciences and Education National Research Council, NATIONAL ACADEMY PRESS, Washington, DC, 2001

6. The concept inventory is adapted from the CCI, as made available from the Journal of Chemical Education.

- http://www.jce.divched.org/JCEDlib/QBank/collection/CQandChP/CQs/ConceptsInventory/Concepts_Inventory.html.

- The Chemical Concepts Inventory was developed by Doug Mulford for his M.S. thesis, (Douglas R. Mulford, M.S., Purdue University, August, 1996. An Inventory for Measuring College Students' Level Of Misconceptions in First Semester Chemistry. Major Professor: William R. Robinson)

- Our ‘in house’ adaptations include new questions on areas of specific interest to us. We have begun the process of test validation.

Appendix A11. Student graduation data

Total Number of Degree Recipients
2001-2002 to 2010-2011 Academic Years
Chemistry Department

Major	Degree	2001-02	2002-03	2003-04	2004-05	2005-06	2006-07	2007-08	2008-09	2009-10	2010-2011
Chemistry	BA	4	3	5	3	10	12	4	19	17	13
Chemistry	BS	4	10	7	4	6	12	11	6	10	3
Chemistry	MS	5	9	2	2	1	5	8	5	4	2
Chemistry	PHD	5	6	7	7	15	14	8	11	6	9
Total Degrees Awarded		18	28	21	16	32	43	31	41	37	27

Appendix A12. Faculty CVs

Section II. Debra Dunaway-Mariano Professional CV

Education

1973 B.S. Biochemistry Texas A & M University
1975 Ph.D. Biochemistry, Texas A & M University
1977-79 Postdoctoral, Biochemistry, University of Wisconsin

Professional Positions

1976-77 Texas A & M University Lecturer Organic Chemistry
1979-84 University of Maryland Assistant Professor of Chemistry and Biochemistry
1985-89 University of Maryland Associate Professor of Chemistry and Biochemistry
1990-96 University of Maryland Professor of Chemistry and Biochemistry
1997-on University of New Mexico Professor of Chemistry and Chemical Biology

Awards

1977-79 NIH Postdoctoral Research Fellow Award
1982-86 NIH Career Development Award
1984-85 Alfred P. Sloan Fellow Award

On-going Professional Appointments in Service

1986-on Associate Editor of *Bioorganic Chemistry*
2008-on ACS *Biochemistry* Editorial Board Member

Classroom Teaching

Undergraduate: Senior level Bioorganic Chemistry (Mechanisms of Molecular Recognition and Catalysis in Small Molecule and Protein/Nucleic Acid Molecules for Chemistry, Biochemistry and Chemical Engineer majors); Senior level Biological Chemistry (Form-to-Function in Proteins, Nucleic Acids, Lipids and Carbohydrates for Chemistry, Biochemistry, and Chemical Engineer majors); Sophomore level Organic Chemistry; Freshman level combined Organic Chemistry/Biochemistry (second semester in a 2 semester track for nutrition/nursing majors).

Graduate level: Bioorganic Chemistry (Mechanisms of Molecular Recognition and Catalysis in Small Molecule and Protein/Nucleic Acid Molecules); Biological Chemistry (Form-to-Function in Proteins, Nucleic Acids, Lipids and Carbohydrates); Mechanistic Enzymology I-Physical Organic Tools (kinetics, isotope effects; stereochemistry, free energy relationships); Mechanistic Enzymology II- Theories of enzyme catalysis and the catalytic mechanisms of enzymes representing the six enzyme classes; Methods for Biological Chemistry Research (Bioinformatics, computer graphics, protein purification; gene cloning and mutagenesis; real time PCR; in vivo protein imaging; protein directed evolution)

Research Program Thrust Areas

Project Topics:

- Molecular and Biological Diversity

• Biological Catalysis
• Mining Genomes for Novel Chemicals and Catalysts
• Drug Targeting and Design
• Enzyme Folding and Dynamics
• Enzyme Engineering for Biofuel Biosynthesis and Pollutant Degradation
• Chemienzymatic Organic Synthesis

Project Subtopics:
•Enzyme Catalysis, Mechanism and Structure
•Protein Engineering
•Natural and Laboratory Directed Evolution of Novel Enzyme Catalysts
• Development and Application of Bioinformatic and Experimental Methods for Bacterial Enzyme Function Determination
•In Cell Protein Imagining for Human Enzyme Function Determination and Drug Targeting
•Mechanism Based Enzyme Inhibitor Design
•Protein Structure and Conformation Analysis via Solution Small Angle Diffraction (SASX) and X-ray Crystallographic Determination
•Thermodynamic and Kinetic Analysis of Protein Folding
•Natural Product and Chemical Library Synthesis Based on Natural Engineered Enzyme Catalyst

Research Publications

1. Nucleoside Phosphorothioates: I. Thiophosphorylation of Nucleosides with Phosphorus Thioxy-anions. D. Dunaway-Mariano, *Tetrahedron 32*: 2991-29996 (1976).
2. The Chemistry of Azocines. Intermediates for the Synthesis of Pyrrolizidines. P. S. Mariano*, M. E. Osborn, D. Dunaway-Mariano, B. C. Gunn and R. C. Pettersen, *J. Organic Chem.* 42: 2903-2910 (1977).
3. 7,8-Dicarbomethoxy-9-oxa-2-azabicyclo(4.2.1)non-7-ene-2-p-Toluene Sulfonamide. R. C. Pettersen*, P.S. Mariano, M. E. Osborn and D. Dunaway-Mariano, *Cryst. Struct. Comm. 6*: 471-476 (1977).
4. Novel Approaches to the Synthesis of Hydroisoquinolines Using Aza-Claisen Rearrangements of N-Vinylisoquniuclidenes. P. S. Mariano, D. Dunaway-Mariano, P. L. Huesmann and R. L. Beamer, *Tetrahedron Lett.*, 4299-5209 (1977).
5. General Synthetic Methods for the Preparation of 1-Substituted-Vinyl-2-Pyridones. P. S. Mariano, E. Krochmal, R. Beamer, P. L. Husemann and D. Dunaway-Mariano, *Tetrahedron 34*: 2609-2616 (1978).
6. The Diels-Adler Chemistry 1-Vinyl-2-Pyrodones. P. S. Mariano, P. S. Huesmann, R. L. Beamer and D. Dunaway-Mariano, *Tetrahedron 34*: 2617-2626 (1978).
7. Specificity of Nucleoside Transport in Neurospora crassa. D. Dunaway-Mariano and J. M. Magill, *J. Bacteriology 136*: 924-928 (1978).
8. Amino-Claisen Rearrangements of N-Vinylisoquinuclidenes in Novel Approaches to the Synthesis of Hydroisoquinolines and Hydrophenanthridines. P. S. Mariano, D. Dunaway-Mariano and P. L. Huesmann, *J. Org. Chem. 44*: 124-133 (1979).
9. Stereospecificity of the Metal-ATP Complex in Reactions of Pyruvate Kinase. D. Dunaway-Mariano, J. Benovic, W. W. Cleland, R. K. Gupta and A. S. Mildvan, *Biochemistry 18*: 4347-4354 (1979).

10. Preparation and Properties of Chromium(III) Adenosine 5'-triphosphate, Chromium(III) Adenosine 5'-diphosphate and Related Chromium(III) Complexes, D. Dunaway-Mariano and W. W. Cleland, *Biochemistry 19*:1496-1505 (1980).
11. Investigations of Substrate Specificity and Reaction Mechanisms of Several Kinases Using Chromium(III) Adenosine 5'-triphosphate and Chromium(III)5'-diphosphate. D. Dunaway-Mariano and W. W. Cleland, *Biochemistry 19*:1506-1515 (1980).
12. Crystal Structure and Chelate Ring Pucker of Bidentate Pyrophosphatotetra-aqua-chromium(III) Trihydrate, a Model for Metal-ADP Coordination. E. A. Merrit, M. Sundaralingam and D. Dunaway-Mariano, *J. Amer. Chem. Soc. 103*: 3565-3567 (1981).
13. Investigation of the Mechanism of Yeast Inorganic Pyrophosphatase. W. B. Knight, S. W. Fitts and D. Dunaway-Mariano, *Biochemistry 20*: 4079-4086 (1981).
14. X-Ray Crystallographic and Nuclear Magnetic Resonance Spectral Studies of the Products from the Yeast Inorganic Pyrophosphatase-Co(NH3)4PP Reaction. Investigation of the Pyrophosphatase Reaction Mechanism. T. P. Haromy, W. B. Knight, M. Sundaralingam and D. Dunaway-Mariano, *Biochemistry 21*: 6950-6956 (1982).
15. Yeast Inorganic Pyrophosphatase Substrate Recognition. W. B. Knight, S.-J. Ting, S. Chuang, , T. P. Haromy, M. Sundaralingam and D. Dunaway-Mariano, *Archives of Biochemistry & Biophysics 227:* 302-309 (1983).
16. Investigation of the Structure, Protonation and Reactivity of Tetraamine(imidodi-phosphato)cobalt(III), A Substrate for Potato Apyrase. T. P.Haromy, W. B. Knight, D. Dunaway-Mariano* and M. Sundaralingam, *Biochemistry 22*: 5015-5121 (1983).
17. An Examination of the Solvent Perturbation Techniques as a Method to Identify Enzyme Catalytic Groups. S. Grace and D. Dunaway-Mariano, *Biochemistry 22*: 4238-4247 (1983).
18. Phosphoryl Group Activation in the Yeast Inorganic Pyrophosphatase Reaction. Su-Jen Ting and D. Dunaway-Mariano, *FEBS Lett. 165*: 251-253 (1984).
19. The Preparation and Characterization of Rh(III) Polyphosphate Complexes. I. Lin, W. B. Knight, S.-J. Ting and D. Dunaway-Mariano, *Inorganic Chemistry 23*: 988-991 (1984).
20. Investigations of the Metal Ion Binding Sites of Yeast Inorganic Pyrophosphatase. W. B. Knight, S. Ransom, J. J. Villafranca and D. Dunaway-Mariano, *J. Biol. Chem. 259*: 2886-2895 (1984).
21. Crystal Structure of Bidentate Tetraamine(pyrophosphato)chromium(III)Dihydrate, Cr(H3)4HP2O7.2H20. T. P. Haromy, W. B. Knight, D. Dunaway-Mariano and M. Sundaralingam, *Acta Crystallography C40*: 223-225 (1984).
22. Crystal Structure and Molecular Conformation of Tetraamine(methylenephosphato)-cobalt(III) Hydrochloride (CoPCP): CoH2P2O6CH2(NH3)4+ .Cl-. T. P. Haromy, W. B. Knight, D. Dunaway-Mariano and M. Sundaralingam, *Inorg. Chem. 23*: 2412-2414 (1984).
23. Preparation and Characterization of Co(III) and Cr(III) Complexes of Adenosine 5'-diphosphate. I. Lin., A. Hseuh and D. Dunaway-Mariano*, *Inorganic Chemistry 23*: 1692 (1984).
24. Stereospecific Synthesis of P^1,P^2-Bidentate $Co(NH_3)_4$(thiopyrophosphate) and P^1,P^2-Bidentate $Cr(H_2O)_4$(thiopyrophosphate) Enantiomers. I. Lin and *D. Dunaway-Mariano**, *J. Amer. Chem. Soc. 106*: 6074 (1984).
25. Recent Advances in the Use of Exchange Inert Complexes of Nucleotides with Cr(III), Co(III) and Rh(III) as Stereochemical Probes. D. Dunaway-Mariano, Stereochemistry of Enzymatic Reactions. Ed. P. Frey, Elsevier Science Publ. Co. N. Y., N. Y. pp. 149-164 (1985).
26. Investigation of the Regiospecificity and Stereospecificity of Proton Transfer in the Yeast Inorganic Pyrophosphatase Catalyzed Reaction. I. Lin, W. B. Knight, A. Hseuh and D. Dunaway-Mariano, *Biochemistry 25*: 4688-4692 (1986).
27. Inhibition and Inactivation of Pyruvate Phosphate Dikinase with Cr(III) Complexes of ATP and PP. L. Ciskanik, and D. Dunaway-Mariano*, *J. Enzyme Inhibition 1*: 113-119 (1986).
28. The Kinetic Mechanism of Yeast Inorganic Pyrophosphatase. R. J. Barry and Debra Dunaway-Mariano. *Archives of Biochemistry and Biophysics 259*:196-203 (1987).

29. Structural and Biochemical Properties of Bidentate Tetraaqua Rh(III) Complexes of Inorganic Pyrophosphate and Adenosine 5'-Diphosphate. A. L. Shorter, T. P. Haromy, T. Scalzo-Brush, W. B. Knight, M. S. Sundaralingam and D. Dunaway-Mariano, *Biochemistry 25*: 2060-2066 (1987).
30. Synthesis and Stereochemical Analysis of exchange Inert Cr(III) Complexes of Adenosine-5'-O-(2-thiodiphosphate) Adenosine-5'-O-(2-thiotriphosphate) and Adenosine-5'-O-(3-thiotriphosphate). Generation of a New Class of Chiral Enzyme Active Site Probes. I. Lin and D. Dunaway-Mariano, *J. Amer. Chem. Soc*. 110: 950-959 (1988).
31. Preparation and configurational analysis of the stereoisomers of β,γ-bidentate $Rh(H_2O)_4ATP$ and α,β,γ-tridentate $Rh(H_2O)_3ATP$. A new class of enzyme active site probes. Lu, Z., Shorter, A. L., Lin, I., Dunaway-Mariano, Debra. *Inorganic Chemistry 27*: 4135-4139 (1988).
32. Investigations of the Partial Reactions Catalyzed by Pyruvate Phosphate Dikinase from Bacteriodes Symbiosus. H.-C. Wang, L. Ciskanik, W. VonderSaal, J. J. Villafranca and D. Dunaway-Mariano, *Biochemistry 27*: 625-634 (1988).
33. Investigation of the Bacillus cereus Phosphonoacetaldehyde Hydrolase. Evidence for a Schiff Base Mechanism and Sequence Analysis of an Active Site Peptide Containing the Catalytic Lysine Residue. D. B. Olsen, T. W. Hepburn, M. Moos, P. S. Mariano and D. Dunaway-Mariano, *Biochemistry 27*: 2229-2236 (1988).
34. Elucidation of the 2-Aminoethylphosphonate Biosynthetic Pathway in Tetrahymena pyriformis. R. Barry, E. Bowman, M. McQueney and D. Dunaway-Mariano*, *Biochem. and Biophys. Res. Comm*.. 153: 177-182 (1988).
35. Catalysis and Thermodynamics of the Rearrangement of Phosphoenol Pyruvate to Phosphonopyruvate. Entry into the Phosphonate Class of Naturally Occurring Organophosphonates. E. Bowman, M. McQueney, R. Barry and D. Dunaway-Mariano, *J. Amer. Chem.Soc.*, 110: 5575-5577 (1988).
36. Investigation of the Substrate Structure and Metal Cofactor Requirements of the Rat Liver Mitochondrial Proton Pump ATPase. S. Hanley-Trawick, M. E. Carpen, P. L. Pedersen, J. Hulliken and D. Dunaway-Mariano*, *Archives of Biochemistry and Biophysics 268*: 116-123 (1989).
37. The mode of triple phosphoryl group transfer in pyruvate phosphate dikinase catalysis. Demonstration of the intermediacy of pyrophosphorylated and phosphorylated enzyme species. Carroll, Lawrence J.; Mehl, Andrew F.; Dunaway-Mariano, Debra. *J. Amer. Chem. Soc. 111*: 5965-5967 (1989).
38. A Remarkable Pericyclic Mechanism for Enzyme-Catalyzed P-C Bond Formation. M. S. McQueney, S.-L. Lee, E. Bowman, P. S. Mariano and D. Dunaway-Mariano, *J. Amer. Chem. Soc., 111*: 6885-6887 (1989).
39. Purification and Characterization of the Tetrahymena Pyriformis P-C Bond Forming Enzyme, Phosphoenol Pyruvate Phosphomutase. E. D. Bowman, M. S. McQueney, J. D. Scholten and D. Dunaway-Mariano, *Biochemistry 29*: 7059-7063 (1990).
40. A Method for Chiral Thiophosphonate Synthesis and its Use in Elucidating the Phosphorus Stereochemistry of the Hydrolytic C-P Bond Cleavage Reaction of Thiophosphono-acetaldehyde. S. L. Lee, T. W. Hepburn, P. S. Mariano and D. Dunaway-Mariano, *J. Organic Chem. 55*: 5435-5445 (1990).
41. Determination of the Catalytic Pathway of C4-Leaf Pyruvate Orthophosphate Dikinase from Maize. L. J. Carroll, , C. M. Smith, R. Chollett, and D. Dunaway-Mariano *FEBS Lett., 274:* 178-180 (1990).
42. Analysis of Sequence Homologies in Plant and Bacterial Pyruvate Phosphate Dikinase, Enzyme I of Bacterial Phosphoenolpyruvate: Sugar Phosphotransferase System and Other PEP-Utilizing Enzymes: Identification of Potential Catalytic and Regulatory Motifs. D. J. Pocalyko, L. J. Carroll, B. M. Martin, P. C. Babbitt and Debra Dunaway-Mariano, *Biochemistry 29*: 10757-10765 (1990).
43. Novel Enzymic Hydrolytic Dehalogenation of a Chlorinated Aromatic. J. D. Scholten, K.-H. Chang P. C. Babbitt, H. Charest, M. Sylvestre and D. Dunaway-Mariano, *Science 253:* 182-185 (1991).
44. Evidence for an Intra Molecular, Stepwise Reaction Pathway for PEP Phosphomutase Catalyzed P-C Bond Formation. M. S. McQueney, S.-L. Lee, W H. Swartz, H. L. Ammon, P. S. Mariano and D. Dunaway-Mariano, J. *Org. Chem. 56*: 7121-7129 (1991).

45. Expression of the 4-Chlorobenzoate Dehalogenase Genes From Pseudomonas sp. CBS-3 in Escherichia coli and Identification of the Gene Translation Products. P. Savard, H. Charest, F. Schareck, M. Sylvestre, J. D. Scholten and D. Dunaway-Mariano, *Canadian J. Microbiol. 38*: 1074-1081 (1992).
46. Investigation of the Substrate Binding and Catalytic Groups of the P-C Bond Cleaving Enzyme Phosphonoacetaldehyde Hydrolase, D. B. Olsen, T. W. Hepburn, S.-L. Lee, B. M. Martin, P. S. Mariano and Debra Dunaway-Mariano, *Arch. Biochem. & Biophys. 296:* 144-151 (1992).
47. Isolation and Characterization of the Three Polypeptide Components of 4-Chlorobenzoate Dehalogenase from Pseudomonas sp. Strain CBS-3. K.-H. Chang, P.-H. Liang, W. Beck, J. D. Scholten and D. Dunaway-Mariano, *Biochemistry 31:* 5605-5610 (1992).
48. Ancestry of the 4-Chlorobenzoate Dehalogenase: Analysis of Amino Acid Sequence Identities Among Families of Acyl: Adenyl Ligases, Enoyl-CoA Hydratases/Isomerases and Acyl-CoA Thioesterases. P. C. Babbitt, G. L. Kenyon, B. M. Martin, H. Charest, M. Sylvestre, J. D. Scholten, K.-H. Chang, P.-H Liang and D. Dunaway-Mariano, *Biochemistry 31*: 5594-5604 (1992).
49. A Stereochemical Probe for the Mechanism of P-C Bond Cleavage Catalyzed by the B. cereus Phosphonoacetaldehyde Hydrolase. S.-L. Lee, T. W. Hepburn, W. H. Swartz, P. S. Mariano and D. Dunaway-Mariano, *J. Am. Chem. Soc. 114:* 7346-7348 (1992).
50. Characterization of the Covalent Enzyme Intermediates Formed During Pyruvate Phosphate Dikinase Catalysis. S. H. Thrall, A. F. Mehl, L. J. Carroll and D. Dunaway-Mariano, *Biochemistry 32*: 1803-1809 (1993).
51. Investigations of Kinase Substrate Specificity with Aqua Rh(III) Complexes of Adenosine 5'-Triphosphate, Z. Lu, A.L. Shorter and D. Dunaway-Mariano, *Biochemistry 32*: 2378-2385 (1993).
52. Specificity of 4-Chlorobenzoate-Coenzyme A Dehalogenase Catalyzed Dehalogenation of Halogenated Aromatics. P.-H. Liang, G. Yang and D. Dunaway-Mariano, *Biochemistry 32: 12245-12250* (1993).
53. Kinetic Evidence for Separate Site Catalysis by Pyruvate Phosphate Dikinase, S.A. Thrall and D. Dunaway-Mariano, *Biochemistry 33*: 1103-1107 (1994).
54. Energetics of Pyruvate Phosphate Dikinase Catalysis. A. Mehl, Y. Xu and D. Dunaway-Mariano, *Biochemistry 33:* 1093-1102 (1994).
55. Substrate Binding Domains in Pyruvate Phosphate Dikinase. L.J. Carroll, Y. Xu, S.H. Thrall, B. M. Martin and D. Dunaway-Mariano, *Biochemistry 33:* 1134-1142 (1994).
56. On the Origins and Functions of the enzymes of the 4-Chlorobenzoate to 4-Hydroxybenzoate Converting Pathway. D. Dunaway-Mariano and P.C. Babbitt, *Biodegradation 5*: 259-276 (1994).
57. Evidence for Nucleophilic Catalysis in the Aromatic Substitution Reaction Catalyzed by (4-Chlorobenzoyl)enzyme A Dehalogenase, G. Yang, P.-H. Liang and D. Dunaway-Mariano *Biochemistry 33:* 8527-8531 (1994).
58. Separate Site Catalysis by Pyruvate Phosphate Dikinase as Revealed by Deletion Mutants, Y. Xu, M. McGuire, B.M. Martin and D. Dunaway-Mariano, *Biochemistry 34*: 2195-2202 (1995).
59. Location of the Catalytic Site for PEP Formation within the Primary Structure of Clostridium Symbiosum Pyruvate Phosphate Dikinase I. Identification of an Essential Cysteine by Chemical Modification with [1-^{14}C]Bromopyruvate and Site Directed Mutagenesis. X. Yu, S. Li, L. Yankie, Y.-S. Jung, P.S. Mariano, B.M. Martin and D. Dunaway-Mariano, *Biochemistry 34*: 2181-2187 (1995).
60. Location of the Catalytic Site for PEP Formation within to Primary Structures of Clostridium Symbiosum Pyruvate Phosphate Dikinase II. Site Directed Mutagenesis of an Essential Arginine. L. Yankie, Y. Xu and D. Dunaway-Mariano, *Biochemistry 34*: 2188-2194 (1995).
61. Transient State Kinetic Analysis of the Chemical Intermediates of the 4-Chlorobenzoyl-Coenzyme A Dehalogenase Catalyzed Aromatic Substitution Reaction. R.Q. Liu, P.O. Liang, J. Scholten and D. Dunaway-Mariano *J. Am. Chem. Soc.*, 117: 5003-5005 (1995).
62. Evidence for Electrophilic Catalysis in the 4-Chlorobenzoyl-CoA Dehalogenase Reaction: UV, Raman, and 13C-NMR Spectral Studies of Dehalogenase Complexes of Benzoyl-CoA Adducts. K. Taylor, R-Q. Liu, P.-H. Liang, J. Price, P.J. Tonge, J. Clarkson, P.R. Carey and D. Dunaway-Mariano, *Biochemistry 34:* 13881-13888 (1995).

63. Swiveling-Domain Mechanism for Enzymatic Phosphotransfer Between Remote Reaction Sites. O. Herzberg, C.C.H. Chen, G. Kapadia, M. McGuire, L.J. Carroll, S. J. Noh and Debra Dunaway-Mariano *Proc. Nat. Acad. Sci. USA, 93:* 2652-2657 (1996).
64. Phosphoenolpyruvate Mutase Catalysis of Phosphoryl Transfer in Phosphoenol Pyruvate: Kinetics and Mechanism of Phosphorus-Carbon Bond Formation. J. Kim and D. Dunaway-Mariano, *Biochemistry 35:* 4628-4635 (1996).
65. Structure of 4-Chlorobenzoyl Coenzyme A Dehalogenase Determined to 1.8 A Resolution: An Enzyme Catalyst Generated via Adaptive Mutation. M. M. Benning, K. L. Taylor, R.-Q. Liu, G. Yang, H. Xiang, G. Wesenberg, D. Dunaway-Mariano and H. Holden, *Biochemistry 35:* 8103-8109 (1996).
66. Determination of the Nucleotide Binding Sites within Clostridium Symbiosum Pyruvate Phosphate Dikinase by Photoaffinity Labeling, Site-Directed Mutagenesis and Structural Analysis. M. McGuire, L.J. Carroll, L. Yankie,, S. Thrall, D. Dunaway-Mariano, O. Herzberg, B. Jayaram and B. Haley *Biochemistry 35:* 8544-8552 (1996).
67. Identification of Active Site Residues Essential to 4-Chlorobenzoyl-Coenzyme A Catalysis by Chemical Modification and Site Directed Mutagenesis.Yang, G., Taylor, K. L., Liu, R.-Q., Xiang, H., Price, J. and Dunaway-Mariano, D. (1996) *Biochemistry 35:* 10879-10885.
68. Determination of the Chemical Pathway for 4-Chlorobenzoate: Coenzyme A Ligase Catalysis. Chang, K.-H. and Dunaway-Mariano, D. Biochemistry 35: 13478-13484 (1996).
69. Investigation of Substrate Activation by 4-Chlorobenzoyl Coenzyme Dehalogenase.Taylor, K. L , Xiang, H., Liu, R.-Q.and Dunaway-Mariano, D. Biochemistry 36: 1349-1361 (1997).
70. Studies on the Structure, Mechanism of Catalysis and Ancestry of 4-Chlorobenzoyl-Coenzyme A Dehalogenase. Dunaway-Mariano, D. *Proced. Nat. Acad. Sci. Netherlands*, 143-156 (1997).
71. Raman-Study of the Polarizing Forces Promoting Catalysis in 4-Chlorobenzoate-CoA Dehalogenase Clarkson J, Tonge P. J., Taylor K. L., Dunaway-Mariano D., Carey P. R., *Biochemistry 36:* 10192-10199 (1997).
72. Acyl-Adenylate Motif of the Acyl-Adenylate/Thioester-Forming Enzyme Superfamily : A Site-Directed Mutagenesis Study with the Pseudomonas Sp. Strain Cbs3 4-Chlorobenzoate-Coenzyme-A Ligase. Chang K. H., Xiang H., Dunaway-Mariano D. *Biochemistry 36:*15650-15659 (1997).
73. Isolation and Characterization ot the Carbon-Phosphorus Bond-Forming Enzyme Phosphoenoylpyruvate Mutase from the Mollusk Mytilus-Edulis. A. Kim, J. Kim, B. M. Martin and D. Dunaway-Mariano. *J. Biol. Chem. 273*: 4443-4448 (1998).
74. Insights Into the Mechanism of Catalysis by the P-C Bond Cleaving Enzyme Phosphonoacetaldehyde Hydrolase Derived from Gene Sequence-Analysis and Mutagenesis. Baker, A.S., Ciocci, M. J., Metcalf, W.W., Kim, J.-B., Babbitt, P. C., Wanner, B. L., Martin, B. M., Dunaway-Mariano, D *Biochemistry 37*: 9305-9315 (1998).
75. Location of the Phosphate Binding Site within Clostridium Symbiosum Pyruvate Phosphate Dikinase M.McGuire, K. Haung, G. Kapadia, O. Herzberg and D. Dunaway-Mariano *Biochemistry 37:* 13463-1374 (1998).
76. The Three-dimensional Structure of 4-Hydroxybenzoyl-CoA Thioesterase from Pseudomonas s. strain CBS-3. M. M. Benning, G. Wesenberg, R. Liu, K. L. Taylor, D. Dunaway-Mariano and H. Holden (1998) *J. Biol. Chem. 273*: 33572-33579.
77. Intermediates and Energetics in Pyruvate Phosphate Dikinase. Dunaway-Mariano *Methods in Enzymology 308*: 149-176 (1999).
78. The Template Mechanism of Enzyme Evolution. Xiang, H., Taylor, K. and Dunaway-Mariano, D. Biomedical Health Research vol 27, Ed. P. Frey & D. Northrop, IOS Press, Washington D.C.224-234 (1999).
79. Product Catalyzes the Deamidation of D154N Dehalogenase to Produce the Wild-Type Enzyme H. Xiang, J. Dong, P. R. Carey and D. Dunaway-Mariano (1999) Biochemistry 38: 4207-4213.
80. Modulating the Elecron Density in the Bound Product, 4-Hydroxybenzoyl-CoA, By Mutations in the 4-Chlorobenzoyl-CoA Dehalogenase Near the 4-Hydroxy-Group. J. Dong, H. Xiang, L. Luo, Debra Dunaway-Mariano and Paul Carey, *Biochemistry 38:* 4198-4206 (1999).

81. Helix swapping between two aa/bbbarrels: crystal structure of phosphoenolpyruvate mutase with bound Mg 2+ oxalate K. Huang, Z. Li, Y. Jia, Dunaway-Mariano, D and O. Herzberg, (1999) Structure 7: 539-548.
82. Interchange of Catalytic Activity within the2-Enoyl-Coenzyme A Hydratase/Isomerase Superfamily Based on a Common Active Site Template H. Xiang, L. Luo, K. L. Taylor, and D. Dunaway-Mariano, *Biochemistry 38:* 7638-7652 (1999).
83. Insight into the mechanism of phosphoenolpyruvate mutase catalysis derived from site-directed mutagenesis studies of active site residues. Y. Jia, Z. Lu, K. Huang, O. Herzberg, and D. Dunaway-Mariano, *Biochemistry 38:* 14165-14173 (1999).
84. Crystallization and preliminary crystallographic analysis of phosphonoacetaldehyde hydrolase. M.C.Morais, A.S. Baker, D.Dunaway-Mariano, and K.N.Allen, *Acta Crytallogr. D. Biol. Crystallogr. 56 (Pt 2):* 206-209 (2000).
85. The crystal structure of Bacillus cereus phosphonoacetaldehyde hydrolase: insight into catalysis of phosphorus bond cleavage and catalytic diversification within the HAD enzyme superfamily, M.C. Morais, W. Zhang, A.S. Baker, G. Zhang, K.N. Allen. and D. Dunaway-Mariano *Biochemistry 39:* 10385-10396 (2000).
86. Identification of Domain-Domain Docking Sites within Clostridium symbiosum Pyruvate Phosphate Dikinase by Amino Acid Replacement. M. Wei, Z. Li, D. Ye, O. Herzberg, and D. Dunaway-Mariano. *J. Biol. Chem. 275:* 41156-41165 (2000).
87. Raman difference spectroscopic studies of dithiobenzoyl substrate and product analogs binding to the enzyme dehologenase: pi-electron polarization is prevented by C=O to C=S substitution. J. Dong, L. Luo, P. Liang, D. Dunaway-Mariano and P. Carey J. Raman Spectroscopy, 31:365-371 (2000).
88. Investigation of the Catalytic Site within the ATP-Grasp Domain of Clostridium symbiosum Pyruvate Phosphate Dikinase.D. Ye, M. Wei, M. McGuire, K. Huang, G. Kapadia, O. Herzberg, B.M. Martin, and D. Dunaway-Mariano. J. Biol. Chem. 276:37630-37639 (2001).
89. Histidine 90 Fuction in 4-Chlorobenzoyl-Coenzyme A Dehalogenase Catalysis. W. Zhang, Y. Wei, L. Luo, K.L.Taylor, G. Yang, and; M.M. Benning and H.M. Holden and D. Dunaway-Mariano *Biochemistry 40*:13474-13482 (2001).
90. Investigation of the Role of the Domain Linkers in Separate Site Catalysis by Clostridium symbiosum Pyruvate Phosphate Dikinase. M. Wei, D. Ye, and D. Dunaway-Mariano, *Biochemistry 40:* 13466-13473 (2001).
91. Role of Active Site Binding Interactions in 4-Chlorobenzoyl-Coenzyme A Dehalogenase Catalysis. L. Luo, K. L. Taylor, H. Xiang, Y. Wei, W. Zhang, and D. Dunaway-Mariano *Biochemistry 40:* 15684-15692 (2001).
92. Pyruvate Site of Pyruvate Phosphate Dikinase: Crystal Structure of the Enzyme-Phosphonopyruvate Complex, and Mutant Analysis.O. Herzberg, C.C.H. Chen, S. Liu, A. Tempczyk, A. Howard, M. Wei, D. Ye, and D. Dunaway-Mariano. *Biochemistry 41:* 780-787(2002).
93 .Determination of the chlorine kinetic isotope effect, on the 4-chlorobenzoyl-CoA dehalogenase-catalyzed nucleophilic aromatic substitution. A. Lewandowicz, J. Rudzinski, L. Luo, D. Dunaway-Mariano and P. Paneth, *Arch. Biochem.and Biophys. 398:* 249-252 (2002).
94. Crystallization and Preliminary X-Ray Diffraction Studies of Beta-Phosphoglucomutase from Lactococcus Lactus. S.D.Lahiri, G. Zhang, P. Radstrom, D. Dunaway-Mariano and K.N. Allen, *Acta Cryst. Section D-Biological Crystallography 58*: 324-326 (2002).
95. The YbgC Protein Encoded by the ybgC Gene of the tol-pal Gene Cluster of Haemophilus Influenzae Catalyzes Acyl-Coenzyme A Thioester Hydrolysis.Z. Zhuang, F. Song, B.M. Martin and D. Dunaway-Mariano*, FEBS Letters 516:*161-163 (2002).
96. Raman Evidence for Meisenheimer Complex Formation in the Hydrolysis Reactions of 4-Fluorobenzoyl- and 4-Nitrobenzoyl-Coenzyme A Catalyzed by 4-Chlorobenzyol-Coenzyme A Dehydrogenese. J. Dong, P.R. Carey; Y. Wei, L. Luo, X. Lu, R. Liu and D.Dunaway-Mariano, *Biochemistry 41*: 7453-7463 (2002).

97. Caught in the Act: The Structure of Phosphorylated Beta-Phosphoglucomutase from Lactococcus lactis. S.D Lahiri, G. Zhang, D. Dunaway-Mariano and K.N.Allen. *Biochemistry 41:* 8351-8359 (2002).
98. The 2-Aminoethylphosphonate-Specific Transaminase of the 2-Aminoethylphosphonate Degradation Pathway. A. D. Kim, A.S. Baker, W.W. Metcalf, B.L. Wanner, Brian M. Martin and D.Dunaway-Mariano,. *J. Bacteriology 184*: 4134-4140 (2002).
99. X-ray Crystallographic Analysis of Inhibitor and Substrate Complexes of Wild-type and Mutant 4-Hydroxybenzoyl-CoA Thioesterase. J. B. Thoden, H. M. Holden, Z. Zhuang, and D. Dunawy-Mariano, *J. Biol. Chem. 277*: 27468-27476 (2002).
100. Dissociative Phosphoryl Transfer in PEP Mutase Catalysis: Structure of the Enzyme/Sulfopyruvate Complex and Kinetic Properties of Mutants. S.Liu, Z. Lu, Y. Jia, D. Dunaway-Mariano, and O. Herzberg, *Biochemistry 41:* 10270-10276 (2002).
101. Kinetic, Raman, NMR, and Site-Directed Mutagenesis Studies of the Pseudomonas Sp. Strain CBS3 4-Hydroxybenzoyl-CoA Thioesterase Active Site. Z. Zhuang, F. Song, W. Zhang, K. Taylor, A. Archambault, D. Dunaway-Mariano; J. Dong and P. R. Carey. *Biochemistry, 41:*11152-11160 (2002).
102. Degradation Pathway of the Phosphonate Ciliatine: Crystal Structure of 2-Aminoethylphosphonate Transaminase. Celia C. H. Chen, H. Zhang, A. D. Kim, A. Howard, G. M. Sheldrick, D. Mariano-Dunaway and O. Herzberg. *Biochemistry 41:* 13162-13169 (2002).
103. Kinetic Evidence for a Substrate-Induced Fit in Phosphonoacetaldehyde Hydrolase Catalysis. G. Zhang, A. S. Mazurkie, K. N. Allen and D. Dunaway-Mariano *Biochemistry 41:*13370-13377 (2002).
104. The Pentacovalent Phosphorous Intermediate of a Phosphoryl Transfer Reaction. S.D Lahiri, G. Zhang, D. Dunaway-Mariano and K.N. Allen. *Science 299*:2067-2071 (2003).
105. Characterization of the 4-Hydroxybenzoyl-Coenzyme A Thioesterase from Arthrobacter sp. Strain SU. Zhihao Zhuang, Karl-Heinz Gartemann, Rudolf Eichenlaub and Debra Dunaway-Mariano. (2003) Applied and Environmental Microbiology, 69(5):2707-2711.
106. The Strength of Dehalogenase-Substrate Hydrogen Bonding Correlates with the Rate of Meisenheimer Intermediate Formation. J. Dong, X. Lu, Y. Wei, L. Luo, D. Dunaway-Mariano and P. R. Carey, *Biochemistry 42:* 9482-9490 (2003).
107. The Structure of 4-Hydroxybenzoyl-CoA Thioesterase from Arthrobacter sp. strain SU. J. B. Thoden, Z. Zhuang, D. Dunaway-Mariano and H. M. Holden. *J. Biol. Chem. 278:* 43709-43716 (2003).
108. The Phosphonopyruvate Decarboxylase from Bacteroides fragilis.G. Zhang, J. Dai, Z. Lu and D. Dunaway-Mariano. *J. Biol. Chem. 278*:41302 – 41308 (2003).
109. Enzymatic synthesis of radiolabeled phosphonoacetaldehyde. G. Zhang, K. N. Allen and D. Dunaway-Mariano. *Analytical Biochemistry 322*: 233-237 (2003).
110. Kinetic Analysis of Enzyme Mutants for Identification of Catalytic Residues. Y. Wei, L. Luo, W. Zhang and D. Dunaway-Mariano. *Kinetic Analysis of Macromolecules-A Practical Approach*: 229-249 (2003).
111. The BH1999 Protein of Bacillus halodurans C-125 Is Gentisyl-Coenzyme A Thioesterase. Z. Zhuang, F. Song, H. Takami, and D. Dunaway-Mariano. *J. Bacteriol. 186:* 393-399 (2004).
112. X-ray Crystallographic and Site-directed Mutagenesis Analysis of the Mechanism of Schiff-Base Formation in Phosphonoacetaldehyde Hydrolase Catalysis. M. C. Morais, G. Zhang, W. Zhang, D. B. Olsen, D. Dunaway-Mariano and K. N. Allen. *J. Biol. Chem. 279:* 9353 – 9361 (2004).
113. Analysis of the Substrate Specificity Loop of the HAD Superfamily Cap Domain. S. D. Lahiri, G. Zhang, J. Dai, Karen N. Allen and Debra Dunaway-Mariano. *Biochemistry 43:* 2812 – 2820 (2004).
114. Conformational Flexibility of PEP Mutase. S. Liu, Z. Lu, Y. Han, Y. Jia, A. Howard, D. Dunaway-Mariano, and O. Herzberg. *Biochemistry 43*: 4447-4453 (2004).
115. Investigation of Metal Ion Binding in Phosphonoacetaldehyde Hydrolase Identifies Sequence Markers for Metal-Activated Enzymes of the HAD Enzyme Superfamily. G. Zhang, M. C. Morais, J. Dai, W. Zhang, Karen N. Allen and Debra Dunaway-Mariano *Biochemistry 43:* 4990 – 4997 (2004).
116. Arginine deiminase uses an active-site cysteine in nucleophilic catalysis of L-arginine hydrolysis. Lu, X., Galkin, A., Herzberg, O. and Dunaway-Mariano, D. *Journal of the American Chemical Society, 126:* 5374-5375 (2004).

117. Crystal Structure of 4-Chlorobenzoate:CoA Ligase/Synthetase in the Unliganded and Aryl Substrate-Bound States. A. M. Gulick, Xuefeng L., and D. Dunaway-Mariano. *Biochemistry 43:* 8670-8679 (2004).
118. Phosphoryl group transfer: evolution of a catalytic scaffold. Allen KN, and Dunaway-Mariano D. *Trends Biochem Sci. 29*: 495-503 (2004).
119. X-ray Crystal Structure of the Hypothetical Phosphotyrosine Phosphatase MDP-1 of the Haloacid Dehalogenase Superfamily. E. Peisach, J. D. Selengut, D. Dunaway-Mariano, and Karen N. Allen, *Biochemistry 43:* 12770-12779 (2004).
120. QM/MM Studies of the Enzyme-Catalyzed Dechlorination of 4-Chlorobenzoyl-CoA Provide Insight into Reaction Energetics. Dingguo Xu, Yanseng Wei, Jingbo Wu, Debra Dunaway-Mariano, Hua Guo, Qiang Cui, and Jiali Gao. *J. Am. Chem. Soc., 126:* 13649-13658 (2004).
121. Crystal structures of 2-methylisocitrate lyase in complex with product and with isocitrate inhibitor provide insight into lyase substrate specificity, catalysis and evolution. Liu S, Lu Z, Han Y, Melamud E, Dunaway-Mariano D, and Herzberg O. (2005) *Biochemistry 44*: 2949-62 (2005).
122. Structure of YciI from Haemophilus influenzae (HI0828) reveals a ferredoxin-like alpha/beta-fold with a histidine/aspartate centered catalytic site. Willis MA, Song F, Zhuang Z, Krajewski W, Chalamasetty VR, Reddy P, Howard A, Dunaway-Mariano D, and Herzberg O. *Proteins 59:* 648-652 (2005).
123. Chemical Confirmation of a Pentavalent Phosphorane in Complex with beta-Phosphoglucomutase. Tremblay L.W., Zhang G., Dai J, Dunaway-Mariano D., and Allen K .N. *J. Amer. Chem. Soc., 127:* 5298-9 (2005).
124. Raman evidence for product binding to the enzyme W137F 4-chlorobenzoyl-CoA dehalogenase in two conformational states. J. Dong, L. Luo, D. Dunaway-Mariano and P. R. Carey. *J. Raman Spectrosc. 36:* 320-325 (2005).
125. HAD Superfamily Phosphotransferase Substrate Diversification: Structure and Function Analysis of HAD Subclass IIB Sugar Phosphatase BT4131. Z. Lu, K. N. Allen and D. Dunaway-Mariano. *Biochemistry 44:* 8684-8696 (2005).
126. Catalytic cycling in beta-phosphoglucomutase: a kinetic and structural analysis. Zhang G, Dai J, Wang L,Tremblay LW, Allen K.N. Dunaway-Mariano D, *Biochemistry 44:* 9404-9416 (2005).
127. Crystal structures representing the Michaelis complex and the Thiouronium reaction intermediate of Pseudomonas aeruginosa arginine deiminase. Galkin A, Lu X, Dunaway-Mariano D, Herzberg O. *J Biol Chem. 280:* 34080-7 (2005).
128. L-Canavanine is a time-controlled mechanism-based inhibitor of *Pseudomonas aeruginosa* arginine deiminase. Lu X, Li L, Feng X, Wu Y, , Engen JR, Mariano PS, Dunaway-Mariano D, *J. Am. Chem. Soc. 127:* 16412-1613 (2005).
129. Diversity of Function in the Isocitrate Lyase Enzyme Superfamily: The Dianthus caryophyllus Petal Death Protein Cleaves alpha-Keto and alpha-Hydroxycarboxylic Acids. Lu Z, Feng X, Song L, Han Y, Kim A, Herzberg O, Woodson WR, Martin BM, Mariano PS and Dunaway-Mariano D. *Biochemistry 44:*16365-16376 (2005).
130. Crystal Structure of the Petal Death Protein from Carnation Flower. Teplyakov A, Liu S, Lu Z, Howard A, Dunaway-Mariano D and Herzberg O. *Biochemistry 44*:16377-16384 (2005).
131. Contributions of Long-Range Electrostatic Interactions to 4-Chlorobenzoyl-CoA Dehalogenase Catalysis: A Combined Theoretical and Experimental Study. Wu J, Xu D, Lu X, Wang C, Guo H, Dunaway-Mariano D. *Biochemistry. 45*:102-112 (2006).
132. Kinetic Analysis of Pseudomonas aeruginosa Arginine Deiminase Mutants and Alternate Substrates Provides Insight into Structural Determinants of Function. Lu X, Li L, Wu R, Feng X, Li Z, Yang H, Wang C, Guo H, Galkin A, Herzberg O, Mariano PS, Martin BM, Dunaway-Mariano D. *Biochemistry.* 45:1162-1172 (2006).
133. Structure and Activity Analyses of Escherichia coli K-12 NagD Provide Insight into the Evolution of Biochemical Function in the Haloalkanoic Acid Dehalogenase Superfamily. Tremblay LW, Allen KN and Dunaway-Mariano D. *Biochemistry* 45:1183-1193 (2006).

134. Examination of the structure, stability, and catalytic potential in the engineered phosphoryl carrier domain of pyruvate phosphate dikinase Lin Y, Lusin JD, Ye D, Dunaway-Mariano D, Ames JB. *Biochemistry 45:*1702-11 (2006).
135. Structure, function and mechanism of the phenylacetate pathway hotdog-fold thioesterase PAAI Song F, Zhuang Z, Finci L, , Kniewel R, Buglino JA, Solorzano V, Wu J, Lima C. and Dunaway-Mariano D, *J. Biol. Chem. 281:* 11028-38 (2006).
136. The X-ray crystal structures of human alpha-phosphomannomutase 1 reveal the structural basis of congenital disorder of glycosylation type 1a. Silvaggi NR, Zhang C, Lu Z, Dai J, Allen KN and Dunaway-Mariano D *J. Biol. Chem. 281*: 14918-26 (2006).
137. Conformational Cycling in beta-Phosphoglucomutase Catalysis: Reorientation of the beta-d-Glucose 1,6-(Bis)phosphate Intermediate.Dai J, Wang L, Allen KN, Radstrom P, and Dunaway-Mariano D. *Biochemistry. 45*, 7818-7824 (2006).
138. Evolutionary Genomics of the HAD Superfamily: Understanding the Structural Adaptations and Catalytic Diversity in a Superfamily of Phosphoesterases and Allied Enzymes. A. Maxwell Burroughs, Karen N. Allen, Debra Dunaway-Mariano and L. Aravind. *J. Mol. Biol. 361*: 1003-1034 (2006).
139. Crystal Structure of Human Thioesterase Superfamily Member 2. Z. Cheng, F. Song, X. Shan, Z. Wei, Y. Wang, D. Dunaway-Mariano, W. Gong. *Biochem. and Biophys. Res. Comm. 349:* 172-177 (2006).
140. Structure and Kinetics of Phosphonopyruvate Hydrolase from VorioVorax sp. Pal2: New Insight into the Divergence of Catalysis within the PEP Mutase/Isocitrate Lyase Superfamily. C. C. H. Chen, Y. Han, W. Niu, A. N. Kulakova, A. Howard, J. P. Quinn, O. Herzberg and Debra Dunaway-Mariano. *Biochemsitry 45:* 11491-11504 (2006**)**.
141. Diversification of Function in the Haloacid Dehalogenase Enzyme Superfamily: The Role of the Cap Domain in Hydrolytic Phosphorus-Carbon Bond Cleavage. S. D. Lahiri, G. Zhang, D. Dunaway-Mariano, K. N. Allen. *Bioorg. Chem. 34:* 394-409 (2006).
142. Structure-activity analysis of base and enzyme-catalyzed 4-hydroxybenzoyl coenzyme A hydrolysis. Song F, Zhuang Z, Dunaway-Mariano D. *Bioorg. Chem. 35:* 1-10 (2007).
143. Characterization, Kinetics, and Crystal Structures of Fructose-1,6-bisphosphate Aldolase from the Human Parasite, *Giardia lamblia*. Galkin A, Kulakova L, Melamud E, Li L, Wu C, Mariano P, Dunaway-Mariano D, Nash TE, Herzberg O. *J. Biol. Chem. 282:* 4859-6 (2007).
144. Oxaloacetate hydrolase: The C-C bond lyase of oxalate secreting fungi. Han Y, Joosten HJ, Niu W, Zhao Z, Mariano PS, McCalman MT, van Kan JA, Schaap PJ, Dunaway-Mariano D. *J. Biol. Chem. 282*: 9581-90 (2007).
145. The X-ray crystallographic structure and activity analysis of a *Pseudomonas*-specific subfamily of the HAD enzyme superfamily evidences a novel biochemical function. Peisach E, Wang L, Burroughs AM, Aravind L, Dunaway-Mariano D, Allen KN. *Proteins 70*; 197-207 (2007).
146. Identification of fungal oxaloacetate hydrolyase within the isocitrate lyase/PEP mutase enzyme superfamily using a sequence marker-based method. Joosten HJ, Han Y, Niu W, Vervoort J, Schaap PJ. and Dunaway-Mariano D *Proteins 70:* 157-166 (2007).
147. Rational redesign of the 4-chlorobenzoate binding site of 4-chlorobenzoate: coenzyme a ligase for expanded substrate range Wu R, Reger AS, Cao J, Gulick AM, Dunaway-Mariano D. *Biochemistry 46:* 14487-14499 (2007).
148. Swiveling Domain Mechanism in Pyruvate Phosphate Dikinase. Lim K, Read RJ, Chen CC, Tempczyk A, Wei M, Ye D, Wu C, Dunaway-Mariano D, Herzberg O *Biochemistry 46:*14845-14853 (2007).
149. Structure and Function of PA4872 from *Pseudomonas aeruginosa*, a Novel Class of Oxaloacetate Decarboxylase from the PEP Mutase/Isocitrate Lyase Superfamily. Narayanan BC, Niu W, Han Y, Zou J, Mariano PS, Herzberg O. and Dunaway-Mariano D, *Biochemistry 47*:167-182 (2008).
150. Inactivation of Microbial Arginine Deiminases by L-Canavanine. Li L, Li Z, Chen D, Lu X, Feng X, Wright EC, Solberg NO, Dunaway-Mariano D, Mariano PS, Galkin A, Kulakova L, Herzberg O, Green-Church KB, Zhang L. *J. Am. Chem. Soc.130*: 1918-1931 (2008).

151. Divergence of function in the hot dog fold enzyme superfamily: the bacterial thioesterase YciA. Zhuang Z, Song F, Zhao H, Li L, Cao J, Eisenstein E, Herzberg O, and Dunaway-Mariano D. *Biochemistry 47:* 2789-2796 (2008).
152. Structure of YciA from Haemophilus influenzae (HI0827), a hexameric broad specificity acyl-coenzyme A thioesterase. Willis MA, Zhuang Z, Song F, Howard A, Dunaway-Mariano D, Herzberg O. *Biochemistry 47:* 2797-2805 (2008).
153. The catalytic scaffold of the haloalkanoic acid dehalogenase enzyme superfamily acts as a mold for the trigonal bipyramidal transition state. Lu Z, Dunaway-Mariano D, Allen KN. *Proc. Nat. Acad. Sci. U S A. 105:* 5687-5692 (2008).
154. The Electrostatic Driving Force for Nucleophilic Catalysis in l-Arginine Deiminase: A Combined Experimental and Theoretical Study. Li L, Li Z, Wang C, Xu D, Mariano PS, Guo H, Dunaway-Mariano D. *Biochemistry 47:* 4721-4732 (2008**)**.
155. Structural characterization of a 140 degrees domain movement in the two-step reaction catalyzed by 4-chlorobenzoate:CoA ligase. Reger AS, Wu R, Dunaway-Mariano D, Gulick AM. *Biochemistry 47:* 8016-8025 (2008).
156. Mechanism of 4-chlorobenzoate:coenzyme a ligase catalysis. Wu R, Cao J, Lu X, Reger AS, Gulick AM, Dunaway-Mariano D. *Biochemistry 47:* 8026-8039 (2008**)**.
157. The catalytic scaffold of the haloalkanoic acid dehalogenase enzyme superfamily acts as a mold for the trigonal bipyramidal transition state. Lu Z, Dunaway-Mariano D, Allen KN. *Proc. Nat. Acad. Sci. U S A. 105:* 5687-92 (2008).
158. Human Symbiont *Bacteroides thetaiotaomicron* synthesizes 2-keto-3-deoxy-D-glycero-D-galacto-nononic Acid (KDN) Wang L., Lu, Z, Allen, K. N., Mariano, P.S.,Dunaway-Mariano D. *Chemistry and Biology 15:* 893 (2008).
159. Enzyme function discovery. Dunaway-Mariano D**.** *Structure. 16,* 1599-1600 (2008).
160. Structure-function analysis of 2-keto-3-deoxy-D-glycero-D-galactonononate-9-phosphate phosphatase defines specificity elements in type C0 haloalkanoate dehalogenase family members. Lu Z, Wang L, Allen KN and Dunaway-Mariano D, *J. Biol. Chem. 284*: 1224-33 (2009).
161. In vitro kinetic analysis of substrate specificity in enterobactin biosynthetic lower pathway enzymes provides insight into the biochemical function of the hot dog-fold thioesterase EntH. Chen D, Wu R, Bryan TL, Dunaway-Mariano D. *Biochemistry 48:* 511-513 (2009).
162. Structure and function of 2,3-dimethylmalate lyase, a PEP mutase/isocitrate lyase superfamily member. Narayanan B, Niu W, Joosten HJ, Li Z, Kuipers RK, Schaap PJ, Herzberg O and Dunaway-Mariano D. *J. Mol. Biol. 386*: 486-503 (2009).
163. Analysis of the Structural Determinants Underlying Discrimination between Substrate and Solvent in beta-Phosphoglucomutase Catalysis. J. Dai, L. Finci, C. Zhang, S. Lahiri, G. Zhang, E. Peisach, K. N. Allen and D. Dunaway-Mariano *Biochemistry 48:* 1984–1995 (2009**)**.
164. The Mechanisms of Human Hotdog-fold Thioesterase 2 (hTHEM2) Substrate Recognition and Catalysis Illuminated by a Structure and Function Based Analysis J. Cao, Hang Xu, H. Zhao, W. Gong and D. Dunaway-Mariano, *Biochemistry 48*: 1293–1304 (2009).
165. Structural insights into substrate binding and stereoselectivity of *Giardia* fructose-1,6-bisphosphate aldolase. Galkin A, Li Z, Li L, Kulakova L, Pal L, Dunaway-Mariano D, Herzberg O. *Biochemistry 48:* 3186-3196 (2009).
166. The Mechanism of Domain Alternation in the Acyl-Adenylate Forming Ligase Superfamily Member 4-Chlorobenzoate: Coenzyme A Ligase. Wu R, Reger A, Lu X, Gulick A, Dunaway-Mariano D. *Biochemistry 48:* 4115-4125 (2009).
167. X-ray Structure and Kinetic Properties of Ornithine Transcarbamoylase from the Human Parasite *Giardia lamblia* Galkin, G., Kulakova, L, Wu, R., Gong M., Dunaway-Mariano, D. and Herzberg, O. *Proteins 76*: 1049-1053 (2009).
168. Monitoring enzyme catalysis in the multimeric state: direct observation of Arthrobacter 4-hydroxybenzoyl-coenzyme A thioesterase catalytic complexes using time-resolved electrospray

ionization mass spectrometry. Li Z, Song F, Zhuang Z, Dunaway-Mariano D, Anderson KS. *Anal. Biochem. 394:* 209-216 (2009).
169. Mechanisms of catalysis and inhibition operative in the arginine deiminase from the human pathogen Giardia lamblia. Li Z, Kulakova L, Li L, Galkin A, Zhao Z, Nash TE, Mariano PS, Herzberg O, Dunaway-Mariano D. *Bioorg Chem. 37:* 149-61 (2009).
170. Mechanisms of catalysis and inhibition operative in the arginine deiminase from the human pathogen Giardia lamblia. Li Z, Kulakova L, Li L, Galkin A, Zhao Z, Nash TE, Mariano PS, Herzberg O, Dunaway-Mariano D. *Bioorg Chem. 37:* 149-61 (2009).
171. Markers of fitness in a successful enzyme superfamily. Allen KN, Dunaway-Mariano D. *Curr Opin Struct Biol. 19*: 658-65 (2009).
172. The Akt C-terminal modulator protein is an acyl-CoA thioesterase of the hotdog-fold family. Zhao H, Martin BM, Bisoffi M, Dunaway-Mariano D. *Biochemistry 48*: 5507-9 (2009).
173. Divergence of biochemical function in the HAD superfamily: D-glycero-D-manno-heptose-1,7-bisphosphate phosphatase (GmhB). Wang L, Huang H, Nguyen HH, Allen KN, Mariano PS, Dunaway-Mariano D. *Biochemistry 49:* 1072-81 (2010).
174. Structural determinants of substrate recognition in the HAD superfamily member D-glycero-D-manno-heptose-1,7-bisphosphate phosphatase (GmhB). Nguyen HH, Wang L, Huang H, Peisach E, Dunaway-Mariano D, Allen KN., *Biochemistry 49:* 1082-92 (2010).
175. X-ray structure and characterization of carbamate kinase from the human parasite Giardia lamblia. Galkin A, Kulakova L, Wu R, Nash TE, Dunaway-Mariano D, Herzberg O. *Acta Crystallogr Sect F Struct Biol Cryst Commun. 66(Pt 4):* 386-90 (2010).
176. Nature and kinetic analysis of carbon-carbon bond fragmentation reactions of cation radicals derived from SET-oxidation of lignin model compounds. Cho DW, Parthasarathi R, Pimentel AS, Maestas GD, Park HJ, Yoon UC, Dunaway-Mariano D, Gnanakaran S, Langan P, Mariano PS. (2010) *J Org Chem*. 75, 6549-62.
177. Rational design, synthesis and evaluation of first generation inhibitors of the Giardia lamblia fructose-1,6-biphosphate aldolase.Li Z, Liu Z, Cho DW, Zou J, Gong M, Breece RM, Galkin A, Li L, Zhao H, Maestas GD, Tierney DL, Herzberg O, Dunaway-Mariano D, Mariano PS. *J Inorg Biochem*. 105, 509-17 (2011).
178. Regioselectivity of enzymatic and photochemical single electron transfer promoted carbon-carbon bond fragmentation reactions of tetrameric lignin model compounds. Cho DW, Latham JA, Park HJ, Yoon UC, Langan P, Dunaway-Mariano D, Mariano PS.
J Org Chem. *76*, 2840-52 (2011).
179. Homo sapiens Dullard Protein Phosphatase Shows a Preference for the Insulin-Dependent Phosphorylation Site of Lipin1. Wu R, Garland M, Dunaway-Mariano D, Allen KN. *Biochemistry 50*, 3045-7 (2011).
180. Divergence of Chemical Function in the Alkaline Phosphatase Superfamily: Structure and Mechanism of the P-C Bond Cleaving Enzyme Phosphonoacetate Hydrolase. Kim A, Benning MM, Oklee S, Quinn J, Martin BM, Holden HM, Dunaway-Mariano D. *Biochemistry.* 50, 3481-94 (2011).
181. The X-ray crystallographic structure and specificity profile of HAD superfamily phosphohydrolase BT1666: Comparison of paralogous functions in B. thetaiotaomicron.Lu Z, Dunaway-Mariano D, Allen KN. *Proteins. 79*, 3099-107 (2011).
182. Divergence of Structure and Function in the Haloacid Dehalogenase Enzyme Superfamily: Bacteroides thetaiotaomicron BT2127 Is an Inorganic Pyrophosphatase.Huang H, Patskovsky Y, Toro R, Farelli JD, Pandya C, Almo SC, Allen KN, Dunaway-Mariano D. *Biochemistry 50*, 8937-49 (2011)
183. The Enzyme Function Initiative. Gerlt JA, Allen KN, Almo SC, Armstrong RN, Babbitt PC, Cronan JE, Dunaway-Mariano D, Imker HJ, Jacobson MP, Minor W, Poulter CD, Raushel FM, Sali A, Shoichet BK, Sweedler JV. *Biochemistry 50*, 9950-62 (2011).
184. A Thioester Substrate Binds to the Enzyme *Arthrobacter* Thioesterase in Two Ionization States; Evidence from Raman Difference Spectroscopy. Jian Dong, Zhihao Zhuang, Feng Song, Debra Dunaway-Mariano and Paul R. Carey *Journal of Raman Spectroscopy 43,* 65-71 (2012).

185. Investigation of the Catalytic Mechanism of the Hotdog-Fold Enzyme Superfamily Pseudomonas sp. Strain CBS3 4-Hydroxybenzoyl-CoA Thioesterase. Zhuang Z, Latham J, Song F, Zhang W, Trujillo M, Dunaway-Mariano D. *Biochemistry*. 51, 786-794 (2012).
186. Human brown fat inducible thioesterase variant 2 cellular localization and catalytic function. Chen D, Latham J, Zhao H, Bisoffi M, Farelli J, Dunaway-Mariano D *Biochemistry 5*, 6990-6999 (2012).
187.The Catalytic Mechanism of the Hotdog-fold Enzyme Superfamily 4-Hydroxybenzoyl-CoA Thioesterase from Arthrobacter sp. Strain SU. Song F, Thoden JB, Zhuang Z, Latham J, Trujillo M, Holden HM, Dunaway-Mariano D *Biochemistry 51*, 7000-7016 (2012).
188. Correlation of Structure and Function in the Human Hotdog-fold Enzyme hTHEM4. Zhao H, Lim K, Choudry A, Latham JA, Pathak MC, Dominguez D, Luo L, Herzberg O, Dunaway-Mariano D. *Biochemistry 51*, 6490-2 (2012).

Biosketch
Deborah G. Evans

(a) Professional Preparation

College/University	Major/Area	Degree &Year
University of the Witwatersrand, Johannesburg, South Africa	Mathematics and Chemistry	B.Sc., 1986
University of the Witwatersrand	Chemistry	B.Sc. Honors, 1987
University of the Witwatersrand	Theoretical Chemistry	M.Sc., 1989
University of Pittsburgh	Chemical Physics	PhD, 1990-1995
University of Tel Aviv	Chemical Physics	Postdoctoral Associate, 1996

(b) Academic/Professional Appointments

Associate Director	Nanoscience and Microsystems Graduate Program	2007-present
Affiliate Research Scientist	New Mexico Consortium (NMC)	2010-2012
Associate Professor	Department of Chemistry, University of New Mexico	2002-present
Visiting Faculty (sabbatical)	Center for Integrated Nanosystems (LANL)	2006-2007
Assistant Professor	University of New Mexico	1996-2001
Research Assistant	University of Pittsburgh, PA	1993-1995
Teaching Assistant	University of Pittsburgh, PA	1991-1993
Junior Lecturer	University of the Witwatersrand, Johannesburg	1988-1990

(c) Publications (40 refereed journal articles, over 60 presentations and invited talks)

Five Most Recent Multidisciplinary Articles in Refereed Journals

1. *A Molecular Dynamics Simulation Study of the Interaction of Cationic Biocides with Lipid Bilayers: Aggregation Effects and Bilayer Damage,* Hill, E; *Stratton, K (REU-2012); Whitten, D and Evans, D, Langmuir, accepted, September **2012**
2. *A Molecular Dynamics and Computational Study of Ligand Docking and Electron Transfer in Ferritins*, Vijaya Subramanian and Deborah G. Evans, *J. Phys. Chem. B*, **2012**, *116* (31), 9287–9302
3. Photochemistry of a Model Cationic *p*-Phenylene Ethynylene in Water, Eric H. Hill, Subhadip Goswami, Deborah G. Evans, Kirk S. Schanze, and David G. Whitten, *The Journal of Physical Chemistry Letters,* **2012** *3* (10), 1363-1368
4. *Synthesis, Self-Assembly, and Photophysical Properties of Cationic Oligo(p-phenyleneethynylene)s*, Yanli Tang, Eric H. Hill, Zhijun Zhou, Deborah G. Evans, Kirk S. Schanze, and David G. Whitten, *Langmuir*, **2011**, *27* (8), pp 4945–4955.
5. *The targeted delivery of multicomponent cargos to cancer cells by nanoporous particle-supported lipid bilayers*, Ashley CE, Carnes EC, Phillips GK, Padilla D, Durfee PN, *Brown PA, Hanna TN, Liu J, Phillips B, Carter MB, Carroll NJ, Jiang X, Dunphy DR, Willman CL, Petsev DN, Evans DG, Parikh AN, Chackerian B, Wharton W, Peabody DS, Brinker CJ., Nature Materials, **2011**, 10(5), pp. 389-9.

(d) Synergistic Activities:

1. **Associate Director of the Nanoscience and Microsystems (NSMS) Graduate Degree Program** at UNM, a multi-department and across-college interdisciplinary degree. Activities include:
 - developing and teaching of a core course in the NSMS degree: Chemistry and Physics at the Nanoscale
 - administration of the Department of Education GAANN Fellowship Program at UNM
 - administration of the NSMS REU program in NSMS (2009-2012)
 - NSMS graduate student recruitment, admission and advisement

- advisement and retention of students in the NSMS IGERT, GAANN and Professional Science Masters (PSM) programs
- coordination and design of curricula offered in the NSMS PhD and MS programs

2. Co-advise two graduate students in the Whitten group at UNM, working on business plans to market the biomedical applications of polyelectrolyte self-assembly.
3. College of Arts and Sciences Scholarships Committee Chair (2006-present): committee oversees all College awards and scholarships, including the Lane Fellowship to the top two incoming female students who are going to major in a STEM discipline. Served as Chair of the Undergraduate Curriculum Committee and as Undergraduate Faculty Advisor in the Chemistry Department (2005-2009)
4. Created a suite of Mathcad^{TM} learning tools for undergraduate chemistry classes. Developed an interdisciplinary capstone course for the BS Chemistry degree at UNM: *Physical Chemistry and Nanoscience*. Obtained funding to establish an undergraduate computer pod for chemistry undergraduates
5. Co-organizer of a physical chemistry symposium at the ACS National Meeting in Boston (August 2007) on "Emergence of Function in Nano and Biomolecular Assemblies"

(e) Research

Collaborators over the last 48 months:

Dr. Andrew Shreve *LANL, Dr. Richard Watt (BYU), Dr. Rob Coalson (Pittsburgh), Dr. David Whitten, UNM, Dr. C Brinker, UNM.*

Graduate and Postdoctoral Advisors:

Graduate Advisor, Prof. Rob D. Coalson (University of Pittsburgh)
Post-Doctoral Advisor, Prof. A. Nitzan (Tel Aviv University)

Postdoctoral Associates and Students in the Last Five Years:

Postdoctoral Associates (total 4): Vijaya Subramaniam
Graduate Students (total 5): Eric Hill, William Cook, Thomas Corbitt, Mark Fleharty, Bea Yu
Undergraduate Research Students (total 24):
Tye Martin, Jeremiah Anderson, Katie Schultz, Page Stiers, Monique Cordova, Tiffany Allen

Current Funding:

NSF BMAT (co-PI), $390K, DOE GAANN 2009 (co-PI), $525K, DOE GAANN 2012 (co-PI), $660K
NSF REU 2009-2012 (co-PI) $345K

(f) Honors and Professional Recognition

1. *The Gunter Starkey Teaching Award,* College of Arts and Sciences, University of New Mexico, March 2005. Annual Award for excellence and breadth of teaching within the College.
2. The Wiley-International Journal of Quantum Chemistry *Young Investigator Award,* 2001.
3. The Dreyfus Foundation: *Camille Dreyfus Teacher-Scholar Award,* 2000-2005.
4. The Research Corporation, *Cottrell Teacher-Scholar,* 1999-2004.
5. *Provost Outstanding Teacher of the Year,* UNM 1999/2000.
6. *NSF-CAREER award*, Electron dynamics in thin films and dendrimers, 1999

Curriculum Vitae
Deborah G. Evans

Educational History

College/University	Major/Area	Degree &Year
University of the Witwatersrand, Johannesburg, South Africa	Mathematics and Chemistry	B.Sc., 1986
University of the Witwatersrand	Chemistry	B.Sc. Honors, 1987
University of the Witwatersrand	Theoretical Chemistry	M.Sc., 1989
University of Pittsburgh	Chemical Physics	PhD, 1990-1995
University of Tel Aviv	Chemical Physics	Postdoctoral Associate, 1996

Employment History

Appointment	Institution	Time Period
Associate Director	Nanoscience and Microsystems Graduate Program	2007-present
Affiliate Research Scientist	New Mexico Consortium (NMC)/LANL	2010-2012
Associate Professor	Department of Chemistry, UNM	2002-present
Visiting Faculty (sabbatical)	Center for Integrated Nanosystems (LANL)	2006-2007
Assistant Professor	Department of Chemistry, UNM	1996-2001
Research Assistant	University of Pittsburgh,	1993-1995
Teaching Assistant	University of Pittsburgh, PA	1991-1993
Junior Lecturer	University of the Witwatersrand, Johannesburg	1988-1990

Honors and Professional Recognition

- *The Gunter Starkey Teaching Award,* College of Arts and Sciences, UNM, March 2005.
- *The Wiley-International Journal of Quantum Chemistry Young Investigator Award, 2001.*
- *The Dreyfus Foundation:* Camille Dreyfus Teacher-Scholar Award, 2000-2005.
- *The Research Corporation,* Cottrell Teacher-Scholar, 1999-2004.
- *Provost Outstanding Teacher of the Year,* UNM 1999/2000.
- NSF-CAREER award, *Electron dynamics in thin films and dendrimers* , 1999
- Postdoctoral Research Scholarship, University of Tel Aviv, 1996
- Andrew D. Mellon pre-doctoral fellow, University of Pittsburgh, 1992-1994
- Chancellor's Medal for the most distinguished graduate of the U. of the Witwatersrand, 1986
- Faculty Honoree (teaching excellence and mentoring) inducted to Phi Eta Sigma National Honor Society, March 2006; inducted into Phi Kappa Phi Honor Society, April 2006 and April 2007

SCHOLARLY ACHIEVEMENTS

Articles in Refereed Journals

40. *A Molecular Dynamics Simulation Study of the Interaction of Cationic Biocides with Lipid Bilayers: Aggregation Effects and Bilayer Damage,* Hill, E; *Stratton, K (REU-2012); Whitten, D and Evans, D, Langmuir, accepted, September 2012

39. *A Molecular Dynamics and Computational Study of Ligand Docking and Electron Transfer in Ferritins*, Vijaya Subramanian and Deborah G. Evans, *J. Phys. Chem. B*, 2012, *116* (31), 9287–9302

38. Photochemistry of a Model Cationic *p*-Phenylene Ethynylene in Water, Eric H. Hill, Subhadip Goswami, Deborah G. Evans, Kirk S. Schanze, and David G. Whitten, *The Journal of Physical Chemistry Letters,* 2012 *3* (10), 1363-1368

37. *Synthesis, Self-Assembly, and Photophysical Properties of Cationic Oligo(p-phenyleneethynylene)s*, Yanli Tang, Eric H. Hill, Zhijun Zhou, Deborah G. Evans, Kirk S. Schanze, and David G. Whitten, *Langmuir*, 2011, *27* (8), pp 4945–4955.

36. *The targeted delivery of multicomponent cargos to cancer cells by nanoporous particle-supported lipid bilayers*, Ashley CE, Carnes EC, Phillips GK, Padilla D, Durfee PN, *Brown PA, Hanna TN, Liu J, Phillips B, Carter MB, Carroll NJ, Jiang X, Dunphy DR, Willman CL, Petsev DN, Evans DG, Parikh AN, Chackerian B, Wharton W, Peabody DS, Brinker CJ., Nature Materials, 2011, 10(5), pp. 389-9.

35. William R. Cook, Rob D. Coalson and Deborah G. Evans, *Effectiveness of Perturbation Theory Approaches for Computing Non-Condon Electron Transfer Dynamics in Condensed Phases*, *J. Phys. Chem. B*, 2009, *113*, 11437–11447

34. S. Peter, D.G. Evans* and R.D. Coalson, *Condensed-phase Relaxation of Multilevel Quantum Systems. I. An Exactly Solvable Model,* J. Phys. Chem. B, 110, 18758 (2006).

33. S. Peter, D.G. Evans* and R.D. Coalson, *Condensed-phase Relaxation of Multilevel Quantum Systems. II. Comparison of Path Integral Calculations and Second-Order Relaxation Theory for a Non-degenerate Three-level System,* invited article, , J. Phys. Chem. B, 110, 18764 (2006).

32. W.R. Cook, D.G. Evans* and R.D. Coalson, *An Exactly Solvable Model of Non-Condon Effects in Electron Transfer*, Chem. Phys. Lett., 420, 362 (2006).

31. R.D. Coalson and D.G. Evans*, *Condensed phase vibrational relaxation: calibration of approximate relaxation theories with analytical and numerically exact results*, Chem. Phys., 296, 117, 2004.

30. V. Subramanian and D.G. Evans and, *Excitation energy transfer in model light-harvesting antennae*, J. Phys. Chem B; 108, 1085 (2004)

29. C.K. Kalyanaraman and D.G. Evans, *Molecular Conductance of Dendritic Wires,* Nanoletters., 2, 437, 2002.

28. C.K. Kalyanaraman and D.G. Evans, *Anharmonic Effects on Photoinduced Electron Transfer: a Redfield Approach*, J. Chem. Phys, 115 (14), 2001.

27. D.G. Evans, *Theoretical Methods in Condensed Phase Chemistry: A book review of Progress in Theoretical Chemistry*, J. Am. Chem. Soc., (2002).

26. T.S. Elicker, J-S Binette and D.G. Evans, *Topological effects in electron transfer: Applications to dendrimers and branched molecules,* J. Phys. Chem. B, 105, 370 (2001).

25. D.G. Evans. *Anharmonic Effects on Photo-induced Electron Transfer*, J. Chem. Phys, 113, 3282 (2000).

24. C.K. Kalyanaraman and D.G. Evans, *Symplectic Integrators for the multilevel Redfield equation*, Chem. Phys. Lett., 324, 459 (2000).

23. D. Evans and R. Wampler, *Electron Transmission through self-assembled monolayers*, J. Phys. Chem. B, 103, 4666 (1999).
22. T.S. Elicker and D. G. Evans, *Electron Dynamics in Dendrimers*, J. Phys. Chem. A, 103, 9423 (1999).
21. Naaman R., Haran A. Nitzan A., Evans D., Galperin M., *Electron Transmission Through Molecular Layers*, J. Phys. Chem. B, 102, 3658 (1998).
20. Evans D., Nitzan A., Ratner M., *Photoinduced Electron-Transfer in mixed-valence compounds : Beyond the Golden-Rule Regime*, J. Chem. Phys., 108, 6387 (1998).
19. Emin, D. ; Evans, D.G. ; McCready, S.S., *Bipolaron formation in icosahedral and octahedral borides.*, Physica Status Solidi B, 205, 311 (1998).
18. R. Naaman, A. Kadyschevich, D. Evans and A. Nitzan, *Electron transmission through band structure in organized organic thin films.*, Chem. Phys. Lett., 268, 475, (1997).
17. I. Benjamin, D. Evans and A. Nitzan, *Asymmetric tunneling through ordered molecular layers*, J. Chem. Phys., 106, 1291 (1997).
16. I. Benjamin, D. Evans and A. Nitzan, *Electron tunneling through water layers: Effect of layer structure and thickness* , J. Chem. Phys., 106, 6647 (1997).
15. D.G. Evans and R.D. Coalson *Simulation of electron transfer in polar solvents: effects of nonequilibrium initial state preparation*, J. Chem. Phys., 104, 3598-3608, 1996.
14. D.G. Evans, R.D. Coalson and Yu. Dakhnovskii, *Induced oscillations in an electron transfer reaction in the presence of a bichromatic electromagnetic field*, J. Chem. Phys., 104, 2287-2296, (1996).
13. D.G. Evans, Yu. Dakhnovskii and R.D. Coalson, *Inducing coherent oscillations in the electron transfer dynamics of a strongly dissipative system with pulsed laser light*, Phys. Rev. Lett., 75, 3649-3652, (1995).
12. Yu. Dakhnovskii, D.G. Evans, H. Kim and R.D. Coalson, *The effect of a laser field on electron transfer in metal complexes : quantum degrees of freedom*, J. Chem. Phys., 103, 5461-5469, (1995).
11. D.G. Evans and R.D. Coalson, *Incorporating backflow into a relaxation theory treatment of the dynamics of nonequilibrium nonadiabatic transition processes*, J. Chem. Phys., 102, 5658-5668, (1995).
10. R.D. Coalson, D.G. Evans and A.Nitzan, *A non-equilibrium Golden rule formula for electronic state populations in nonadiabatically coupled systems*, J. Chem. Phys., 101, 436-448, (1994).
9. D.G. Evans and R.D. Coalson, *System-bath relaxation theory approach to nonadiabatic coupling effects on condensed phase electronic absorption spectra*, J. Chem. Phys., 100, 5605-5616, (1994).
8. D.G. Evans and R.D. Coalson, *Relaxation theory for curve crossing corrections to electronic absorption line shapes in condensed phases*, J. Chem. Phys., 99, 6264-6277, (1993).
7. D.G. Evans and R.D. Coalson, *Using relaxation theory to compute the electronic absorption spectrum of a chromophore coupled to a condensed phase environment* , J. Chem. Phys., 97, 5081-5097, (1992).
6. D.G. Evans and J.C.A. Boeyens, *The conformation of nine-membered rings*, Acta Cryst., B46, 524-532, (1990).
5. D.G. Evans and J.C.A. Boeyens, *Conformational analysis of ring pucker*, Acta Cryst., B45, 581-590, (1989).
4. J.C.A. Boeyens and D.G. Evans, *Group Theory of Ring Pucker*, Acta Cryst., B45, 577-581, (1989).

3. D.G. Evans, G.A. Yeo and T.A. Ford, *The boron trifluoride complex : a matrix isolation infrared spectroscopic and ab initio theoretical study*, Faraday Discuss. Chem. Soc., 86, 55-64, (1988).
2. D.G. Evans and J.C.A. Boeyens, *Mapping the conformation of eight-membered rings* , Acta Cryst., B44, 663-671, (1988).
1. J.C.A. Boeyens, L.Denner and D.G. Evans, *Crystallographic Study of Restricted Rotation in o-formanilides*, J. Cryst. & Spec. Res., 18, 175-187, (1988).

<u>Invited Oral Presentations</u> at Professional Meetings

28. Cottrell Scholar Conference, Tucson, July 8 2011, Transforming Science Education in PhD-Granting Institutions.
27. Simulations of Ion Dynamics through Ferritin Pores, D. Evans, 16 July 2010, Telluride Science Research Center Workshop on "Ions in Aqueous Solutions and Molecular Biology: Theory, simulation, modeling".
26. Co-organizer of the ACS symposium, *"Emergence of Function in Molecular Assemblies"*, ACS National meeting, Boston 2007
25. Modeling Electron Transfer in Mixed-valence compounds, Theoretical Chemistry at Pitt: Past, Present and Future, University of Pittsburgh, May 2007
24. *Electron Transfer in Mixed-valence Compounds: Effects of Strong Off-diagonal Vibronic Coupling*, 21 October 2006, ACS meeting, Houston, TX
23. *Exactly Solvable Condensed-phase Problems in Quantum Dynamics*, June 2006, ACS meeting, Reno, NV
22. *Exactly Solvable Condensed-phase Quantum Systems*, April 2006, Center for Advanced Studies, Department of Physics, UNM
21. *Non-Condon Effects in Electron Transfer and Molecular-scale Control*, 2005, Plenary Lecture, Workshop on Classical and Quantum Dynamical Simulations, The Max-Planck Institute, Dresden, Germany
20. *Exact Solutions for the non-Condon Problem*, 2005 Mesilla Theoretical Chemistry Workshop.
19. *Exact Solutions for Dissipative Dynamics,* ACS National Spring Meeting, Anaheim, March 2004.
18. *Energy Transfer in Molecular Arrays,* ACS National Spring Meeting, New Orleans, March 2003.
17. *Electron Dynamics in Dendritic Wires*, Invited Lecturer, U. Wyoming, School on Molecular Wires, August, 2002.
16. *Exciton dynamics in polymeric muscles*, Plenary Lecture, ACTC, PA, July 2002.
15. *Anharmonic effects on photo-induced electron dynamics*, ACS NORM meeting, Seattle WA, July 2001.
14. *Methods for Electron Transfer in solvated Dendrimers*: Plenary Lecture, Sanibel Conference, Florida, Feb. 2001.
13. *Multilevel Redfield Equations for electron transfer in Dendrimers*, Wyoming School on numerical methods in chemistry and biology, Laramie, July 2000.
12. *Visualization of physical chemistry concepts*: First Annual Meeting of the Research Corporation Cottrell Scholars, Tucson, Arizona, July 2000.
11. *Electron Transfer in Dendrimers*, Plenary Lecture, Sanibel Conference, Florida, February 2000.

10. *Electron transmission in thin films*, Southwest and Rocky Mountain Regional ACS meeting, 21 October 1999.
9. *Electron dynamics in dendrimers*, ACS National Meeting, New Orleans, August 1999.
8. *Electron Transfer in Mixed-Valence Systems*, Workshop on Mixed Valence compounds in chemistry and physics, Los Alamos National Laboratory, July 1999.
7. *Electron dynamics in dendrimers*, Workshop on quantum dynamics, Utah, March 1999.
6. *Electron Transmission Though self-assembled monolayers*, at the international symposium on `Electron transmission through Molecules and Molecular Interfaces', Maagan, Israel, December 1998.
5. *Electron hopping transport in high fields*, at the Annual Meeting of the International Society for Optical Engineering (SPIE), San Diego, July 1998.
4. *Photoinduced electron transfer*, Dallas, March 1998, Americal Chemical Society Meeting.
3. *Electron tranmission through Organic thin films*, Las Vegas, August 1997, Americal Chemical Society Meeting.
2. *Photoinduced Electron Transfer*, at Physics via High Performance Computing: Approaches and Tools, Albuquerque, May 1997.
1. *Tunneling and transmission in Thin Films*, Classical and Quantum Dynamics, Mesilla, NM, 9-12 February 1997.

Poster Presentations at Professional Meetings
12. V. Subramaniam and D. Evans, "Exciton Dynamics in Model Photosynthetic Antennae Systems", ACTC, July, 2002.
11. C. Kalyanaraman and D. Evans, ``Redfield Theory for molecular wires", ACS meeting, Chicago, August 2001.
10. G. Mallick, R. Pati, S. Karna and D.G. Evans, ``Ab initio Hartree-Fock calculations of electron transfer coupling elements in solution", Sanibel, 2001.
9. T.S. Elicker and D. Evans, ``Dendrimers as Molecular Wires'', at the Electron transport in polymers conference at Argonne National Laboratory, June 2000.
8. C. Kalyanaraman and D.G. Evans, ``Symplectic integrators for the multilevel Redfield Equation''. , Sanibel 2000.
7. First PURSUE Program Principal Investigators Conference, October 1999, ``Visualization of Quantum Chemical Processes as Teaching Tools'', D.G. Evans, J. Binette and M. Fleharty.
6. Ben Porter, D.G. Evans, ``Controlling electron transfer reactions in laser fields'', American Chemical Society National Meeting, March 1999.
5. D. Evans and R. Wampler, ``Electron transmission through thiol thin films'', Gordon conference on Electron Donor-Acceptor Interactions, Newport RI, August 1998.
4. D. Emin, S. McCready and D. Evans, *A novel type of bipolaron*, at the Annual Meeting of the International Society for Optical Engineering (SPIE), San Diego, July 1998.
3. D. Emin, S. McCready and D. Evans, Budapest August 1997; ``Bipolaron formation and transport'' at the International Conference on hopping and related phenomena''.
2. Nitzan A, Benjamin I, Evans D, Galperin M, `` Numerical Simulations of electron transmission through molecular layers'', American Chemical Society National Meeting, September 1997.
1. D. Evans and R.D. Coalson, ``Relaxation theory approach to condensed phase spectroscopy'', NATO meeting, Snowbird, 1992.

Invited Seminars at Scientific Institutions

17. Modeling Ferritin as a Synthetic Machine, South Florida University, in Fall 2009.
16. Electron Transfer in Mixed Valence Compounds, Michigan Tech, in Fall 2009.
15. *Electron Dynamics in polymeric systems,* Emory University, 10/2002.
14. *Exciton Dynamics in polymeric nanomuscles,* Georgia Tech, 10/2002.
13. *Solvation of Dendrimers ,* University of Rhode Island, 3/2002.
12. *Photoinduced electron transfer in dendrimers ,* University of California Irvine, 6/2002.
11. *Redfield Methods in Electron Transfer,* University of Oregon, 10/22/2001.
10. *Transport properties of dendrimers:* University of Cincinnati, OH, 11/20/2001.
9. *Transport properties of dendrimers*: Ohio State University, 11/19/2001.
8. *Transport and dynamics of dendrimers*: UCLA, 11/5/2001.
7. *Electron Transfer in Dendrimers*: University of Pittsburgh, Department of Chemistry, 3/2001
6. *Electron Transfer in Dendrimers*: Carnegie Mellon University, Department of Chemistry, 3/2001
5. *Path Integral calculations of electron transfer processes in condensed phases*, University of New Mexico, Physics Department, ``High Performance Computing Symposium", 5/1997.
4. *Computational and theoretical studies of electron transfer*, New Mexico State University, Las Cruces, 11/1997.
3. *Electron transmission in disordered layers*, Sandia National Laboratory, Albuquerque, 4/1997.
2. *Manipulation of electron transfer reactions*, Los Alamos National Laboratory, Los Alamos, 11/1997.
1. Northwestern University: *Electron transfer in mixed valence compounds*, 10/96.

Funding:

Current Funding:

Title: **Biocidal conjugated polyelectrolyte polymers and oligomers**
Agency: NSF, DMR Biomaterials Program
PI: Chi EY Co-PIs: Whitten DG, Evans D
Duration: 8/15/2012-7/31/2015
Amount: $390,000

Title: **Graduate Assistantships in Areas of National Need**
Agency: Department of Education
PI: Datye AK Co-PI: Evans D
Duration: 08/25/2012-08/24/2015
Amount: $660,000

Title: **Graduate Assistantships in Areas of National Need**
Agency: Department of Education
PI: Datye AK Co-PI: Evans D
Duration: 8/20/2009-8/19/2013
Amount: $525,000

Title: **Research Experience for Undergraduates in Nanoscience and Microsystems**
Agency: NSF, DMR 1005217
PI: Datye, AK Co-PI: Evans D
Duration: 04/15/2010-04/14/2013
Amount: $345,000

Previous Funding
15. Pittsburgh Supercomputing Center: Medium Allocation Research Grant, "Simulation of pore opening in ferritin", Computing Grant, 50K computing hours. D. Evans (PI), V. Subramaniam (coPI), extended to 2011
14. Center for Integrated Nanotechnologies (CINT): "Simulations of Ru nanoclusters for optical and photonic applications", Users Grant – 20K computing.
13. ACS Petroleum Research Fund, Deborah Evans (PI), $3500 – organizational funds for the symposium on "Emergence of Function in Molecular Assemblies", Feb. 2007.
12. UNM-LANL JSTL, D.G. Evans, PI and J. Brozik, co-PI, *An Integrated Experimental/Theoretical Approach for Understanding and Controlling Electronic Communication in Nanoscale Molecular Assemblies,* April 2006, 90K, no overhead.
11. ACS-PRF, D.G. Evans, PI and R. Watt, co-PI, *Synthesis and Simulation of Molecular Control in a Novel Class of Bionanoassemblies*, Aug. 2005, 80K for 2yrs
10. Membrane Bound Amphiphilic and Biamphiphilic Oligomers With Photo-initiated Electron and Energy Transfer Properties, J. Brozik, A. Shreve, and D. Evans: DOE, 2004-2008, $300000 total
9. Camille Dreyfus Teacher-Scholar Award, Deborah Evans PI, *Computational Methods for teaching and condensed phase electron transfer*, 2000-2005, Total $60 000.
8. Studies of Response to Pulsed RF fields, J. Tyo, E. Shamiloglu, C. Christodoulou (EE) and D. Evans (chemistry): DepScor , 2002-2004, $80000
7. Research Corporation Cottrell Scholar Award, Deborah Evans PI, *Electron and exciton dynamics in dendrimeric macromolecules* 2000-2004, Total $50 000.
6. NSF-CAREER award, *Electron dynamics in thin films and dendrimers* , Deborah Evans PI, 1999, Total $330 000.
5. ACS- Petroleum Research Fund AC-grant, D.G. Evans PI, *Quantum Mechanical Calculations of Electron Dynamics in Organic Macromolecules*, 2001-2003, Total $60 000.
4. Exxon-Mobil, D.G. Evans PI, *Simulation of kerogens*, 2000, Total $50 000.
3. Electron transport in organic macromolecules and carbides, Deborah Evans (PI), American Chemical Society - Petroleum Research Fund - type G grant, August 1998-August 2000), $20000 over 2 years (no indirect costs).
2. Electron Transport in Materials, by Deborah Evans (PI). Funded by Sandia National Laboratory, August 1997-July 1998. Total $35000 (Direct=$23 647; Indirect=$11353).
1. Electron Transport in Materials, by Deborah Evans (PI). Funded by Sandia National Laboratory, August 1996-July 1997. Total $35000 (Direct=$23 647; Indirect=$11353).

TEACHING
Research Teaching and Advisement
Post-doctoral Fellows
3. Vijaya Subramanian, June 2001-July 2004, Research Associate Professor Aug. 2006-present.
2. Chakrapani Kalyanaraman, August 1999-September 2002.
1. Irene Newhouse, May 1999-2002
Post-graduate Advisement [retraining Sandians program at UNM]
2. Eric Lundgren, Sandia/UNM retraining program, Spring 1998.
1. Allen Sault, Sandia/UNM retraining program, Summer 1998.

Ph.D. Advisement
6. Eric Hill, Simulations of Bio-active Polyelectrolytes and their Nano applications, Phd
5. Bea Yu: Path integral Calculations of Electron Transfer in Nanomaterials: MS (2007)

4. Tom Corbitt, Self-assembly of photo-active membranes and vesicles: theory and experiment Jan. 2003-
3. Bill Cook; Non-Condon Effects in Electron Transfer, graduated August 2005, PhD.
2. T. Sean Elicker; Quantum methods for transport in dendrimers. [awarded 2003]
1. G. Mallick; Simulation of dendrimers in solvent [graduated 03/2002, PhD].

M.S. Advisement
3. Mark Fleharty, Algorithms to model Dendritic Polymers, Fall 2010
2. C. Churchwell, Semi-group analysis of dissipative systems. Graduated in July 2001.
1. J. Mattila; Electron transmission in thin films. Graduated 12/98.

B.S. Advisement
18. Tye Martin, 2011-
17. Jeremiah Anderson, 2011-
16. Katie Schultz, 2009-2010
15. Page Stiers, 2009-2011
14. Monique Cordova, research 2007
13. Tiffany Allen, research 2006
12. Joshua Hewitt, Undergraduate Research, Summer 2005 – 2006
11. Mirvat Abdelhaq, Undergraduate Research, Summer 2005 – 2006
10. Bea Yu, undergraduate research, Summer 2003-Summer 2004
9. Eric Heatwole, undergraduate research, Summer 2001.
8. Ladonna Malone, undergraduate research, August 2000-Summer 2003.
7. Mandy Flores, undergraduate research, Fall 2000.
6. Kasey Hutt, undergraduate research, August 2000-March 2001.
5. Nouvelle Gebhart; Summer 1999-Summer 2000, Undergraduate Research Project. (simulation of polymeric materials).
4. Ben Porter; NSF/REU scholar, summer, 1998.
3. Undergraduate research program: R. Wampler - simulation of dendrimers and thin films.
2. R. Wampler; NSF/REU scholar, summer, 1997.
1. K. Patton and R. Ingam, NASA summer program for High School Seniors

Undergraduate Mentoring
Mark Fleharty, Jean-Sebastien Binette, Rob Wampler

Classroom Teaching

SEMESTER	COURSE	ICES rating (if available)
Spring, 1997	CHEM 501: Molecular structure	
Fall, 1997	CHEM 567: Supercomputing and quantum simulations	6.0
Spring 1998	CHEM 501 Molecular structure	6.0
Fall, 1998	CHEM 311 Undergraduate Physical Chemistry	6.0
Fall, 1999	CHEM 311 Undergraduate Physical Chemistry	5.7
Spring, 2000	CHEM 312 Undergraduate Physical Chemistry II	5.9
Fall, 2000	CHEM 311 Undergraduate Physical Chemistry	5.8
Spring, 2001	CHEM 312 Undergraduate Physical Chemistry II	5.8

Fall, 2001	CHEM 311 Undergraduate Physical Chemistry	5.9
Spring, 2002	CHEM 312 Undergraduate Physical Chemistry II	5.9
Fall, 2002	CHEM 121: Undergraduate Freshman Chemistry	5.8
Spring, 2003	CHEM 122: Undergraduate Freshman Chemistry II	5.9
Fall, 2003	CHEM 131: Honors Freshman Chemistry I	5.7
Spring 2004	CHEM 132: Honors Freshman Chemistry II	6.0
Fall, 2004	CHEM 131: Honors Freshman Chemistry I	5.9
Spring 2005	CHEM 132: Honors Freshman Chemistry II	6.0
Fall, 2005	CHEM 131: Honors Freshman Chemistry CHEM 315: Undergraduate BioPhysical Chemistry	5.4 5.7
Spring, 2006	CHEM 132: Honors Freshman Chemistry II	
Fall 2007	CHEM 315 Undergraduate Biophysical Chemistry	
Spring 2008	NSMS 510/CHEM471/PHYC410: Chemistry and Physics at the Nanoscale	
Fall 2008	CHEM 315 Undergraduate Biophysical Chemistry	
Spring 2009	CHEM471 Physical Chemistry at the Nanoscale	
Fall 2009	NSMS 595: Professional Development in NSMS	
Spring 2010	NSMS 510: Chemisty and Physics at the Nanoscale CHEM471: Physical Chemistry of Nanoscale Phenomena	
Fall 2010	NSMS 595: Professional Development in NSMS	
Spring 2011	NSMS 510: Chemisty and Physics at the Nanoscale CHEM471: Physical Chemistry of Nanoscale Phenomena	
Fall 2011	NSMS510: Chemistry and Physics at the Nanoscale	
Spring 2012	CHEM471: Physical Chemistry of Nanoscale Phenomena	
Fall 2012	NSMS510: Chemistry and Physics at the Nanoscale	

Curriculum Development

4. CHEM 471: Physical Chemistry of Nano Phenomena, upper division CHEM, ChNE elective
3. NSMS 510: new core course for the NSMS graduate degree program
2. ``Introduction to Quantum Dynamics"; a second quantum mechanics course for graduate students.
1. ``Visualization of Physical Chemistry Concepts": a suite of computational exercises for undergraduate Physical Chemistry Education: www.unm.edu/~pchem/CHEM311 and www.unm.edu/~pchem/CHEM312

Teaching Funding

6. Wolfram Research Grant Award - the Wolfram Technology in Education Grant (2006). $3000 in Mathematica Software.
5. Teaching Allocation Grant, 2003 ($2500). Used to purchase 10 copies of the Spartan software for the computer pod.
4. Small Equipment Grant, Intel Corporation, ten 866 MHz Pentium computers for undergraduate computer pod start-up.
3. Visualization of Physical Chemistry Concepts": Development of Undergraduate Teaching Tools, $ 4500 [01/01-01/03]. NASA Preparation for University Research of Students in Undergraduate Education Program.

2. ``Visualization of Physical Chemistry Concepts": Development of Undergraduate Teaching Tools, $10 000 [04/00-12/00]. NASA Preparation for University Research of Students in Undergraduate Education Program.
1. ``Visualization of Physical Chemistry Concepts": Development of Undergraduate Teaching Tools, $10 000 [05/99-03/00]. NASA Preparation for University Research of Students in Undergraduate Education Program.

SERVICE

Reviewing:
Peer Reviews:
Journal reviewer for: Chemical Physics Letters ; Journal of Chemical Physics ; Journal of Physical Chemistry and Chemical Physics.
Proposal reviewer for: Israel-US binational scientific Foundation (BSF). ; Research Corporation; NSF, ACS-PRF.
University Reviewing:
Internal UNM reviewer for the Dreyfus Foundation Awards (2003).
Internal UNM reviewer for the Provost Teacher of the Year Award.
Internal Reviewer for the Lane Scholarship awarded to the best incoming female freshman majoring in the science
Internal UNM reviewer for several NSF proposals in limited competitions
Internal reviewer for the UNM-SURP program
Local and National Committee Work:
Faculty Search Committees -: searches for positions in physical and educational chemistry.
Member of the "Scientific and Engineering Certificate" recruitment committee at UNM.
Member of the User Alliance board for the National Computational Science Alliance (NCSA).
July 2001: Search Committee member for the position of Chair, Department of Chemical and Nuclear Engineering at UNM.
Faculty Advisor for the ACS student chapter at UNM.
Department Seminar Program Coordinator.
Chair of the Student Awards Committee, Department of Chemistry
Chair of the Undergraduate Studies Committee, Department of Chemistry
The Faculty Undergraduate Advisor, Department of Chemistry
Chair, Faculty Search Committee for a Freshman Chemistry Coordinator
Member of the Freshman Chemistry Committee, Department of Chemistry.
Member of the College of Arts and Sciences Student Awards Committee, Spring 2004-present. (Selection of College Awards, including the Annual Lane Fellowship for the best incoming female freshman into the College)
Chair of the College of Arts and Sciences Scholarships and Awards Committee, March 2005-present
Member: Steering committee for the hpc@unm high-performance computing center on campus, chaired by Marc Ingber (2002-2004).
Member: Steering committee for the establishment of a graduate program in Nanotechnology, chaired by Rob Duncan and A. Datye
Member of the High Performance Computing Center Review Board

Ramesh Giri
University of New Mexico
Department of Chemistry and Chemical Biology, MSC03 2060
1 University of New Mexico, Albuquerque, NM 87131-0001
505-277-1070 (Office); rgiri@unm.edu

Professional Preparation

Tribhuvan University	Chemistry, Biology	B.Sc.	1995
Tribhuvan University	Chemistry	M.Sc.	1998
University of Cambridge	Bioorganic Chemistry	M.Phil.	2003
The Scripps Research Institute	Chemistry	Ph.D.	2009
University of Illinois, Urbana-Champaign	Transition metal catalysis	Postdoc	2009 – 2011
University of California, Berkeley	Transition metal catalysis	Postdoc	2011 – 2012

Appointments

2012-present	Assistant Professor, Department of Chemistry and Chemical Biology, University of New Mexico
2000-2002	Researcher, Research Center for Applied Science and Technology, Tribhuvan University
2000-2002	Assistant Lecturer, Trichandra College, Tribhuvan University

Honors and Awards

Graduate Student Symposium Award, The Scripps Research Institute, La Jolla	2007
Myron Rosenblum Endowed Fellowship, Brandeis University, Waltham	2006 – 2007
Outstanding Teaching Fellow Award, Brandeis University, Waltham	2007
Cambridge Overseas Trust Scholarship, University of Cambridge, UK	2002 – 2003
Nepal Academy of Science and Technology Research Grant, Nepal	1999

Publications

20. Giri, R.; Lan, Yu.; Liu, P.; Houk, K. N.; Yu, J.-Q., 2012. Understanding Reactivity and Stereoselectivity in Palladium-Catalyzed Diastereoselective sp^3 C–H Bond Activation: Intermediate Characterization and Computational Studies. *Journal of the American Chemical Society* 134, 14118-14126.

19. Giri, R.; Hartwig, J. F., 2010. Cu(I) Amido Complexes in the Ullmann Reaction. Reactions of Cu(I)-Amido Complexes with Iodoarenes with and without Autocatalysis by CuI. *Journal of the American Chemical Society* 132, 15860-15863.

18. Tye, J. W.; Weng, Z.; Giri, R.; Hartwig, J. F., 2010. Copper(I) Phenoxide Complexes in the Etherification of Aryl Halides. *Angewandte Chemie International Edition* 49, 2185-2189.

17. Giri, R.; Lam, J. K.; Yu, J.-Q., 2010. Synthetic Applications of Pd(II)-Catalyzed C–H Carboxylation and Mechanistic Insights: Expedient Routes to Anthranilic Acids, Oxazolinones, and Quinazolinones. *Journal of the American Chemical Society* 132, 686-693.

16. Chen, X.; Dobereiner, G.; Hao, X.-S.; Giri, R.; Maugel, N.; Yu, J.-Q., 2009. Cu(II)-Mediated Oxidative Dimerization of 2-Phenylpyridine Derivatives. *Tetrahedron* 65, 3085-3089.

15. Giri, R.; Shi, B.-F.; Engle, K. M.; Maugel, N.; Yu, J.-Q., 2009. Transition Metal-Catalyzed C–H Activation Reactions: Diastereoselectivity and Enantioselectivity. *Chemical Society Reviews* 38, 3242-3272.

14. Giri, R.; Yu, J.-Q., 2008. Synthesis of 1,2-and 1,3-Dicarboxylic Acids via Pd(II)-Catalyzed Carboxylation of Aryl and Vinyl C–H Bonds. *Journal of the American Chemical Society* 130, 14082-14083.

13. Giri, R.; Maugel, N.; Foxman, B. M.; Yu, J.-Q., 2008. Dehydrogenation of Alkyl Groups via Remote C–H Activation: Converting a Propyl Group into a π-Allylic Complex. *Organometallics* 27, 1667-1670.

12. Li, J.-J.; Giri, R.; Yu, J.-Q., 2008. Remote C–H Bond Functionalization Reveals the Distance-dependant Isotope Effect. *Tetrahedron* 64, 6979-6987.

11. Mei, T.-S.; Giri, R.; Maugel, N.; Yu, J.-Q., 2008. Pd(II)-Catalyzed mono-Selective *ortho*-Halogenation of Arene Carboxylic Acids Assisted by Counter Cations: An Orthogonal Method to Directed ortho-Lithiation. *Angewandte Chemie International Edition* 47, 5215-5219.

10. Wang, D.-H; Wasa, M.; Giri, R.; Yu, J.-Q., 2008. Pd(II)-catalyzed Cross-Coupling of sp^2 and sp^3 Boronic Acids Using Air as the Oxidant. *Journal of the American Chemical Society* 130, 7190-7191.

9. Giri, R.; Yu, J.-Q., 2008. Iodine Monoacetate. *Electronic Encyclopaedia of the Reagents for Organic Synthesis (eEROS)*. http://onlinelibrary.wiley.com/o/eros/articles/rn00915/frame.html.

8. Giri, R.; Maugel, N.; Li, J.-J.; Wang, D.-H; Breazzano, S. P.; Saunders, L. B.; Yu, J.-Q., 2007. Palladium-Catalyzed Methylation and Arylation of sp^2 and sp^3 C–H Bonds in Simple Carboxylic Acids. *Journal of the American Chemical Society* 129, 3510-3511.

7. Giri, R.; Wasa, M.; Breazzano, S. P.; Yu, J.-Q., 2006. Converting *gem*-Dimethyl Groups into Cyclopropanes via Pd-Catalyzed Sequential C–H Activation and Radical Cyclization. *Organic Letters* 8, 5685-5688.

6. Yu, J.-Q.; Giri, R.; Chen, X., 2006. σ-Chelation-directed C–H Functionalizations using Pd(II) and Cu(II) Catalysts: Regioselectivity, Stereoselectivity and Catalytic Turnover. *Organic & Biomolecular Chemistry* 4, 4041-4047.

5. Giri, R.; Chen, X.; Yu, J.-Q., 2005. Palladium-Catalyzed Asymmetric Iodination of Unactivated C–H Bonds under Mild Conditions. *Angewandte Chemie International Edition* 44, 2112-2115.

4. Giri, R.; Liang, J.; Lei, J.-G.; Li, J.-J.; Wang, D.-H.; Chen, X.; Naggar, I. C.; Guo, C.; Foxman, B. M.; Yu, J. Q., 2005. Palladium-Catalyzed Stereoselective Oxidation of Methyl Groups by Inexpensive Oxidants under Mild Conditions: a Dual Role for Carboxylic Anhydrides in Catalytic C–H Bond Oxidation. *Angewandte Chemie International Edition* 44, 7420-7424.

3. Giri, R.; Chen, X.; Hao, X.-H.; Li, J.-J.; Liang, J.; Fan, Z.-P.; Yu, J.-Q., 2005. Catalytic and Stereoselective Iodination of Prochiral C–H Bonds. *Tetrahedron: Asymmetry* 16, 3502-3505.

2. Li, Y.; Llewellyn, N. M.; Giri, R.; Huang, F.; Spencer, J. B., 2005. Biosynthesis of the Unique Amino Acid Side Chain of Butirosin: Possible Protective-Group Chemistry in an Acyl Carrier Protein-Mediated Pathway. *Chemistry & Biology* 12, 665-675.

1. Bajracharya, G. B.; Pokhrel, D.; Giri, R.; Tuladhar, S. M., 2000. Potentially Anti-carcinogenic Flavonoids in Vegetables, Fruits and Spices. *Nepal Journal of Science and Technology* 2, 17-26.

Scholarly and Professional Activities:

Editorial Service – Guest Editor, *Molecules*, special issue “Transition Metals Catalysis”, 2012.

Member – American Chemical Society, 2007-present.

College of Arts and Sciences
Curriculum Vitae

Name	**Department**	**Date**
John K. Grey	Chemistry and Chemical Biology	09/10/2012

Educational History:
Ph.D., October 2004, McGill University, Montreal, Quebec, Chemistry
B.Sc., November 1999, Michigan Technological University, Houghton, MI, Chemistry

Employment History
Assistant Professor (August 2007-present) Department of Chemistry and Chemical Biology, University of New Mexico

Postdoctoral Research Associate (July 2004–July 2007) Advisor: Paul F. Barbara. Department of Chemistry and Biochemistry, University of Texas, Austin. Topic: "*Single Molecule Spectroscopic Investigations of Energy Transfer in Conjugated Polymers*"

Graduate Research Assistant (January 2000–June 2004) Advisors: Christian Reber and Ian Butler. Department of Chemistry, McGill University. Topic: "*Vibronic Luminescence Properties of Tetragonal Transition Metal Complexes*"

Teaching Assistant (January 2000–May 2002) General and Analytical Chemistry. Department of Chemistry, McGill University.

(principal positions prior the Bachelor's degree)
Undergraduate Research Assistant (May–September 1999) Advisor: Bahne Cornilsen. Department of Chemistry, Michigan Technological University. Topic: "*Structural Studies of Layered Materials*"

Undergraduate Research Assistant (July–November 1998) Supervisor: Larry Stevens. Indium Corporation/ Department of Chemistry, Michigan Technological University. Topic: "*Removal of Trace Impurities from Post-Process Indium Metal*"

Corporal, United States Marine Corps (June 1990–June 1994) Communications Security (COMSEC) technician, Camp Pendleton, CA

Professional Recognition, Honors, etc.
CAREER award, National Science Foundation (2010)
Doctoral New Investigator award, Petroleum Research Fund, American Chemical Society (2009)
Ralph Powe Junior Faculty award, Oak Ridge Associated Universities (2008)
Alternative Energy Fellow Petroleum Research Fund, American Chemical Society (2004-2006)
Postdoctoral Fellowship – Natural Sciences and Engineering Research Council of Canada (2004, not tenured)

Postdoctoral Fellowship – Fonds de Recherche sur la Nature et les Technologies du Quebec (2004, not tenured)
Robert Zamboni Prize (research award) – McGill University (2003)
Udho, Parsini, Diwan Award (best graduate research paper), McGill University (2002)
Graduate Scholarship Natural Sciences and Engineering Research Council, Canada (2002-2004)
Graduate Scholarship - Fonds de Recherche sur la Nature et les Technologies, Québec (2002)
Departmental Scholar Award (Chemistry) - Michigan Technological University (1999)
Ted G. Rosza Scholarship - Michigan Technological University (1997–1999)

Short Narrative Description of Research, Teaching and Service Interests.

Research: ***The primary goal of my research is to elucidate and understand the structure-function relationships of conjugated polymer semiconductor molecules and functional forms.*** My independent research work primarily emphasizes next generation polymeric donor/acceptor (D/A) based solar cells, which can potentially deliver efficient, clean and relatively inexpensive electrical energy. However, the extreme morphological heterogeneity present in these D/A systems gives rise to large fluctuations in the rates of key photophysical processes (i.e., charge and energy transfer) over the nano- to micrometer distance scales. *We are particularly interested in understanding how structural and electronic interactions between polymer molecules (aggregation) and other molecules (D/A systems) vary with local morphology and their influence on material performance figures-of-merit (i.e., photocurrent production).*

My research relies on innovative *top-down* and *bottom-up* physical approaches designed to unravel molecular-level structure-function information entangled with material morphology. The following highlights three distinct, but interrelated, themes in support of this overall mission: ***i) understand the roles of morphology-dependent polymer aggregation properties on material performance in D/A thin film solar cell composites; ii) elucidate the dependence of electronic coupling on polymer conformation and packing in new nanoscale self-assembled polymer functional forms; iii) characterize excited state structural displacements of D/A interfacial charge transfer states and their dependence on molecular structural and electronic interactions***.

Teaching: The primary goal of my teaching is the integration of cutting-edge research themes and computer-based tools into the classroom with particular emphasis on context-rich examples with significant societal impact, such as energy. *Two broad educational goals that I am interested in addressing are,* ***i) undergraduate curriculum improvement in physical chemistry courses that traditionally have low interest amongst students; and ii) improving graduate student knowledge of state-of-the-art research and enhancing communication skills necessary to excel in interdisciplinary settings***. I have mainly relied on computer-based learning tools and cutting-edge research themes to provide context for clarifying complex physical concepts that often represent large hurdles for students. This effort primarily involves the use of MATLAB modules developed by my research group that re now being implemented in graduate and undergraduate courses. This integrated approach was a key objective of my NSF CAREER award and I plan to continue to merge cutting-edge research tools and topics into the classroom far beyond the duration of this award.

Service: I am currently participating in faculty recruitment, graduate student recruitment, and graduate curriculum committees, which I hope to continue in support of strengthening our graduate program. Outside of UNM, I have actively served as a reviewer for several top journals and national funding agencies. In addition, I have participated in national and regional conferences (as a symposium chair and speaker) as well as given numerous research seminars at top universities. I was also recently elected to the User Executive Committee at the nearby Center for Integrated Nanotechnologies (CINT) facility and to optimize access and functionality of these facilities. My relationship with CINT will then be leveraged to increase participation of UNM students at this state-of-the-art facility. I have also participated in local outreach activities involving K-12 students and will continue this in hopes of attracting students to pursue careers in science and engineering.

Scholarly Achievements:

Brief Synopsis of Accomplishments (please see expanded statement for full details)

UNM Independent Research Work (8 papers published, 3 submitted, 2 in preparation)

1) Combined Raman spectroscopic and electrical imaging of disordered polymeric solar cell materials. My group has pioneered combined resonance Raman spectroscopic and photocurrent imaging studies of disordered polymeric D/A solar cells. The apparatus was entirely homebuilt (including homemade software) and our approach permits detailed, in situ studies of molecular structure, composition and packing on size scales comparable to most scanned probe techniques that have already seen extensive use. *Importantly, polymer solar cells contain other moieties that can contribute to Raman signals often making it exceedingly difficult to disentangle the signal from the molecule of interest.* ***However, our approach offers a level of selectivity not readily attainable by any other physical technique that can easily discriminate between the material of interest by taking advantage of a strong resonance enhancement effect.*** Our initial results were published in the *Journal of the American Chemical Society* followed by several related articles. Additionally, my graduate student responsible for the development of this technique (Yongqian Gao) was recognized for his achievements at the Spring 2009 American Chemical Society National Meeting with a best poster presentation award and a travel award for the 2010 Electronic Processes in Organic Materials (EPOM) Gordon Research Conference.

2) Characterization of exciton coupling in aggregates of nanoscale polymer functional forms. Following our initial successes of using resonance Raman spectroscopic imaging probes, we embarked on studies of new self-assembled aggregated polymer forms, namely, polymer nanofibers. These systems offer tremendous promise over conventional polymer thin films by effectively managing the boundaries between ordered and disordered regions which is not currently possible in conventional processing approaches. Along with collaborators from University of California, Davis (Moulé group) and Temple University (Spano group), we demonstrated that coupling of optical excitations (excitons) of nanofibers can be tuned by simply inducing minor, but reversible, structural perturbations. Based on this work, we have recently constructed a high resolution, low temperature optical microscope capable of studying single nanofibers to better understand the apparent delicate interplay between structural order and exciton coupling within the aggregate. Additionally, we have entered into new collaborative efforts with the Park group at the University of Pennsylvania to encapsulate and grow superstructures of polymer nanofibers. This work has recently spawned two submitted papers with additional submissions in the near future.

3) Characterization of ground and excited state structures of D/A charge transfer complexes. Despite the influence of charge transfer states at molecular D/A interfaces on solar cell performance figures-of-merit (i.e., device open circuit voltage, V_{OC}), surprisingly little is understood about molecular-level structure interactions and displacements when charge is transferred between the D/A molecules. We recently brought our powerful resonance Raman spectroscopy and imaging techniques to bear on the study of charge transfer interactions and excited state structural displacements using a series polymer D/A charge transfer complexes with various electron acceptors of different redox properties and structure. Resonance Raman spectra of these systems produced an unprecedented level of detail where long and resolved progressions of overtone and combination bands were observed. These features are rarely, if ever, observed in Raman spectra of polymers and are especially sensitive to specific D/A structural and electronic interactions. *Moreover, overtone-combination bands permit a quantitative analysis of vibrational mode-specific excited state structural displacements, which have a profound influence on the rates of charge transfer, and therefore the performance attributes of solar cells*. Our results were published recently and we are currently expanding this work to perform multi-dimensional Raman overtone and photocurrent imaging which, when combined with photocurrent imaging in (1), can yield vast amounts of new and valuable information about the morphology dependence of vibrational displacements at D/A interfaces.

Postdoctoral Research Work (7 papers published)

1) Single molecule studies of energy transfer in conjugated polymers. The central focus of my postdoctoral research involved the elucidation and understanding of the relation between polymer conformational factors and excitation energy transfer efficiencies. The fact that bulk polymer systems – the most common functional form used in device applications – possess conformational and morphological heterogeneity makes the study of energy transfer difficult owing to the random orientations of chromophores. These issues can be circumvented by studying polymers at the single molecule level thus affording valuable pictures of the nascent morphology on energy transfer characteristics. Using a prototype polymer system with varying size (i.e. molecular weight), functional forms and medium polarity, we were able to show the prevalence of intra-chain contacts as low-energy traps at the bottom of a complex array of energy funnels within the molecules. *Importantly, this work provided unambiguous proof that bulk-like polymer photophysics originates at the single chain level due to chain folding characteristics in various media*.

2) Single molecule spectroelectrochemistry studies of ground and excited electronic states of polymers. The interaction of charges on polymer molecules with complicated conformational heterogeneity has remained a difficult area to probe owing to the complicated nature of interactions and relatively small signals on the sub-100 nm size scale. To help overcome these barriers, *I developed a new combined time-resolved single molecule and electrochemical imaging technique capable of interrogating both ground and excited state charge transfer processes in model device structures*. This approach was used to study excited state redox processes in single polymer molecules and nanoparticles which provided new insights into the role of polymer conformational heterogeneity on interfacial charge transfer processes in the electronically excited states. Because conjugated polymer molecules are highly sensitive to oxygen and water, I constructed a variant of this technique housed inside a nitrogen glovebox, which was the first of its kind and allowed the study of single particles in model devices without exposure to air leading to undesirable side reactions.

Graduate Research Work (9 papers published, 1 book chapter, 1 review)

1) Exploring electronic coupling between states by applied structural perturbations. Many important chemical and physical properties of molecules are dictated by the structural conformation of the molecule. My graduate thesis work involved the study of the interdependence between structural and light-emitting (optical) properties in a series of light emitting transition metal complexes. These systems exhibit strong electronic coupling interactions between electronic states that are highly tunable by inducing minor geometry changes. I developed a new emission spectroscopic imaging technique based on a diamond-anvil cell to apply high external pressures to materials at cryogenic temperatures (i.e., 5K) that allowed for detailed studies of variable electronic coupling effects. This approach offers a new means to study small changes in molecular geometry without the need for time-consuming chemical synthesis since high pressures can stabilize structures that would not normally exist under ambient conditions. This information can help materials scientists in the endeavor to use chemical structure and geometry to arrive at a particular desired outcome of physical properties.

2) Tuning fundamental excited state decay rates by applied pressures. Achieving high emission quantum yields in transition metal complexes is often plagued by efficient nonradiative processes that effectively dump the energy of the excited state before it can emit a photon. I developed a new time-resolved, pressure-dependent emission experiment that measured the kinetic competition between radiative and nonradiative excited state decay processes with varying molecular structure, which reveals an entirely new aspect of molecular photophysical properties not observed by conventional methods. Because the excited state is utilized in optoelectronic applications, e.g., to participate in charge and energy transfer, a detailed knowledge of molecular excited state properties as a function of molecular structure is especially useful in materials development. This research showed for the first time that the nonradiative rate constant could be tuned by orders of magnitude that resulted in a ~100-fold increase in the relative emission quantum yield.

Articles in Refereed Journals: (* corresponding author, † undergraduate student)

Martin, Thomas P.; Wise, Adam J.; Busby, Erik; Gao, Jian; Ford, Michael J.; Moulé, Adam J.; Larsen, Delmar; Grey, John K.* "*Packing-dependent exciton coupling in single poly(3-hexylthiophene) H- and J-aggregate nanofibers*" ***Journal of Physical Chemistry B*** *(Paul Barbara Festschrift*) (2012) *ASAP* DOI: 10.1021/jp308586k

Cativo, Ma. Helen M.; Kamps, Amanda C.; Gao, Jian; Grey, John K.; Hutchison, Geoffrey R.; Park, So-Jung *"Oxidation-induced photoluminescence of conjugated polymers"* ***Journal of Physical Chemistry B*** (2012) *ASAP* DOI: 10.1021/jp308638w

Gao, Jian; Kamps, Amanda C.; Park, So-Jung; Grey, John K.* *"Encapsulation of poly(3-hexylthiophene) J-aggregate nanofibers with an amphiphilic co-polymer"* ***Langmuir*** (2012) *28*, 16401-16407.

Wise, Adam J.; Grey, John K.* *"Resonance Raman studies of excited state displacements of conjugated polymer donor/acceptor charge transfer complexes"* ***Physical Chemistry Chemical Physics*** (2012) *14,* 11273-11276.

Niles, Edwards T.; Roehling, John D.; Yamagata, Hajime; Wise, Adam J.; Spano, Frank C.; Moule, Adam J.; Grey, John K.* "*J-Aggregate behavior in poly(3-hexylthiophene) nanofibers*" ***Journal of Physical Chemistry Letters*** (2012) *3*, 259-263.

Gao, Jian; Grey, John K.* "*Spectroscopic studies of energy transfer in fluorene co-polymer blend nanoparticles*" ***Chemical Physics Letters*** (2012) *522,* 86-91.

Wise, Adam J.; Precit, Mimi R.;† Papp, Alexandra M.;† Grey, John K.* "*Effect of fullerene intercalation on the conformation and packing of poly-(2-methoxy-5-(3'-7'-dimethyloctyloxy)-1,4-phenylenevinylene)*" ***ACS Applied Materials and Interfaces*** (2011) *3*, 3011–3019.

Wise, Adam J.; Martin, Thomas P;† Van Der Geest, Kori;† Grey, John K.* "*Observation of the missing mode effect in polyphenylenevinylenes: Effect of chain packing, conformation and morphology*" ***Journal of Chemical Physics*** (2010) *133*, 174901-174910.

Wakeland, Stephen; Martinez, Ricardo; Grey, John K., Luhrs, Claudia C. "*Production of graphene from graphite oxide using urea as expansion–reduction agent*" ***Carbon*** (2010) *48*, 3463-3470.

Gao, Yongqian; Martin, Thomas P.;† Thomas, Alan K.;† Niles, Edwards T.; Wise, Adam J.; Grey, John K.* *"Understanding Morphology-Dependent Polymer aggregation properties and Photocurrent Generation in Polythiophene/Fullerene Solar Cells of Variable Compositions"* ***Journal of Physical Chemistry C*** (2010) *114,* 15121-15128.

Gao, Yongqian; Martin, Thomas P.;† Thomas, Alan K.;† Grey, John K.* "*Resonance Raman spectroscopic- and photocurrent imaging of polythiophene/fullerene solar cells*" ***Journal of Physical Chemistry Letters*** (2010) *1*, 178-182.

Gao, Yongqian; Grey, John K.* "*Resonance chemical imaging of polythiophene/fullerene photovoltaic thin films: Mapping morphology-dependent aggregated and unaggregated C=C species*" ***Journal of the American Chemical Society*** (2009) *131*, 9654-9662.

<u>Postdoctoral Studies</u>

Palacios, Rodrigo E.; Chang, Wei-Shun; Grey, John K.; Chang, Ya-Lan; Miller, William L.; Lu, C-Y.; Henkelman, Graeme; Zepeda, Daniel; Ferraris, John P.; Barbara, Paul F. "*Detailed single-molecule spectroelectrochemical studies of the oxidation of conjugated polymers*" ***Journal of Physical Chemistry B*** (2009) *13*, 14619–14628.

Palacios, Rodrigo E.; Fan, Fu-Ren F.; Grey, John K.; Suk, Jungdon; Bard, Allen J.; Barbara, Paul F. "*Charging and discharging of single conjugated polymer nanoparticles*" ***Nature Materials*** (2007) *6*, 680-685.

Grey, John K.; Kim, Doo Young; Norris, Brent C.; Miller, William L.; Barbara, Paul F. "*Size-dependent spectroscopic properties of conjugated polymer nanoparticles*" ***Journal of Physical Chemistry B*** (2006) *110*, 25568-25572.

Grey, John K.; Kim, Doo Young; Donley, Carrie L.; Miller, William L.; Kim, Ji Seon; Silva, Carlos; Friend, Richard H.; Barbara, Paul F. *"Effect of temperature and chain length on the bimodal emission properties of single polyfluorene copolymer molecules"* ***Journal of Physical Chemistry B*** (Robert Silbey Festschrift) (2006) *110*, 18898-18903.

Kim, Doo Young; Grey, John K.; Barbara, Paul F. *"A detailed single molecule spectroscopy study of the vibronic states and energy transfer pathways of the conjugated polymer MEH-PPV"* ***Synthetic Metals*** (2006) *156*, 336-345.

Lee, Young Jong; Kim, Doo Young; Grey, John K.; Barbara, Paul F. *"Variable temperature single-molecule dynamics of MEH-PPV"* ***ChemPhysChem*** (2005) *6*, 2404-2409.

Grey, John K.; Kim, Doo Young; Lee, Young Jong; Gutierrez, Jose J.; Luong, Nam; Ferraris, John P.; Barbara, Paul F. *"Single-molecule studies of electronic energy transfer in a diblock conjugated polymer"* ***Angewandte Chemie, International Edition*** (2005) *44*, 6207-6210.

<u>Graduate studies</u>

Grey, John K.; Butler, Ian S.; Reber, Christian. *"Emitting-state displacements in ligand-centered vibrational modes in the trans-*$[OsO_2(NCS)_4]^{2-}$ *complex determined from near-infrared luminescence spectroscopy"* ***Inorganic Chemistry*** (2004) *43*, 5103-5111.

Grey, John K.; Butler, Ian S.; Reber, Christian. *"Temperature- and pressure-dependent luminescence spectroscopy on the trans-*$[ReO_2(pyridine)_4]^{+}$ *complex - analysis of vibronic structure, luminescence energies, and bonding characteristics"* ***Canadian Journal of Chemistry*** (2004) *82*, 1083-1091.

Grey, John K.; Butler, Ian S.; Reber, Christian. *"Pressure-induced enhancements of luminescence intensities and lifetimes correlated with emitting-state distortions for thiocyanate and selenocyanate complexes of platinum(II) and palladium(II)"* ***Inorganic Chemistry*** (2003) *42*, 6503-6518.

Cohen, Yair; Hatton, Benjamin; Miguez, Hernan; Coombs, Neil; Fournier-Bidoz, Sebastien; Grey, John K.; Beaulac, Remi; Reber, Christian; Ozin, Geoffrey A. *"Spin-on nanostructured silicon-silica film displaying room-temperature nanosecond lifetime photoluminescence"* ***Advanced Materials*** (2003) *15*, 572-576.

Grey, John K.; Marguerit, Melanie; Butler, Ian S.; Reber, Christian. *"Pressure-dependent Raman spectroscopy of metal-oxo multiple bonds in rhenium(V) and osmium(VI) complexes"* ***Chemical Physics Letters*** (2002) *366*, 361-367.

Grey, John K.; Butler, Ian S.; Reber, Christian. *"Effect of pressure on coupled electronic ground and excited states determined from luminescence spectra of trans-dioxorhenium(V) complexes"* ***Journal of the American Chemical Society*** (2002) *124*, 11699-11708.

Grey, John K.; Butler, Ian S.; Reber, Christian. *"Large pressure-induced increase in luminescence intensity for the* $[Pd(SCN)_4]^{2-}$ *complex"* ***Journal of the American Chemical***

Society (2002) *124*, 9384-9385.

Grey, John K.; Butler, Ian S. *"Effects of high external pressures on the electronic spectra of coordination compounds"* ***Coordination Chemistry Reviews*** (2001) *219-221*, 713-759.

Grey, John K.; Triest, Myriam; Butler, Ian S.; Reber, Christian. *"Effect of pressure on the vibronic luminescence spectrum of a trans-dioxo rhenium(V) complex"* ***Journal of Physical Chemistry A*** (2001) *105*, 6269-6272.

Triest, Myriam; Masson, Steve; Grey, John K.; Reber, Christian. *"Vibronic structure in the luminescence spectra of tetragonal d^2 and d^8 complexes analyzed by wavepacket dynamics on two-dimensional potential surfaces"* ***PhysChemComm*** (2000) *3*, Article No. 12.

Articles Appearing in Chapters in Edited Volumes:

Reber, Christian; Grey, John; Lanthier, Etienne; Frantzen, Kari. *"Pressure-induced change of d-d luminescence energies, vibronic structure and band intensities in transition metal complexes"* ***Comments on Inorganic Chemistry*** (2005) *26*, 233-254.

Works in Progress:

In preparation:

Wise, Adam J.; Gao, Yongqian; Martin, Thomas P.; Thomas, Alan K.; Grey, John K. *"Combined frequency-dependent photocurrent and resonance Raman spectroscopic mapping of polymer/fullerene solar cells"*

Wise, Adam J.; Martin, Thomas P.; Grey, John K. *"Single molecule spectroscopic studies of conformation-dependent emitting state displacements"*

Invited or Refereed Abstracts and/or Presentations at Professional Meetings: (2007-present) *symposium chair

Invited presentations

242nd ACS national meeting, Physical Chemistry Division (Paul Barbara memorial symposium) Denver, CO; August 22-26, 2011*

9th Annual Optical Probes of Conjugated Polymers and Organic Nanostructures, Santa Fe, NM; June 19-24 2011

National Synchotron Light Source Workshop "*Optical Studies of Solar Nanomaterials****" Center for Functional Nanostructures,*** Brookhaven National Laboratory, Upton, NY; May 23, 2011

User Workshop: Center for Integrated Nanotechnologies, Albuquerque, NM; August 10-11 2010*

SPIE, NanoScience and Engineering conference *"Physical Chemistry of Interfaces and Nanomaterials"*, San Diego, CA; August 5 2010

"Functional Nanomaterials: Bio helps Nano" ***Los Alamos National Laboratory***, April 26-28 2010

239th ACS National Meeting, Polymer and Materials Science and Engineering, San Francisco, CA, March 21-25, 2010*

237th ACS National Meeting, Physical Chemistry Division, Salt Lake City, UT, March 21-25, 2009

Transatlantic Frontiers of Chemistry, Cranage Hall, Cheshire, UK, July 31 - August 3 2008

Non-invited presentations

Electronic Processes in Organic Materials: Gordon Research Conference, Mount Holyoke College, July 28-Aug. 1, 2010

64th Northwest Regional Meeting of the American Chemical Society, Tacoma, WA, United States, June 28-July 1, 2009

Joint 63rd Northwest and 21st Rocky Mountain Regional Meeting of the American Chemical Society, Park City, UT, United States, June 15-18, 2008

Seminars:

Department of Chemistry and Biochemistry, University of North Carolina, Chapel Hill (to be given 10/2012)
Department of Physics, Université de Montréal, (to be given 10/2012)
Department of Chemistry, University of California, Riverside (to be given 11/2012)
Department of Chemistry, ***Emory University***, March 19 2012
Department of Chemistry, ***Michigan State University***, March 9 2012
Department of Chemistry and Biochemistry, ***Arizona State University***, Feb. 24 2012
Department of Chemistry, ***University of Massachusetts, Amherst***, Feb. 9 2012
Department of Chemistry, ***University of Pennsylvania***, Dec. 6 2011
National Renewable Energy Laboratory, Nov. 17 2011
Department of Chemistry, ***Rice University***, Oct. 26 2011
Department of Chemistry, ***Carnegie Mellon University***, Sept. 27 2011
Department of Chemistry, ***New Mexico State University***, March 17 2011
Los Alamos National Laboratory, Oct. 30 2010
Sandia National Laboratory, May 20 2010
Department of Chemistry, ***New Mexico Technological University***, March 18 2010
Department of Chemistry, ***Idaho State University***, April 2010
Department of Chemistry, ***Miami University***, Feb. 25 2010
Department of Chemistry, ***Temple University***, Feb. 4 2010

Department of Chemistry, ***University of Washington***, March 18 2009
Department of Chemistry, ***University of Central Florida***, Sept. 26 2008

Research Funding:

"CAREER: Understanding Structure-Function Relationships in Polymer Semiconductor Materials from Top-Down and Bottom-up Perspectives"
John Grey (PI)
National Science Foundation
Division of Chemistry and Materials Research
$575,000 (50.5% F&A)
03/01/10 - 03/01/15

"Controllable Adhesion, Detection, and Release of CBW Agents by Multifunctional "SMART" Nanoscale Surfaces"
John Grey (co-PI)
Defense Threat Reduction Agency
$1,500,000 (51% F&A)
09/01/11-09/01/14

"Spatial Mapping of Charge Mobilities in Polymer Solar Cells"
John Grey (PI)
University of New Mexico – Research Allocations Committee funds (large grant)
$7,500 (50% F&A)
12/01/09-09/01/10

"Uncovering and understanding morphology-dependent charge transport and trapping in polymer photovoltaic materials"
John Grey (PI)
ACS Petroleum Research Fund
$100,000 (0% F&A)
01/01/09 - 08/01/10

"Mapping Structure-Function Relationships in Molecular Photovoltaic Devices"
John Grey (PI)
Oak Ridge Associated Universities - Ralph E. Powe award
$10,000 (0% F&A)
05/01/08 - 05/01/09

"Resonance Raman Imaging of Charge Transfer in Polymer Donor/Acceptor Solar Cells"
John Grey
University of New Mexico – Research Allocations Committee funds
$4,000 (50% F&A)
12/01/07-08/31/08

Pending Research Funding:

"NUE: Ethics and Policy Implications of Nanotechnology"
John Grey (co-PI)
National Science Foundation

Teaching

Doctoral Advisement:

Yongqian Gao (Ph.D., Chemistry, 2011) Mapping aggregation properties and photocurrent generation efficiency in polymer solar cells ***(postdoctoral fellow, Los Alamos National Laboratory)***

Adam Wise (Ph.D., Chemical Engineering-NSMS, 2012) Molecular spectroscopic studies of conformation, packing and morphology in a prototypical conjugated polymer ***(postdoctoral fellow, University of Massachusetts, Amherst)***

Jian Gao (2008-present) Uncovering structure-function relationships in nanoscale conjugated polymer functional forms

Eric Martin (Chemical Engineering-NSMS; 2011-present) Resonance Raman studies of polymer charge transfer complexes

Edwards Niles (2008-present) New hybrid materials for solar cells and their spectroscopic properties

Alan Thomas (2011-present) Spectroscopic and electrical imaging of polymer/fullerene solar cells with charge transfer additives

Stephen Myers (01/08-05/08) *Nanoscience and Microsystems, IGERT rotation student*

Undergraduate Student Mentoring:

Kathleen Martin (06/12-present) undergraduate research, *Whaley fellow* (*undergraduate student, University of New Mexico*)

Jeffrey Parrish (06/11-08/11) NSMS REU student (*undergraduate student, University of Arizona*)

Jon Rabinowitz (01/11-08/11) undergraduate research, *Whaley fellow* (*B.S., University of New Mexico*)

Alexandra Papp (08/10-12/10) undergraduate research (*medical student, Uniformed Services Medical School*)

Mimi Precit (08/10-12/10) undergraduate research (*medical student, University of Washington, M.D.-Ph.D. program*)

Kori van Der Geest (06/10-08/10) NSMS REU student, (*undergraduate student, Pomona College*)

Alan Thomas (01/09-05/09) undergraduate research (*graduate student, University of New Mexico)*

Krista Anaya (01/09-05/09) undergraduate research (*B.S., University of New Mexico*)

Thomas Martin (06/08-08/12) visiting undergraduate student (*graduate student, University of Florida*)

Anh Ta Phuong (06/08-09/08) undergraduate research (*B.S., University of New Mexico*)

Jared Najjar (01/08-05/08) undergraduate research (*B.S., University of New Mexico*)

Classroom Teaching:

Fall 2007: *Characterization of Nanomaterials* (CH567) 5 students

Spring 2008: research semester
Fall 2008: *Characterization Methods of Nanostructured Materials* (CH567, NSMS/ChNE 512) 15 students
Spring 2009: *Instrumental Analysis* (CH351) 12 students
Fall 2009: *Characterization Methods of Nanostructured Materials* (CH471-567, ChNE 499, NSMS/ChNE 512) 55 students
Spring 2010: *Introduction to Physical Chemistry* (CH315) 95 students
Fall 2010: *Characterization Methods of Nanostructured Materials* (CH471-567, ChNE 499, NSMS/ChNE 512) 35 students
Spring 2011: *Physical Chemistry II* (CH312) 43 students
Fall 2011: *Characterization Methods of Nanostructured Materials* (CH471-567, ChNE 499, NSMS/ChNE 512) 30 students
Spring 2012: *Physical Chemistry II* (CH312) 39 students; *Introduction to Computational Simulations* (CH545) 8 students
Fall 2012: *Spectroscopy* (CH 471-545, ChNE 499-515, NSMS 595) 15 students

Curriculum Development or Teaching Administrative Positions:

CH351 Instrumental Analysis: Developed MATLAB computer data acquisition and processing routines for students. These routines replace Excel based analysis methods that expose students to cutting-edge scientific programming techniques; 06/2009-08/2009

CH545 Simulations: Developed MATLAB based time-dependent wavepacket simulation software for calculating electronic and Raman spectra. *These scripts are also used by my research group in accordance with my proposed integrated research and teaching plan*. 01/2012-05/2012

Service:

Member, User Executive Committee (2012-present)
Center for Integrated Nanotechnologies, Albuquerque, NM

Adjunct Faculty Member, Department of Chemical and Nuclear Engineering, University of New Mexico

Reviewing for journals
Journal of the American Chemical Society; The Journal of Physical Chemistry; Chemical Physics Letters; The Journal of Chemical Physics; Langmuir; ACS Nano; Materials Science and Engineering; Diamond; Synthetic Metals

Reviewing user proposals for DOE sponsored facilities
Center for Integrated Nanotechnologies (CINT), Los Alamos National Laboratory
Center for Functional Nanomaterials (CFN), Brookhaven National Laboratory

Reviewing proposals for funding agencies

National Science Foundation
Department of Energy
Petroleum Research Fund
University of Cyprus (internal funding)

Administrative work in Department, College, University committees
1) Graduate studies and recruitment committee
Fall 2007-present

2) Department seminar coordinator (01/2009-01/2012)

3) Graduate thesis committees
Fei Li (Chemistry)
Reed Weber (Physics)
Raid Haddad (Ph.D. Chemical Engineering)
Rosalba Rincon (Ph.D. Chemical Engineering)
Ron Slaby (Ph.D. Chemical Engineering)
David Kissel (Ph.D. Chemical Engineering)
Sireesha Chemburu (Ph.D. Chemical Engineering)
Anita Parmer (Ph.D. Physics)
Virginia Severns (M.S. Chemistry)
Amanda Heath (M.S. Chemistry)
Wei Jiang (Ph.D. Chemistry)

4) Faculty Advisor (2009-2010)
Graduate Student Association
UNM Chemistry and Chemical Biology

5) Faculty search committee
Jan.-April 2010; Jan.-April 2012

Community service, etc.
Faculty coach
Nanoscience and Micro-systems IGERT outreach program
Harry S. Truman middle school
09/2007

Lab tour for honors chemistry students
Sandia High School
04/2011-2012

CURRICULUM VITAE

PERSONAL DETAILS

NAME :	Hua GUO
DATE OF BIRTH :	20, August 1962
CITIZENSHIP:	USA
ADDRESS :	Department of Chemistry and Chemical Biology University of New Mexico, Albuquerque, NM 87131, USA
PHONE :	(505) 277 1716
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WWW:	http://www.unm.edu/~hguo

EDUCATION AND OCCUPATIONS

2010 – present	Professor of Physics and Astronomy
2001 – present	Professor of Chemistry
1998 - 2001	Associate Professor of Chemistry Department of Chemistry and Chemical Biology University of New Mexico, Albuquerque, NM 87131, USA
1995-1998	Associate Professor of Chemistry
1990-1995	Assistant Professor of Chemistry Department of Chemistry University of Toledo, Toledo, OH 43606, USA
1988—1990	Postdoctoral Fellow (with Prof. G. C. Schatz) Department of Chemistry Northwestern University, Evanston, IL 60208, USA
1985—1988	D. Phil. in Theoretical Chemistry (with Prof. J. N. Murrell, FRS) School of Chemistry and Molecular Sciences Sussex University, Brighton, Sussex, U.K.
1982—1985	M.Sc. in Theoretical Chemistry Department of Chemistry Sichuan University, Chengdu, China
1978—1982	B.Sc. in Chemistry Department of Basic Sciences, Chengdu Institute of Electronic Engineering, Chengdu, China

MEMBERSHIP

Member, American Physical Society (since 1990)

Member, American Chemical Society (since 1990)

AWARDS AND PROFESSIONAL EXPERIENCE

Overseas Research Student Award, Sussex University, U.K., 1986-1988

Visiting Research Student, University of Crete, Crete, Greece, 1988

Panelist, Department of Energy/Basic Energy Sciences Review Panel, 1992

Visiting Associate/Lecturer, California Institute of Technology, 1993

Dean's Merit Award, College of Arts and Sciences, University of Toledo, 1993

Dean's Merit Award, College of Arts and Sciences, University of Toledo, 1994

D. D. Raftopolous Award for Outstanding Research, Sigma Xi Society, University of Toledo, 1995

Session Chairman, SPIE conference, San Diego, 1995

Outstanding Faculty Research Award, University of Toledo, 1996

Dean's Merit Award, College of Arts and Sciences, University of Toledo, 1996

Session Chairman, DMC Conference, Gull Lake, Minnesota, 1997

Advisory board, Institute of Theoretical and Computational Chemistry, Nanjing University, China, since 2001

Editorial board, Journal of Theoretical and Computational Chemistry, since 2002

Symposium organizer, 225th national ACS meeting, New Orleans, 2003

Guest Editor, Special Issue of Journal of Theoretical and Computational Chemistry, 2003

Conference co-organizer, the 4th conference of worldwide young Chinese chemists, 2004

Member, National Institutes of Health Study Section, 2006

Member, advisory board of the Chinese American Chemistry Professor Association, since 2006

Advisory committee member, the 10th Chinese National Conference on Quantum Chemistry, 2008

Member, National Science Foundation panel on Theoretical and Computational Chemistry, 2008

Member, Department of Energy Panel on Theoretical and Computational Chemistry, 2009

Member, Department of Energy Panel on Early Career Awards, 2010

Member, Editorial Advisory Board, Theoretical Chemical Accounts, 2010-2012

50th Anniversary Editor, Theoretical Chemical Accounts, 2010.

Vice Chair, Conference on Dynamics of Molecular Collisions, Snow Bird, Utah, 2011

Organizer, International Workshop on Reactive Quantum Scattering, Santa Fe, 2011

Member, Department of Energy Review Panel, 2012

Organizer, Conference on Dynamics of Molecular Collisions, Granlibakken, 2013

GRANTS RECEIVED

1. National Science Foundation, 1991-1994, "Non-adiabatic Effects in Photodissociation Dynamics of Small Molecules"
2. American Chemical Society/Petroleum Research Fund, Type G, 1992-1994, "Quantum/Classical Hybrid Theory of Photoinduced Reaction Dynamics on Surfaces"
3. National Science Foundation, 1994-1997, "Theoretical Study of Photodissociation Dynamics in the Gaseous and Condensed Phases"
4. American Chemical Society/Petroleum Research Fund, Type AC, 1996-1998, "Multidimensional Dynamics of Photochemistry on Metal Surfaces"
5. National Science Foundation, 1997-2000, "Theoretical Studies of Spectroscopy and Dynamics of Molecular Systems"
6. American Chemical Society/Petroleum Research Fund, Type AC, 2000-2002, "Quantum Dynamics of Scattering and Desorption of Polyatomic Molecules from Solid Surfaces"
7. National Science Foundation, 2000-2003, "Theoretical Studies of Spectroscopy and Dynamics of Molecular Systems"
8. American Chemical Society/Petroleum Research Fund, Type SE, 2003, for ACS symposium titled "Recent advances in Iterative Methods and their Applications to Chemistry"
9. National Science Foundation, 2003-2006, "Collaborative Research of Proton Transfers in Enzymes: A Synergetic Theory-Experiment Approach"
10. National Science Foundation, 2004-2007, "Theoretical Studies of Spectroscopy and Dynamics of Molecular Systems"
11. National Science Foundation, 2004-2007, "Acquisition of a High Performance Shared-memory Computer Cluster for Computational Science and Engineering in the University of New Mexico"
12. Department of Energy, 2005-2008, "Wave Packet based Statistical Approaches to Complex-forming Reactions"
13. National Institutes of Health, 2006-2008, "Substrate Binding and Catalysis of Subclass B2 β-Lactamases"
14. Department of Energy, 2008-2011, "Quantum Dynamics of Elementary Chemical Reactions"
15. American Chemical Society/Petroleum Research Fund, 2009-2011, "Catalytic Mechanisms for Hydrogen Production by Methanol Steam Reforming"

16. National Institute of Health, 2009-2011, "Mechanism and Inhibition of Arginine Deiminase"
17. National Science Foundation, 2009-2012, "Dynamical Effects in Heterogeneous Catalytic Reactions"
18. National Institutes of Health (subcontract from Utah State), 2009-2011, "Mechanisms of Phosphoryl Transfer"
19. Defense Threat Reduction Agency (CoPI), 2010-2013, "Controllable adhesion, detection and release of CBW agents by multifunctional smart nanoscale surfaces"
20. National Science Foundation (CoPI), 2010-2013, "MRI: Acquisition of a GPU-Accelerated Parallel Supercomputer for Computational Science and Engineering Research at the University of New Mexico"
21. Defense Threat Reduction Agency (PI), 2011 – 2013, "Modeling Case-Enhanced Explosives with Coupled Chemistry and Hydrocodes"
22. Department of Energy (PI), 2011 – 2014, "Quantum Dynamics of Elementary Chemical Reactions"

PUBLICATIONS

1. **H. Guo**, A. M. Tian and G. S. Yan, J. Mole. Struct. (THEOCHEM) (Herzberg special issue), 34, 105 (1987). Non-empirical calculations of the spin-orbit constants for some diatomic molecules.

2. J. N. Murrell and **H. Guo**, J. Chem. Soc. Faraday II, 83, 683 (1987). Potential energy functions for the ground states of CO_2, CS_2 and OCS, and dynamical calculations on the reaction O + CS $\rightarrow$ S + CO.

3. L. J. Dunne, **H. Guo** and J. N. Murrell, Mole. Phys., 62, 283 (1987). The role of the *B-X* conical intersection in the photodissociation of water.

4. J. P. Braga, **H. Guo**, J. N. Murrell and L. J. Dunne, Mole. Phys., 65, 909 (1988). A comparative study of quantum mechanical and classical trajectory calculations for an A+BC collinear non-adiabatic collision.

5. **H. Guo** and J. N. Murrell, J. Chem. Soc. Faraday II, 84, 949 (1988). A classical trajectory study of the *A*-state photodissociation of the water molecule.

6. **H. Guo** and J. N. Murrell, Mole. Phys., 65, 821 (1988). Dynamics of the *A*-state photodissociation of H_2O at 193 nm.

7. **H. Guo**, D.Phil. Thesis, Sussex University, 1988. Classical trajectory studies on the dynamics of chemical reaction and photodissociation.

8. **H. Guo**, Mole. Phys., 68, 249 (1989). The B-state photodissociation of water, a classical trajectory study.

9. S. Zhu, H. Zhao, **H. Guo**, J. Zhang, J. Mol. Sci. 6, 86 (1990), Study on configuration of meso-tetra-substituted phenyl porphyrin by EHMO method and four circular X-ray diffraction on single crystal.

10. **H. Guo** and G. C. Schatz, J. Chem. Phys., 92, 1634 (1990). Non-adiabatic effects in photodissociation dynamics: a quantum mechanical study of ICN photodissociation in the *A* continuum.

11. **H. Guo** and G. C. Schatz, J. Chem. Phys., 93, 393 (1990). Time-dependent dynamics of methyl iodide photodissociation in the first continuum.

12. **H. Guo** and G. C. Schatz, J. Chem. Phys., 94, 379 (1991) A reduced dimension quantum wave packet study of photodissociation dynamics of diatomic molecules on surfaces.

13. **H. Guo** and G. C. Schatz, J. Phys. Chem., 95, 3091 (1991). Polarized resonance Raman spectrum as a probe of nonadiabatic transitions in photodissociation: a theoretical treatment.

14. **H. Guo**, K.-Q. Lao, G. C. Schatz and A. D. Hammerich, J. Chem. Phys., 94, 6562 (1991). Quantum nonadiabatic effects in the photodissociation of vibrationally excited CH_3I.

15. **H. Guo** and G. C. Schatz, Chem. Phys. Lett., 184, 245 (1991). A mechanism for the quenching of I* in photodissociation of methyl iodide adsorbed on a MgO surface.

16. **H. Guo**, Chem. Phys. Lett., 187, 360 (1991). A three-dimensional wavepacket study on photodissociation dynamics of methyl iodide.

17. **H. Guo**, J. Chem. Phys., 96, 2731 (1992). A wave-packet study on non-adiabatic transition dynamics in photodissociation: the importance of parent bending motion.

18. **H. Guo**, J. Chem. Phys., 96, 6629 (1992). Three-dimensional photodissociation dynamics of methyl iodide.

19. Z.-H. Huang and **H. Guo**, J. Chem. Phys., 96, 8564 (1992). Simulation of photodissociation dynamics of HBr adsorbed on a LiF (001) surface.

20. **H. Guo**, Chem. Phys. Lett., 193, 527 (1992). Femtosecond dynamics of a predissociative Rydberg state of methyl iodide.

21. Z.-H. Huang and **H. Guo**, J. Chem. Phys., 97, 2110 (1992). Dynamical simulations of the photodissociation of CH_3Br on a LiF (001) surface.

22. **H. Guo** and G. C. Schatz, J. Chem. Phys., 97, 7853 (1992). Comment on: Time-dependent Hartree approximation applied to the photodissociation of ICN.

23. Z.-H. Huang and **H. Guo**, J. Chem. Phys., 98, 3395 (1993). Theoretical modeling of photodissociation dynamics of CH_3I on LiF (001).

24. **H. Guo**, J. Phys. Chem., 97, 2602 (1993). Time-dependent quantum dynamical study of the photodissociation of HOCl.

25. Z.-H. Huang and **H. Guo**, Surf. Sci., 286, 182 (1993). A novel method for simulating atoms and molecules interacting with ionic surfaces.

26. Z.-H. Huang and **H. Guo**, J. Chem. Phys., 98, 7412 (1993). The orientation of adsorbed methyl halides on a LiF(001) surface: a Monte Carlo study.

27. **H. Guo**, J. Chem. Phys., 99, 1685 (1993). The effect of non-adiabatic coupling in the predissociation dynamics of IBr.

28. **H. Guo**, The Spectrum (BGSU Photochemical Center), 6, 9 (1993). Photodissociation of adsorbed molecules.

29. M. H. M. Janssen, M. Dantus, **H. Guo** and A. H. Zewail, Chem. Phys. Lett., 214, 281 (1993). Femtosecond reaction dynamics of Rydberg states: methyl iodide.

30. **H. Guo**, L. Liu and K.-Q. Lao, Chem. Phys. Lett., 218, 212 (1994). Non-perturbative time-dependent quantal dynamics of superexchange in electron transfer processes.

31. **H. Guo** and A. H. Zewail, Can. J. Chem. (Polanyi Special Issue), 72, 947 (1994). Femtosecond real-time probe of reactions. XIV. Rydberg states of methyl iodide.

32. J.-Y. Fang and **H. Guo**, J. Chem. Phys., 101, 1231 (1994). Exact quantum and time-dependent Hartree studies of the HBr/LiF(001) photodissociation dynamics.

33. J.-Y. Fang and **H. Guo**, J. Chem. Phys., 101, 5831 (1994). Multiconfiguration time-dependent Hartree studies on the CH_3I/MgO photodissociation dynamics.

34. J.-Y. Fang and **H. Guo**, J. Chem. Phys., 102, 1944 (1995). Multiconfiguration time-dependent Hartree studies of the Cl_2Ne vibrational predissociation dynamics.

35. L. Liu, J.-Y. Fang and **H. Guo**, J. Chem. Phys., 102, 2404 (1995). How many configurations are needed in a time-dependent Hartree treatment of the photodissociation of ICN ?

36. J.-Y. Fang and **H. Guo**, Chem. Phys. Lett., 235, 341 (1995). Four-dimensional quantum study of photodissociation of adsorbed CH_3I.

37. L. Liu and **H. Guo**, Chem. Phys. Lett., 237, 299 (1995). Quantum/classical hybrid dynamics of I_2(A) photodissociation and recombination dynamics in matrix Ar, linear chain model.

38. **H. Guo** and J. Setzler, Heterogeneous Chem. Rev. (invited), 2, 17 (1995). Photodissociation dynamics of adsorbed molecules on insulator surfaces.

39. **H. Guo**, Chem. Phys. Lett., 240, 393 (1995). Wave packet dynamics of photon and

electron-stimulated desorption of ammonia from surfaces.

40. T. Seideman and **H. Guo**, J. Chem. Phys., 103, 2745 (1995). Photodissociation of HCl^+/MgO(001): the static and dynamic effects of the surface.

41. J. V. Setzler, Z.-H. Huang and **H. Guo**, J. Chem. Phys., 103, 4300 (1995). Theoretical modeling of photodissociation dynamics of CH_3I on MgO(001)

42. J.-Y. Fang and **H. Guo**, J. Mole. Struct. (THEOCHEM) (Murrell special issue, invited), 341, 201 (1995). Quantum dynamics within the multiconfiguration time-dependent Hartree approximation.

43. **H. Guo** and T. Seideman, SPIE Proceedings, 2547, 411 (1995). Quantum and classical photodissociation of HCl^+ adsorbed on MgO(001).

44. L. Liu and **H. Guo**, J. Chem. Phys., 103, 7851 (1995). A linear chain hybrid quantum/classical model for the photodissociation and recombination of I_2(A) in rare gas matrices.

45. **H. Guo** and T. Seideman, J. Chem. Phys., 103, 9062 (1995). Quantum mechanical studies of photodesorption of ammonia from a metal surface: isotope effect, final state distributions and desorption mechanisms.

46. L. Liu and **H. Guo**, J. Chem. Phys., 104, 528 (1996). Validity of the hybrid quantum/classical approach in photodissociation/recombination of I_2 in rare gas matrices.

47. L. Liu and **H. Guo**, Chem. Phys. (Special Issue on Surface Dynamics), 205, 179, (1996). Theoretical study on vibrational excitation of ammonia scattered from Cu.

48. R. Chen and **H. Guo**, Chem. Phys. Lett., 252, 201 (1996). An accurate spectral method with arbitrarily large time step sizes.

49. L. Liu, **H. Guo** and T. Seideman, J. Chem. Phys., 104, 8757 (1996). A coherent transition model for photodesorption from metals: NH_3/Cu.

50. R. Chen and **H. Guo**, J. Chem. Phys., 105, 1311 (1996). A general and efficient filter-diagonalization method without time propagation.

51. R. Chen and **H. Guo,** J. Chem. Phys., 105, 3569 (1996). Evolution of quantum system in order domain of Chebychev operator.

52. R. Chen and **H. Guo**, Chem. Phys. Lett., 261, 605(1996). Extraction of resonances with Hermitian Hamiltonian: collinear $H + H_2$ scattering.

53. **H. Guo** and L. Liu, Int. J. Quantum Chem., Quantum Chem. Symp. 30, 267 (1996). Hybrid quantum/classical studies of photodissociation and recombination of I_2(A) in rare gas matrices: a linear chain model.

54. **H. Guo** and L. Liu, Surf. Sci., 372, 337 (1997). Perturbative treatments of photo-stimulated desorption and dissociation on metal surfaces induced by single and multiple electronic transitions.

55. **H. Guo**, J. Chem. Phys., 106, 1967 (1997). Two-dimensional wave packet studies of photon-stimulated desorption of NO from a metal surface induced by single and multiple electronic excitations.

56. J. V. Setzler, **H. Guo**, and G. C. Schatz, J. Phys. Chem., B101, 5352 (1997). Photo-initiated chemical reactions dynamics between aligned adsorbates on solid surfaces: A theoretical exploration of the H + CO_2 system on LiF(001).

57. R. Chen and **H. Guo**, Chem. Phys. Lett., 277, 191 (1997). Benchmark calculations of bound states of HO_2 via basic Lanczos algorithm.

58. R. Chen and **H. Guo**, J. Comput. Phys., 136, 494 (1997). Determination of eigenstates via Lanczos based forward substitution and filter-diagonalization.

59. T. Seideman and **H. Guo**, J. Chem. Phys., 107, 8627 (1997). Theory of desorption induced by electronic transitions II: The strong interaction regime.

60. R. Chen and **H. Guo**, Chem. Phys. Lett., 279, 252 (1997). Calculation of matrix elements in filter diagonalization: A generalized method based on Fourier transform.

61. J. Setzler, J. Bechtel, **H. Guo** and G. C. Schatz, J. Chem. Phys., 107, 9176 (1997). A further theoretical exploration of the surface-aligned photo-initiated H + CO_2 reaction: Surface motion and temperature dependence.

62. **H. Guo** and F. Chen, Faraday Discussions, 108, 309 (1997). Dynamics of substrate mediated photodesorption: The role of the excited state potential.

63. **H. Guo**, J. Chem. Phys., 108, 2466 (1998). A time-independent theory of photodissociation based on polynomial propagation.

64. R. Chen and **H. Guo** J. Chem. Phys., 108, 6068 (1998). Discrete energy representation and generalized propagation of physical systems.

65. F. Chen and **H. Guo**, Chem. Phys. Lett., 286, 205 (1998). Influence of the ground state potential on the rotational/translational correlation in photon-stimulated desorption of NO.

66. **H. Guo**, Chem. Phys. Lett, 289, 396 (1998), An efficient method to calculate resonance Raman amplitudes via polynomial propagation.

67. R. Chen and **H. Guo**, Phys. Rev. E, 57, 7288 (1998). Symmetry enhanced spectral analysis via spectral method and filter-diagonalization.

68. R. Chen, **H. Guo**, L. Liu, and J. T. Muckerman, J. Chem. Phys., 109, 7128 (1998). Symmetry-adapted filter-diagonalization: Calculation of the vibrational spectrum of

planar acetylene from correlation functions.

69. **H. Guo**, in 'Comparisons of Classical and Quantum Dynamics', Edited by W. L. Hase, JAI Press, 1998, (invited). Classical and quantum dynamical studies of photon-induced processes on solid surfaces.

70. R. Chen and **H. Guo**, J. Chem. Phys., 110, 2771 (1999). Extended symmetry-adapted discrete variable representation and accelerated evaluation of $\hat{H}\psi$.

71. **H. Guo** and T. Seideman, Phys. Chem. Chem. Phys., 1, 1265 (1999). Quantum mechanical study of photodissociation of oriented ClNO(S_1).

72. **H. Guo** and R. Chen, J. Chem. Phys., 110, 6626 (1999). Short-time Chebyshev propagator for the Liouville-von Neumann equation.

73. G. Ma, R. Chen, and **H. Guo**, J. Chem. Phys., 110, 8408 (1999). Quantum calculations of highly excited vibrational spectrum of sulfur dioxide. I. Eigenenergies and assignments up to 15000 cm^{-1}.

74. R. Chen and **H. Guo**, Comput. Phys. Comm., 119, 19 (1999). The Chebyshev propagator for quantum systems.

75. R. Chen and **H. Guo**, J. Chem. Phys., 111, 464 (1999). Efficient calculation of matrix elements in low storage filter diagonalization.

76. D. Xie and **H. Guo**, Chem. Phys. Lett., 307, 109 (1999). A refined potential energy surface and the absorption spectrum of OClO(A^2A_2).

77. R. Chen and **H. Guo**, Chem. Phys. Lett., 308, 123 (1999). A low-storage filter-diagonalization method to calculate expectation values of operators non-commutative with the Hamiltonian: vibrational assignment of HOCl

78. G. Ma and **H. Guo**, J. Chem. Phys., 111, 4032 (1999). Quantum calculations of highly excited vibrational spectrum of sulfur dioxide. II. Normal to local mode transition and quantum stochasticity.

79. R. Prosmiti, S. C. Farantos, and **H. Guo**, Chem. Phys. Lett., 311, 241 (1999). Assigning the transition from normal to local vibrational mode in SO_2 by periodic orbits.

80. **H. Guo**, P. Saalfrank, and T. Seideman, Prog. Surf. Sci. 62, 239 (1999) (invited). Theory of photoinduced surface reactions of admolecules.

81. R. Chen, **H. Guo**, S. Skokov, and J. M. Bowman, J. Chem. Phys., 111, 7290 (1999). Theoretical studies of rotation induced Fermi resonances in HOCl.

82. D. Xie, G. Ma, and **H. Guo**, J. Chem. Phys., 111, 7782 (1999). Quantum calculations of highly excited vibrational spectrum of sulfur dioxide. III. Emission spectra from the C^1B_2

state.

83. **H. Guo** and G. Ma, J. Chem. Phys., 111, 8595 (1999). Dissipative quantum dynamics in energy representation: photodesorption of NO from metals.

84. R. Chen and **H. Guo**, J. Chem. Phys., 111, 9944 (1999). A single Lanczos propagation method for calculating transition amplitudes

85. D. Xie, **H. Guo**, Y. Amatatsu, R. Kosloff, J. Phys. Chem., 104, 1009 (2000). Three-dimensional photodissociation dynamics of rotational state selected methyl iodide.

86. D. Xie and **H. Guo**, Surf. Sci. 447, 219 (2000). Dynamics of rare gas desorption from Pt(111) induced by photogenerated hot oxygen atoms.

87. G. Ma and **H. Guo**, Chem, Phys. Lett., 317, 315 (2000). Barrier crossing in a dissipative environment: a density matrix treatment of STM-induced atom transfer dynamics.

88. D. Xie, R. Chen, and **H. Guo**, J. Chem. Phys., 112, 5263 (2000). Comparison of Chebyshev, Faber, and Lanczos propagation-based methods for calculating resonances

89. B. Parsons, L. J. Butler, D. Xie, and **H. Guo**, Chem. Phys. Lett., 320, 499 (2000). A combined experimental and theoretical study of resonance emission spectra of $SO_2(C^1B_2)$.

90. R. Chen, G. Ma, and **H. Guo**, Chem. Phys. Lett., 320, 567 (2000). Full-dimensional quantum calculation of the vibrational energy levels of hydrogen peroxide (HOOH).

91. **H. Guo** and G. Ma, Surf. Sci., 451, 7 (2000). Effect of vibrational relaxation on DIET: A density matrix treatment.

92. D. Xie, **H. Guo**, and K. A. Peterson, J. Chem. Phys., 112, 8387 (2000). Accurate ab initio near-equilibrium potential energy and dipole moment functions of the ground electronic state of ozone.

93. D. Xie, **H. Guo**, O. Bludsky, and P. Nachtigall, Chem. Phys. Lett., 329, 503 (2000). Absorption and resonance emission spectra of SO_2 (X^1A_1/ C^1B_2) calculated from ab initio potential energy and transition dipole moment surfaces.

94. R. Chen and **H. Guo**, J. Chem. Phys., 114, 1467 (2001). A single Lanczos propagation method for calculating transition amplitudes II. Modified QL and symmetry adaptation.

95. G. Li and **H. Guo**, Chem. Phys. Lett., 336, 143 (2001). Doubling of Chebyshev correlation function for calculating resonances using low-storage filter-diagonalization.

96. R. Chen, G. Ma, and **H. Guo**, J. Chem. Phys., 114, 4763 (2001). Six-dimensional quantum calculations of highly excited vibrational energy levels of hydrogen peroxide and its deuterated isotopomers.

97. S. Li and **H. Guo**, J. Chem. Phys. 115, 3330 (2001). Corrugation induced rotational

excitation in photon/electron-induced desorption of ammonia: a three-dimensional quantum calculation.

98. D. Xu, D. Xie, and **H. Guo**, Chem. Phys. Lett. 345, 517 (2001). A new ab initio potential energy surface of HCN(1^1A”) and the predissociative resonances of HCN and DCN.

99. G. Li and **H. Guo**, Chem. Phys. Lett. 347, 443 (2001). Efficient calculation of collisional resonances using doubled Chebyshev autocorrelation functions.

100. G. Li and **H. Guo**, J. Mole. Spectrosc. 210, 90 (2001). Vibrational level spectrum of $H_2O(X^1A')$ on Partridge-Schwenke potential up to dissociation limit.

101. S. Li, G. Li, and **H. Guo**, J. Chem. Phys. 115, 9637 (2001). A single Lanczos propagation method for calculating transition amplitudes: III. S-matrix elements with a complex-symmetric Hamiltonian.

102. D. Xie, **H. Guo**, and K. A. Peterson, J. Chem. Phys. 115, 10404 (2001). Ab initio characterization of low-lying triplet potential energy surfaces and vibrational frequencies in the Wulf band of ozone.

103. **H. Guo**, J. Comp. Meth. Sci. and Eng., 1, 251 (2001), invited. Lanczos approach to molecular spectroscopy without explicit calculation of eigenfunctions.

104. C. Zhou, D. Xie, R. Chen, G. Yan, **H. Guo**, V. Tyng, and M. E. Kellman, Spectrochim Acta. (special issue) A58, 727 (2002), invited. Quantum calculation of highly excited vibrational energy levels of $CS_2(X)$ on a new empirical potential energy surface and semiclassical analysis of 1:2 Fermi resonance.

105. D. Xie, S. Li, and **H. Guo**, J. Chem. Phys., 116, 6391 (2002). Direct calculation of cumulative reaction probabilities from Chebyshev correlation functions.

106. D. Xu, D. Xie, and **H. Guo**, J. Chem. Phys., 116, 10626 (2002). Theoretical study of predissociation dynamics of HCN/DCN in their first absorption bands.

107. S. Li and **H. Guo**, J. Chem. Phys., 117, 4499 (2002). Monte Carlo wave packet study of negative ion mediated vibrationally inelastic scattering of NO from metal surface.

108. **H. Guo**, R. Chen, and D. Xie, J. Theo. Comp. Chem., 1, 173 (2002). Calculation of transition amplitudes with a single Lanczos propagation

109. S. Y. Lin and **H. Guo**, J. Chem. Phys., 117, 5183 (2002). Full-dimensional quantum wave packet study of rotationally inelastic transitions in $H_2 + H_2$ collision.

110. D. Xu, D. Xie, and **H. Guo**, J. Phys. Chem., A106, 10174 (2002). Predissociation of HCN/DCN in two lowest-lying singlet excited states: Effect of Fermi resonances on spectra and dynamics.

111. D. Xu, G. Li, D. Xie, and **H. Guo**, Chem. Phys. Lett., 365, 480 (2002). Full-dimensional

quantum calculations of vibrational energy levels of acetylene (HCCH) up to 13000 cm^{-1}.

112. R. Chen and **H. Guo**, Chem. Phys. Lett., 369, 650 (2003). Effect of spectral range on the convergence in Lanczos algorithm, a numerical study.

113. S. Y. Lin and **H. Guo**, Chem. Phys., 289, 191 (2003). Full-dimensional quantum wave packet study of collision-induced vibrational relaxation between *para*-H_2.

114. D. Xu, R. Chen, and **H. Guo**, J. Chem. Phys., 118, 7273 (2003). Probing highly excited vibrational states of acetylene using a modified single Lanczos propagation method.

115. D. Xu, **H. Guo**, S. Zou and J. M. Bowman, Chem. Phys. Lett., 377, 582 (2003), A scaled ab initio potential energy surface for acetylene and vinylidene.

116. R. Chen and **H. Guo**, J. Chem. Phys., 119, 5762 (2003), On the convergence scaling laws of Lanczos and Chebyshev recursion methods.

117. S. Y. Lin and **H. Guo**, J. Chem. Phys., 119, 5876 (2003), Exact quantum mechanical calculation of rovibrational energy levels of hydrogen peroxide (HOOH).

118. S. Y. Lin and **H. Guo**, J. Phys. Chem. A (invited article in the Kouri Festschrift), 107, 7197 (2003). Full-dimensional quantum wave packet studies of collisional vibrational relaxation of both *p*- and *o*-H_2.

119. D. Xu, D. Xie, and **H. Guo**, J. Theo. Comp. Chem., (Special Issue on Iterative Methods) 2, 639 (2003). Theoretical studies of $\tilde{A}^1A'' \rightarrow \tilde{X}^1A'$ resonance emission spectra of HCN/DCN using single Lanczos propagation method.

120. S. Y. Lin and **H. Guo**, J. Chem. Phys., 119, 11602 (2003), Quantum wave packet study of reactive and inelastic scattering between $C(^1D)$ and H_2.

121. S. Y. Lin and **H. Guo**, Chem. Phys. Lett, 385, 193 (2004), Quantum integral cross-section and rate constant of the $O(^1D) + H_2 \rightarrow OH + H$ reaction on a new potential energy surface.

122. H. Li, D. Xie, and **H. Guo**, J. Chem. Phys., 120, 4273 (2004), An ab initio potential energy surface and predissociative resonances of HArF.

123. S. Y. Lin and **H. Guo**, J. Phys. Chem. A108, 2141 (2004), Quantum wave packet studies of the $C(^1D) + H_2 \rightarrow CH + H$ reaction: integral cross-section and rate constant.

124. D. Xu, **H. Guo**, J. Gao, and Q. Cui, Chem. Comm., 891 (2004), A QM/MM study of nucleophilic aromatic substitution reaction catalyzed by 4-chlorobenzoyl-CoA dehalogenase.

125. S. Y. Lin and **H. Guo**, J. Chem. Phys., 120, 9907 (2004), A wave packet based statistical approach to complex-forming reactions.

126. S. Y. Lin and **H. Guo**, J. Chem. Phys., 121, 1285 (2004), Reactions of $C(^1D)$ with H_2 and

its deuterated isotopomers, a wave packet study.

127. **H. Guo**, Chebyshev propagation and applications to scattering problems, in Theory of Chemical Reaction Dynamics, edited by A. Lagana and G. Lendvay, Kluwer, 2004, Dordrecht.

128. H. Li, D. Xie, and **H. Guo**, J. Chem. Phys., 121, 4156 (2004), An ab initio potential energy surface and vibrational states of $MgH_2(1^1A')$.

129. L. Yang, W. Feng, K. Yamato, A. R. Sanford, D. Xu, **H. Guo**, B. Gong, J. Am. Chem. Soc. 126, 11120 (2004), Highly efficient, one-step macrocyclizations assisted by the folding and preorganization of precursor oligomers.

130. D. Xu, Y. Wei, J. Wu, D. Dunaway-Mariano, **H. Guo**, Q. Cui, and J. Gao, J. Am. Chem. Soc., 126, 13649 (2004), QM/MM studies of enzyme-catalyzed dechlorination of 4-chlorobenzoyl-CoA provide insight into reaction energetics.

131. S. Y. Lin, **H. Guo**, J. Phys. Chem., A108, 10066 (2004), Case study of a prototypical elementary insertion reaction: $C(^1D) + H_2 \rightarrow CH + H$.

132. S. C. Farantos, S. Y. Lin and **H. Guo**, Chem. Phys. Lett., 399, 260 (2004), A regular isomerization path among chaotic vibrational states of $CH_2(a^1A_1)$.

133. S. Y. Lin and **H. Guo**, J. Chem. Phys., 122, 074304 (2005), Quantum statistical and wave packet studies of insertion reactions of $S(^1D)$ with H_2, HD and D_2.

134. D. Xie, D. Xu, L. Zhang, and **H. Guo**, J. Phys. Chem., B109, 5259 (2005), Theoretical studies of general base-catalyzed hydrolysis of aryl esters and implications for enzymatic reactions.

135. S. Y. Lin and **H. Guo** and S. C. Farantos, J. Chem. Phys., 122, 124308 (2005), Resonances of $CH_2(a^1A_1)$ and their roles in unimolecular and bimolecular reactions.

136. H. Li, D. Xie, and **H. Guo**, J. Chem. Phys., 122, 144314 (2005), A reliable ab initio potential energy surface and vibrational states for the ground electronic state of $HgH_2(1^1\Sigma^+_g)$.

137. D. Xie, Y. Zhou, D. Xu, and **H. Guo**, Org. Lett., 7, 2093 (2005), Solvent effect on concertedness of transition state for hydrolysis of *p*-nitrophenyl acetate.

138. C. Xu, D. Xie, D. H. Zhang, S. Y. Lin, and **H. Guo**, J. Chem. Phys., 122, 244305 (2005), A new *ab initio* potential energy surface of $HO_2(X^2A'')$ and quantum studies of HO_2 vibrational spectrum and rate constants for the $H + O_2 \leftrightarrow O + OH$ reactions.

139. J. Wang, H. Li, Y. Mei, B. Lou, D. Xu, D. Xie, **H. Guo**, and W. Wang, J. Org. Chem., 70, 5678 (2005) Direct, facile L-prolinamide and pyrrolidine sulfonamide organocatalyst promoted aldehyde and ketone-selenenylation reactions.

140. D. Xu, **H. Guo**, Y. Liu, and D. M. York, J. Phys. Chem., B109, 13827 (2005), Theoretical studies of dissociative phosphoryl transfer in interconversion of phosphoenolpyruvate to phosphonopyruvate: solvent effects, thio effects, and implications for enzymatic reactions.

141. S. Li, D. Xie, B. Gong, and **H. Guo**, Chem. Phys. Lett., 410, 264 (2005), Stability of a new class of unnatural hydrogen-bonded molecular duplexes: a computational study.

142. D. Xu and **H. Guo**, FEBS Lett., 579, 4249 (2005), Electrostatic influence of active-site waters on the nucleophilic aromatic substitution catalyzed by 4-chlorobenzoyl-CoA dehalogenase.

143. Z. Zhao, E. Duesler, C. Wang, **H. Guo**, P. S. Mariano, J. Org. Chem., 70, 8508 (2005), Photocyclization reactions of cyclohexa- and cyclopenta-fused pyridinium salts. Factors governing regioselectivity.

144. D. Xu, Y. Zhou, D. Xie, and **H. Guo**, J. Med. Chem., 48, 6679 (2005), Antibiotic binding to monozinc CphA β-lactamase from *Aeromonas hydrophila*: quantum mechanical/molecular mechanical and density functional theory studies.

145. L. Zhang, D. Xie, D. Xu, **H. Guo**, J. Phys. Chem., A109 11295 (2005), Reactivity of metaphosphate and thiometaphosphate in water: a DFT study.

146. J. Wu, D. Xu, X. Lu, C. Wang, **H. Guo** and D. Dunaway-Mariano, Biochem, 45, 102 (2006), Contributions of long-range electrostatic interactions to 4-chlorobenzoyl-CoA dehalogenase catalysis: A combined theoretical and experimental study.

147. S. Y. Lin, and **H. Guo**, J. Chem. Phys.,124, 031101 (2006). Exact quantum dynamics of $N(^2D) + H_2 \rightarrow NH + H$ reaction: Cross-sections, rate constants, and dependence on reactant rotation.

148. X. Lu, L. Li, X. Feng, Z. Li, H. Yang, C. Wang, **H. Guo**, A. Galkin, O. Herzberg, P. S. Mariano, B. M. Martin and D. Dunaway-Mariano, Biochem., 45, 1162-1172 (2006) Kinetic analysis of *Pseudomonas aeruginosa* arginine deiminase mutants and alternate substrates provides insight into structural determinants of function.

149. S. Y. Lin, E. J. Rackham, and **H. Guo**, J. Phys. Chem. (invited article in the Hase Festschrift), 110, 1534 (2006), Quantum mechanical rate constants for $H + O_2 \leftrightarrow O + OH$ and $H + O_2 \rightarrow HO_2$ reactions.

150. D. Xu, D. Xie, and **H. Guo**, J. Biol. Chem., 281, 8740 (2006). Catalytic mechanism of class B2 β-lactamase.

151. D. Riccardi, P. Schaefer, Y. Yang, H. Yu, N. Ghosh, X. Prat-Resina, P. König, G. Li, D. Xu, **H. Guo**, M. Elstner and Q. Cui, J. Phys. Chem., B110, 6458 (2006), (feature article and cover) Development of effective quantum mechanical/molecular mechanical (QM/MM) methods for complex biological processes.

152. S. Y. Lin and **H. Guo**, J. Phys. Chem. (invited article in the Light Festschrift), A110, 5305

(2006), Quantum statistical study of O + O_2 isotopic exchange reactions: Cross sections and rate constants.

153. J. Wang, H. Li, B. Lou, L. Zu, **H. Guo**, and W. Wang, Chem. Eur. J., 12, 4321 (2006). Enantio- and diastereoselective Michael addition reactions of unmodified aldehydes and ketones with nitroolefins catalyzed by a pyrrolidine sulfonamide.

154. S. Y. Lin and **H. Guo**, Phys. Rev. A, 74, 022703 (2006). Quantum state-to-state cross sections for atom-diatom reactions, A Chebyshev real wave packet approach.

155. S. Y. Lin, D. Xie, and **H. Guo**, J. Chem. Phys., 125, 091103 (2006). Revelation of non-statistical behavior in HO_2 vibration by a new *ab initio* potential energy surface.

156. S. Y. Lin, **H. Guo**, P. Honvault, D. Xie, J. Phys. Chem. B, 110, 23641 (2006), Quantum dynamics of the H + $O_2 \rightarrow$ O + OH reaction on an accurate *ab initio* potential energy surface.

157. D. Xie, C. Xu, T.-S. Ho, H. Rabitz, G. Lendvay, S. Y. Lin, and **H. Guo**, J. Chem. Phys., 126, 074315 (2007), Global analytical potential energy surfaces for $HO_2(\tilde{X}^2A'')$ based on high level *ab initio* calculations.

158. A. Van Wyngarden, K. Mar, K. Boering, J. J. Lin, Y. T. Lee, S. Y. Lin, **H. Guo**, G. Lendvay, J. Am. Chem. Soc., 129, 2866 (2007). Non-statistical behavior of reactive scattering in the $^{18}O + {}^{32}O_2$ isotope exchange reaction.

159. C. Wang, D. Xu, L. Zhang, D. Xie, and **H. Guo**, J. Phys. Chem. B, 111, 3267 (2007), Molecular dynamics and density functional studies of substrate binding and catalysis of arginine deiminase.

160. S. Y. Lin, L. Banares, and **H. Guo**, J. Phys. Chem. A, 111, 2376 (2007), Differential and integral cross sections of the $N(^2D) + H_2 \rightarrow$ NH + H reaction from exact quantum and quasi-classical trajectory calculations.

161. L. Zhang, D. Xie, D. Xu, and **H. Guo**, Chem. Comm., 1638 (2007), Supermolecular density functional calculations suggest a key role for solvent in alkaline hydrolysis of *p*-nitrophenyl phosphate.

162. H. Ran, D. Xie, and **H. Guo**, Chem. Phys. Lett., 439, 280 (2007). Theoretical studies of C^1B_2 absorption spectra of SO_2 isotopomers.

163. P. Honvault, S. Y. Lin, D. Xie, and **H. Guo**, J. Phys. Chem. A, 111, 5349 (2007), Differential and integral cross sections for the H + $O_2 \rightarrow$ HO + O combustion reaction.

164. D. Xu, **H. Guo,** and Q. Cui, J. Phys. Chem. A, (special issue on SCC-DFTB), 111, 5630 (2007), Antibiotic binding to dizinc β-lactamase L1 from *Stenotrophomonas maltophilia*: SCC-DFTB/CHARMM and DFT studies.

165. C. Xu, D. Xie, P. Honvault, S. Y. Lin, and **H. Guo**, J. Chem. Phys., 127, 024304 (2007),

Rate constant for $OH(^2\Pi) + O(^3P) \rightarrow H(^2S) + O_2(^3\Sigma_g^-)$ reaction on an improved *ab initio* potential energy surface and implications for the interstellar oxygen problem.

166. C. Wang and **H. Guo**, J. Phys. Chem. B., 111, 9986 (2007). Inhibitor binding by metallo-β-lactamase IMP-1 from *Pseudomonas aeruginosa*: Quantum mechanical/ molecular mechanical simulations.

167. D. Xu, **H. Guo**, Q. Cui, J. Am. Chem. Soc., 129, 10814 (2007), Antibiotic deactivation by dizinc β-lactamase: Mechanistic insights from QM/MM and DFT studies.

168. C. Xu, B. Jiang, D. Xie, S. C. Farantos, S. Y. Lin, and **H. Guo**, J. Phys. Chem. A (invited article in the Wyatt Festschrift), 111, 10353 (2007), Analysis of the HO_2 vibrational spectrum on an accurate ab initio potential energy surface.

169. **H. Guo**, Rev. Comput. Chem., 25, 285 (2007), Recursive solutions to large eigenproblems in molecular spectroscopy and reaction dynamics.

170. S. Y. Lin, **H. Guo**, P. Honvault, C. Xu, and D. Xie, J. Chem. Phys., 128, 014303 (2008), Accurate quantum mechanical calculations of differential and integral cross sections and rate constant for the O + OH reaction using an *ab initio* potential energy surface.

171. S. Y. Lin, Z. Sun, **H. Guo**, D. H. Zhang, P. Honvault, D. Xie, and S.-Y. Lee, J. Phys. Chem. A., 112, 602 (2008), Fully Coriolis coupled quantum studies of the $H + O_2$ (υ_i=0-2, j_i=0,1) → OH + O reaction on an accurate potential energy surface: integral cross sections and rate constants.

172. S. Y. Lin, **H. Guo**, P. Honvault, Chem. Phys. Lett., 453, 140 (2008), Quantum dynamics of $C(^3P) + OH(^2\Pi) \rightarrow H(^2S) + CO(X^1\Sigma^+)$ reaction.

173. D. Riccardi, P. Konig, **H. Guo**, and Q. Cui, Biochem., 47, 2369 (2008), Proton transfer in carbonic anhydrase is controlled by electrostatics rather than the orientation of the acceptor.

174. D. Xu and **H. Guo**, J. Phys. Chem. B., 112, 4102 (2008), Ab initio QM/MM studies of phosphoryl transfer reaction catalyzed by PEP mutase suggest a dissociative metaphosphate transition state.

175. S. Zhou, D. Xie, D. Xu, **H. Guo**, R. W. Field, Chem. Phys. Lett., 455, 145 (2008), Theoretical emission spectra of HNC($\tilde{A}^1A''$) on a new ab initio potential energy surface.

176. L. Li, Z. Li, C. Wang, D. Xu, P. S. Mariano, **H. Guo**, and D. Dunaway-Mariano, Biochem., 47, 4721 (2008), The electrostatic driving force for nucleophilic catalysis in L-arginine deiminase: A combined experimental and theoretical study.

177. G. Lendvay, D. Xie, and **H. Guo**, Chem. Phys., 349, 181 (2008) (Special issue on electron correlation and molecular dynamics for excited state and photochemistry in honor of Hans Lischka), Mechanistic insights into the $H + O_2 \rightarrow OH + O$ reaction from quasi-classical

trajectory studies on a new ab initio potential energy surface.

178. S. Zhou, D. Xie, S. Y. Lin, and **H. Guo**, J. Chem. Phys., 128, 224316 (2008), A new *ab initio* potential-energy surface for $NH_2(X^2A'')$ and quantum studies of NH_2 vibrational spectrum and rate constant for the $N(^2D) + H_2 \rightarrow NH + H$ reaction.

179. Z. Li, L. Wang, H. Ran, D. Xie, N. Blinov, P.-N. Roy, and **H. Guo**, J. Chem. Phys., 128, 224513 (2008), Path integral Monte Carlo study of CO_2 solvation in ^4He clusters.

180. D. Quan, E. Herbst, T. Millar, S. Y. Lin, **H. Guo**, P. Honvault, and D. Xie, Astrophys. J. 68, 1318 (2008), New theoretical results concerning the interstellar abundance of molecular oxygen.

181. J. Momb, C. Wang, D. Liu, P. W. Thomas, G. A. Petsko, **H. Guo**, D. Ringe and W. Fast, Biochem., 47, 7715 (2008), On the mechanism of the quorum-quenching lactonase (AiiA) from *Bacillus thuringiensis*: 2. Substrate docking and active site mutations.

182. M. Jorfi, P. Honvault, P. Halvick, S.Y. Lin, and **H. Guo**, Chem. Phys. Lett., 462, 53 (2008), Quasiclassical trajectory scattering calculations for the $OH + O \rightarrow H + O_2$ reaction: cross sections and rate constants

183. L. Pei, J. Zhang, and W. Kong, D. Xu, and **H. Guo**, Chem. Phys. Lett. 462, 173 (2008), Polarization spectroscopy of aluminum phthalocyanine hydroxide embedded in superfluid helium droplets.

184. S. Y. Lin, and **H. Guo**, J. Chem. Phys., 129, 124311 (2008), Energy dependence of the differential and integral cross section for the $O(^1D) + H_2 \rightarrow OH + H$ reaction.

185. W. Lai, S. Y. Lin, D. Xie, and **H. Guo**, J. Chem. Phys., 129, 154311 (2008), Full-dimensional quantum dynamics of *A*-state photodissociation of ammonia. Absorption spectra.

186. S. Lin, D. Xie, and **H. Guo**, J. Chem. Phys., 129, 154313 (2008), *Ab initio* potential energy surfaces for both the ground (X^1A') and excited (A^1A'') electronic states of HGeCl and the absorption and emission spectra of HGeCl/DGeCl.

187. Z. Sun, D. Zhang, C. Xu, S. Zhou, D. Xie, G. Lendvay, S.-Y. Lee, S. Y. Lin, and **H. Guo**, J. Am. Chem. Soc. (communication), 130, 14962 (2008), State-to-state dynamics of H + O_2 reaction, evidence for non-statistical behaviors.

188. S. Y. Lin and **H. Guo**, J. Phys. Chem. A (invited article in the Schatz Festschrift), 113, 4285 (2009), Adiabatic and non-adiabatic state-to-state quantum dynamics for $O(^1D)$ + $H_2(X^1\Sigma_g^+,\ \upsilon_i = j_i = 0) \rightarrow OH(X^2\Pi, \upsilon_f, j_f) + H(^2S)$ reaction.

189. Z. Sun, S.-Y. Lee, **H. Guo**, D. H. Zhang, J. Chem. Phys., 130, 174102 (2009), Comparison of second-order split operator and Chebyshev propagator in wave packet based state-to-state reactive scattering calculations. (*One of 20 most downloaded articles*

from J. Chem. Phys., May 2009)

190. S. Zhou, Z. Li, D. Xie, S. Y. Lin, and **H. Guo**, J. Chem. Phys., 130, 184307 (2009), An *ab initio* global potential-energy surface for $NH_2(A^2A')$ and vibrational spectrum of the Renner-Teller A^2A'- X^2A'' system.

191. S. Y. Lin, **H. Guo**, G. Lendvay, and D. Xie, Phys. Chem. Chem. Phys. (Special Issue on Electronic Structures and Reaction Dynamics of Open-shell Species), 11, 4715 (2009), Effects of reactant rotational excitation on H + O_2 → OH + O reaction rate constant: quantum wave packet, quasi-classical trajectory, and phase space theory calculations.

192. S. Lin, D. Xie, and **H. Guo**, J. Phys. Chem. A (invited article in the Gerber Festschrift), 113, 7314 (2009), *Ab initio* potential energy surfaces for the ground ($\tilde{X}^1A'$) and excited ($\tilde{A}^1A''$) electronic states of HGeBr and the absorption and emission spectra of HGeBr/DGeBr.

193. D. Xu and **H. Guo**, J. Am. Chem. Soc., 131, 9780 (2009), Quantum mechanical/molecular mechanical and density functional theory studies of a prototypical zinc peptidase (carboxypeptidase A) suggest a general acid-general base mechanism.

194. S. C. Farantos, R. Schinke, **H. Guo**, and M. Joyeux, Chem. Rev., 109, 4248 (2009), Energy localization in molecules, bifurcation phenomena and their spectroscopic signatures: The global view.

195. Z. Li, D. Xie, Z. Sun, D. H. Zhang, S. Y. Lin and **H. Guo**, J. Chem. Phys., 131, 124313 (2009), NH($X^3\Sigma$) + H/D(^2S) → H(^2S) + NH/ND($X^3\Sigma$) exchange reactions: State-to-state quantum scattering and applicability of statistical model.

196. G. K. Smith, Z. Ke, A. C. Hengge, D. Xu, D. Xie, and **H. Guo**, J. Phys. Chem. B., 113, 15327 (2009), Active-site dynamics of SpvC virulence factor from *Salmonella Typhimurium* and density functional theory study of phosphothreonine lyase catalysis. (Cover article)

197. F. Lique, M. Jorfi, P. Honvault, P. Halvick, S. Y. Lin, **H. Guo**, D. Xie, J. Kłos, P. J. Dagdigian, and M. H. Alexander, J. Chem. Phys., 131, 221104 (2009), O + OH → O_2 + H: A key, and exemplary, reaction for interstellar chemistry. New theoretical results and comparison with experiment. (*One of 20 most downloaded articles from J. Chem. Phys., December 2009*)

198. Z. Sun, L. Liu, S. Y. Lin, R. Schinke, **H. Guo** and D. H. Zhang, Proc. Natl. Acad. Sci. USA, 107, 555 (2010), State-to-state quantum dynamics of O + O_2 isotope exchange reactions reveals non-statistical behavior at atmospheric conditions.

199. Z. Sun, **H. Guo** and D. H. Zhang, J. Chem. Phys., 132, 084112 (2010), Extraction of state-to-state reactive scattering attributes from wave packet in reactant Jacobi coordinates.

200. W. Lai, S. Y. Lin, D. Xie and **H. Guo**, J. Phys. Chem. A (invited article in the Soep

Festschrift), 114, 3121 (2010), Non-adiabatic dynamics of $\tilde{A}$-state photodissociation of ammonia: a four-dimensional wave packet study.

201. S. Wu, C. Zhang, D. Xu and **H. Guo**, J. Phys. Chem. B., 114, 9259 (2010), Catalysis of carboxypeptidase A: Promoted water vs. nucleophilic pathways**.**

202. J. Ma, S. Y. Lin, **H. Guo**, Z. Sun, D. H. Zhang, D. Xie, J. Chem. Phys., 133, 054302 (2010), State-to-state quantum dynamics of the $O(^3P) + OH(^2\Pi)$ □ $H(^2S) + O_2(^3\Sigma^-_g)$ reaction**.** (*Cover article and one of 20 most downloaded articles from J. Chem. Phys., August 2010*)

203. S. Y. Lin, **H. Guo**, B. Jiang, S. Zhou, and D. Xie, J. Phys. Chem. A (invited article in the Schinke Festschrift), 114, 9655 (2010), Non-Born-Oppenheimer state-to-state dynamics of the $N(^2D) + H_2 \rightarrow NH(\tilde{X}^3\Sigma^-) + H$ reaction: Influence of the Renner-Teller coupling.

204. A. Li, D. Xie, R. Dawes, A. W. Jasper, J. Ma, and **H. Guo**, J. Chem. Phys., 133, 144306 (2010), Global potential energy surface, vibrational spectrum, and reaction dynamics of the first excited (A^2A') state of HO_2.

205. S. Wu, D. Xu, and **H. Guo**, J. Am. Chem. Soc. (communication), 132, 17986 (2010), QM/MM studies of mono-zinc β-lactamase CphA suggest that the crystal structure of an enzyme-intermediate complex represents a minor pathway.

206. C. R. Smith, Z. Yang, G. K. Smith, D. Xu, **H. Guo**, Theo. Chem. Acc., 128, 83 (2011), Catalytic mechanism of anthrax lethal factor: The role of Tyr728.

207. G. K. Smith, S. Lin, W. Lai, A. Datye, D. Xie, and **H. Guo**, Surf. Sci., 605, 750 (2011), Density functional theory studies of the initial steps in methanol steam reforming on PdZn and ZnO surfaces.

208. Z. Ke, **H. Guo**, D. Xie, S. Wang, and Y. Zhang, J. Phys. Chem. B, 115, 3725 (2011), Ab initio QM/MM free-energy study of arginine deiminase catalysis: The protonation state of the Cys nucleophile.

209. Z. Li, C. Xie, B. Jiang, D. Xie, L. Lan, Z. Sun, D. H. Zhang, and **H. Guo**, J. Chem. Phys., 134, 134303 (2011), Quantum and quasi-classical state-to-state dynamics of the NH + H reaction: Competition between abstraction and exchange channels.

210. J. Ma, **H. Guo**, C. Xie, A. Li, D. Xie, Phys. Chem. Chem. Phys., 13, 8407 (2011), State-to-state quantum dynamics of the $H(^2S) + O_2(a^1\Delta_g) \rightarrow O(^3P) + OH(X^2\Pi)$ reaction on the first excited state of $HO_2(A^2A')$.

211. S. Lin, R. Johnson, G. K. Smith, D. Xie, and **H. Guo**, Phys. Chem. Chem. Phys., 13, 9622 (2011), Pathways for methanol steam reforming involving adsorbed formaldehyde and hydroxyl intermediates on Cu(111): density functional theory studies.

212. X. Wang, S. Wu, D. Xu, D. Xie, and **H. Guo**, J. Chem. Info. Model., 51, 1074 (2011),

Inhibitor and substrate binding by angiotensin-converting enzyme: Quantum mechanical/molecular mechanical molecular dynamics studies.

213. A. Li, C. Xie, D. Xie, and **H. Guo**, J. Chem. Phys., 134, 194309 (2011), A global *ab initio* potential energy surface for HNO (a^3A'') and quantum mechanical studies of vibrational states and reaction dynamics.

214. L. Wang, D. Xie, **H. Guo**, H. Li, and R. J. LeRoy, P.-N. Roy, J. Mole. Spectrosc. (Bunker and McKellar special issue), 267, 136 (2011), Superfluid response of ^4He_N-N_2O clusters probed by path integral Monte Carlo simulations.

215. B. Jiang, D. Xie, and **H. Guo**, J. Chem. Phys., 134, 231103 (2011), Communication: State-to-state differential cross sections for $H_2O(B)$ photodissociation.

216. C. M. Johnson, A. F. Monzingo, Z. Ke, D.-W. Yoon, T. W. Linsky, **H. Guo**, J. D. Robertus, and W. Fast, J. Am. Chem. Soc., 133, 10951 (2011), On the mechanism of dimethylarginine dimethylaminohydrolase inactivation by 4-halopyridines.

217. Z. Ke, G. K. Smith, Y. Zhang, and **H. Guo**, J. Am. Chem. Soc. (communication), 133, 11103 (2011), Molecular mechanism for eliminylation, a newly discovered post-translational modification. (Featured on C&E News.)

218. J. Ma and **H. Guo**, Chem. Phys. Lett. (*Editor's Choice*), 511, 193 (2011), Full-dimensional quantum state resolved predissociation dynamics HCO_2 prepared by photodetaching HCO_2^-.

219. R. Dawes, P. Lolur, J. Ma, and **H. Guo**, J. Chem. Phys. 135, 081102 (2011). Communication: Highly accurate ozone formation potential and implications for kinetics.

220. B. Jiang, D. Xie, and **H. Guo**, J. Chem. Phys., 135, 084112 (2011), Calculating of multiple initial state selected reaction probabilities from Chebyshev flux-flux correlation functions: Influence of reactant internal excitations on $H + H_2O \rightarrow OH + H_2$.

221. S. Wu, C. Zhang, D. Xu, and **H. Guo**, J. Phys. Chem. B., 115, 10360 (2011), pH-dependent reactivity for Glycyl-L-Tyrosine in carboxypeptidase A catalyzed hydrolysis.

222. S. Lin, D. Xie, and **H. Guo**, ACS Catal., 1, 1263 (2011), The methyl formate pathway in methanol steam reforming on copper: Density functional calculations.

223. S. Lin, D. Xie, and **H. Guo**, J. Phys. Chem. C., 115, 20583 (2011). Pathways of methanol steam reforming on PdZn and comparison with Cu.

224. C. Xie, A. Li, D. Xie, and **H. Guo**, J. Chem. Phys., 135, 164312 (2011), State-to-state quantum dynamics of the $N(^4S) + OH(X^2\Pi) \rightarrow H(^2S) + NO(X^2\Pi)$ reaction.

225. G. K. Smith, Z. Ke, **H. Guo**, and A. C. Hengge, J. Phys. Chem. B., 115, 13713 (2011), Insights into the phosphoryl transfer mechanism of cyclin-dependent protein kinases from ab initio QM/MM free-energy studies.

226. P. W. Thomas, M. Zheng, S. Wu, **H. Guo**, D. Liu, D. Xu and W. Fast, Biochem., 50, 10102 (2011), Characterization of purified New Delhi metallo-β-lactamase-1 (NDM-1).

227. J. Daranlot, M. Jorfi, C. Xie, A. Bergeat, M. Costes, P. Caubet, D. Xie, **H. Guo**, P. Honvault, K. M. Hickson, Science, 334, 1538 (2011), Revealing atom – radical reactivity at low temperature through the N + OH reaction. (Featured in Science and C&E News, Dec, 2011)

228. J. Ma, D. Xu, **H. Guo**, V. Ting, M. E. Kellman, J. Chem. Phys., 136, 014304 (2012), Isotope effect in normal-to-local transition of acetylene bending modes.

229. B. Jiang, D. Xie, and **H. Guo**, J. Chem. Phys., 136, 034302 (2012), State-to-state photodissociation dynamics of triatomic molecules: H_2O in its B band.

230. J. Li, Y. Wang, B. Jiang, J. Ma, R. Dawes, D. Xie, J. M. Bowman, and **H. Guo**, J. Chem. Phys., 136, 041103 (2012), Communication: A chemically accurate potential energy surface for the HO + CO → H + CO_2 reaction. *(Top 20 most read article on J. Chem. Phys., January and February 2012)*

231. **H. Guo**, Theo. Chem. Acc., 131, 1077 (2012), Theoretical characterization of reaction dynamics in the gas phase and at interfaces (Editorial, 50^{th} anniversary issue).

232. **H. Guo**, Int. Rev. Phys. Chem., 31, 1 (2012), Quantum dynamics of complex-forming reactions (invited review, featured on cover, and one of the most read articles in 2012).

233. S. Lin, D. Xie, and **H. Guo**, J. Mole. Catal. A, 356, 165 (2012), First-principles study of the methyl formate pathway of methanol steam reforming on PdZn(111) with comparison to Cu(111).

234. J. Li, C. Xie, J. Ma, Y. Wang, R. Dawes, D. Xie, J. M. Bowman, **H. Guo**, J. Phys. Chem. A, 116, 5057-5067 (2012), Quasi-classical dynamics of the HO + CO → H + CO_2 reaction on a new ab initio based potential energy surface.

235. X. Zhu, J. Ma, D. R. Yarkony, and **H. Guo**, J. Chem. Phys., 136, 234301 (2012), Computational determination of $\tilde{A}$ state absorption spectrum of NH_3 and ND_3 using a new quasi diabatic representation of the $\tilde{X}$ and $\tilde{A}$ states and full six dimensional quantum dynamics.

236. B. Jiang, X. Ren, D. Xie, and **H. Guo**, Proc. Natl. Acad. Sci. USA., 109, 10224 (2012), Enhancing dissociative chemisorption of H_2O on Cu(111) via vibrational excitation.

237. C. Xie, J. Li, D. Xie, and **H. Guo**, J. Chem. Phys., 137, 024308 (2012), Quasi-classical trajectory studies of the H + CO_2 → HO + CO reaction on a new ab initio based potential energy surface.

238. J. Ma, J. Li, and **H. Guo**, Phys. Rev. Lett., 109, 063202 (2012), Tunneling facilitated dissociation to H + CO_2 in $HOCO^-$ photodetachment.

239. J. Ma, **H. Guo**, R. Dawes, Phys. Chem. Chem. Phys., 14, 12090 (2012), Low temperature rat constants for the N + CN → N_2 + C reaction: two-dimensional quantum capture calculations on an accurate potential energy surface.

240. J. Ma, J. Li, **H. Guo**, J. Phys. Chem. Lett., 3, 2482 (2012), Quantum dynamics of the HO + CO → H + CO_2 reaction on an accurate potential energy surface.

241. J. Li, R. Dawes, and **H. Guo**, J. Chem. Phys., 137, 094304 (2012), An ab initio based full-dimensional global potential energy surface for FH_2O (X^2A') and dynamics for the F + H_2O → HF + HO reaction.

242. J. Ma, X. Zhu, D. R. Yarkony, **H. Guo**, J. Chem. Phys. (Non-adiabatic dynamics special issue), 137, 22A541 (2012), First principles determination of the $NH_2/ND_2(\tilde{A}, \tilde{X})$ branching ratios for photodissociation of NH_3/ND_3 *via* full-dimensional quantum dynamics based on a new quasi-diabatic representation of coupled *ab initio* potential energy surfaces.

243. R. Liu, M. Yang, G. Czakó, J. M. Bowman, J. Li, and **H. Guo**, J. Phys. Chem. Lett., 3, 3776 (2012), Mode selectivity for a central barrier reaction: Eight-dimensional quantum studies of the $O(^3P)$ + CH_4 → OH + CH_3 reaction on an accurate potential energy surface.

244. B. Jiang, D. Xie, and **H. Guo**, Chem. Sci., 4, 503 (2013), Vibrationally mediated bond selective dissociative chemisorption of HOD on Cu(111).

245. Y. Li and **H. Guo**, Theo. Chem. Acc., 132, 1303 (2013), Atomistic simulations of antimicrobial conjugated polyelectrolyte interacting with model bacterial membrane.

246. Y. Li, Y. V. Suleimanov, M. Yang, W. H. Green, and **H. Guo**, J. Phys. Chem. Lett., 4, 48 (2013), Ring polymer molecular dynamics calculations of thermal rate constants for the $O(^3P)$ + CH_4 → OH + CH_3 reaction: Contributions of quantum effects.

247. J. Li, B. Jiang, **H. Guo**, Chem. Sci., 4, 629 (2013), Enhancement of bimolecular reactivity by a pre-reaction van der Waals complex: the case of F + H_2O → HF + HO.

248. S. Lin, J. Ma, L. Zhou, C. Huang, D. Xie, **H. Guo**, J. Phys. Chem. C., 117, 451 (2013), Influence of defects on methanol decomposition: Periodic density functional studies on Pd(211) and kinetic Monte Carlo simulations.

249. A. Li, C. Xie, D. Xie, and **H. Guo**, J. Chem. Phys., 138, 024308 (2013), State-to-state quantum dynamics of the $\mathrm{O}(^3P) + \mathrm{NH}(X^3\Sigma^-)$ reaction on the three lowest-lying electronic states of HNO/HON.

250. B. Jiang, J. Li, D. Xie, and **H. Guo**, J. Chem. Phys., 138, 044704 (2013), Effects of reactant internal excitation and orientation on dissociative chemisorption of H_2O on Cu(111): Quasi-seven-dimensional quantum dynamics on a refined potential energy surface.

251. J. Li, B. Jiang, **H. Guo**, J. Am. Chem. Soc., 135, 982 (2013), Reactant vibrational excitations are more effective than translational energy in promoting an early-barrier reaction F + H_2O → HF + OH.

252. L. Zhou, B. Jiang, D. Xie, and **H. Guo**, J. Phys. Chem. A. (invited article for Bowman Festschrift), in press, State-to-state photodissociation dynamics of H_2O in the *B*-band: Competition between two coexisting non-adiabatic pathways.

253. J. C. Corchado, J. Espinosa-Garcia, J. Li, and **H. Guo**, J. Phys. Chem. A. (invited article for Wittig Festschrift), in press, CO_2 vibrational state distributions from quasi-classical trajectory studies of the HO + CO → H + CO_2 reaction and H + CO_2 inelastic collision.

254. B. Halevi, S. Lin, A. Roy, Z. He, E. Jeroro, J. Vohs, Y. Wang, **H. Guo**, and A. K. Datye, J. Phys. Chem. C, submitted, High CO_2 selectivity of ZnO powder catalysts for methanol steam reforming.

255. J. Li, B. Jiang, and **H. Guo**, J. Chem. Phys., submitted, Spin-orbit corrected full-dimensional potential energy surfaces for the two lowest-lying electronic states of FH_2O and dynamics for the F + H_2O → HF + OH reaction.

256. R. S. Johnson, A. DeLaRiva, V. Ashbacher, B. Halevi, C. J. Villanueva, G. K. Smith, S. Lin, and A. K. Datye, and **H. Guo**, Phys. Chem. Chem. Phys., submitted, CO oxidation mechanism and reactivity on PdZn alloys.

257. Y. Li, Y. V. Suleimanov, J. Li, W. H. Green, and **H. Guo**, J. Chem. Phys., submitted, Rate constants and kinetic isotope effects of the X + CH_4 → CH_3 + HX (X= H, D, Mu) reactions from ring polymer molecular dynamics.

258. J. J. Melko, S. G. Ard, J. A. Fournier, J. Li, N. S. Shuman, **H. Guo**, J. Troe, and A. A. Viggiano, Phys. Chem. Chem. Phys., to be submitted, Iron-catalyzed reduction of N_2O by CO: Gas-phase temperature dependent kinetics.

259. K. Prozument, R. G. Shaver, M. Ciuba, J. S. Muenter, G. B. Park, J. F. Stanton, **H. Guo**, B. M. Wong, D. S. Perry, and R. W. Field, Faraday Disc. Submitted, A new approach toward transition state spectroscopy.

260. **H. Guo**, D. Xu, and Q. Cui, Inter. Rev. Phys. Chem., to be submitted, Quantum mechanical/molecular mechanical studies of zinc hydrolases.

PRESENTATIONS

Seminars and Colloquia

Chemistry, University of Toledo, 1991

Chemistry, Indiana University-Prudue University at Fort Wayne, 1992

Physics, University of Toledo, 1992

Chemistry, University of Michigan, 1993

Chemistry, Bowling Green State University, 1993

Chemistry, University of Southern California, 1993

NASA Ames Research Laboratory, 1993

Chemistry, University of California, San Diego, 1993

Chemistry, University of Notre Dame, 1993

Chemistry, Michigan State University, 1993

Chemistry, Northwestern University, 1993

Naval Research Laboratory, Washington D.C., 1994

Chemistry, Wayne State University, 1994

Chemistry, University of Cincinnati, 1994

Chemistry, Western Michigan University, 1994

Chemistry, Ohio State University, 1995

Chemical Engineering, University of Toledo, 1996

Chemistry, Marquette University, 1996

Mathematics, University of Toledo, 1996

Chemistry, Bowling Green State University, 1996

Chemistry, Southern Illinois University, 1997

Physics, University of Toledo, 1997

Chemistry, University of New Mexico, 1997

Chemistry, University of Illinois at Urbana-Champaign, 1997

Chemistry, University of Virginia, 1997

Medicinal Chemistry, University of Toledo, 1997

Chemistry, University of Manchester, 1997

Theoretical Chemistry, Oxford University, 1997

Chemistry, University College London, 1997

Chemistry, University of Bristol, 1997

Chemistry, Sichuan University, 1997
Chemistry, Emory University, 1998
Chemistry, Case Western Reserve University, 1998
Chemistry, New York University, 1999
Physics, University of Alberta, 2000
Chemistry, University of New Mexico, 2000
Albuquerque High Performance Computing Center, 2000
Center for Advanced Studies, University of New Mexico, 2002
Chemistry, University of Oregon, 2003
Biocomputing, University of New Mexico, 2004
Chemistry, Texas Tech University, 2005
Chemistry, Washington State University, 2005
Chemistry, University of Colorado, 2005
Biocomputing, University of New Mexico, 2006
Chemistry, Nanjing University, 2006
Drug Discovery and Design Center, Shanghai Institute of Materia Medica, 2006
Combustion Research Facility, Sandia Livermore National Laboratory, 2006
Center for Computational Sciences, University of Kentucky, 2007
Department of Chemistry, Oregon State University, 2007
Department of Chemistry, University of Crete, Greece, 2007
Institute of Molecular Biophysics, Florida State University, 2007
UNM Center for High Tech Materials, 2008
Department of Chemistry, New Mexico State University, 2008
Department of Chemistry, Marquette University, 2008
Department of Chemistry, University of California Riverside, 2009
Department of Chemistry, Utah State University, 2009
C-PCS, Los Alamos National Laboratory, 2009
Department of Chemistry, University of Houston, 2009
Department of Chemistry, North Texas University, 2010
Department of Chemistry, New York University, 2010
School of Chemical Science and Engineering, Yunnan University, China, 2010
Institute of Modern Physics, Northwest University, China, 2010
Institute of Theoretical and Computational Chemistry, Nanjing University, China, 2010

College of Chemistry, Beijing Normal University, China, 2010
Dalian Institute of Chemical Physics, China, 2010
Department of Physics, University of New Mexico, 2011
Department of Chemistry, Xiamen University, 2012
Center for Photocatalysis, Fuzhou University, 2012
Wuhan Institute of Physics and Mathematics, Chinese Academy of Sciences, 2012
Institute for Theoretical Chemistry, Jilin University, 2012

Conferences:

Faraday Discussion, 82, 1986, Bristol, **posters**
Midwest Theoretical Chemistry Conference, Indianapolis, 1989, **poster**
Conference on Dynamics of Molecular Collisions, Asilomar, 1989, **poster**
Midwest Theoretical Chemistry Conference, 1990, Madison, **poster**
50th Annual Conference on Physical Electronics, 1990, Gaithersburg, **invited talk**
XIXth informal conference on photochemistry, 1990, Ann Arbor, **poster**
Air Force Workshop on Surface Reactions in Space Environment, 1990, Evanston, **invited talk**
American Physical Society National Meeting, 1991, Washington DC, **poster**
Conference on Dynamics of Molecular Collisions. Lake George, 1991, **poster**
American Chemical Society Central Regional Meeting, Cincinnati, 1992, **invited talk**
Midwest Theoretical Chemistry Conference, E. Lansing, 1992, **poster and talk**
American Physical Society National Meeting, Seattle, 1993, **poster and talk**
American Chemical Society National Meeting, Chicago, 1993, **poster**
American Physical Society National Meeting, Crystal City, 1994, **invited talk**
International Symposium on Molecular Spectroscopy, Columbus, Ohio, 1994, **talk**
American Chemical Society National Meeting, Washington DC, 1994, **invited talk**
International Symposium on Molecular Spectroscopy, Columbus, Ohio, 1995, **talk**
American Chemical Society Central Regional Meeting, Akron, 1995, **invited talk**
Midwest Theoretical Chemistry Conference, Evanston, Illinois, 1995, **poster**
SPIE, Laser Techniques for Surface Sciences II, San Diego, California, 1995, **poster**
Conference on Dynamics of Molecular Collisions, Asilomar, California, 1995, **posters**
Sanibel Symposium on Quantum Theory, St. Augustine, Florida, 1996, **invited talk**
Midwest Theoretical Chemistry Conference, Indianapolis, 1996, **talk**
American Chemical Society National Meeting, San Francisco, 1997, **talk**

57th Annual Conference on Physical Electronics, 1997, Eugene, **invited talk**

Conference on Dynamics of Molecular Collisions, 1997, Gull Lake, MN, **invited talk**, **posters**

John Murrell Retirement Symposium, 1997. University of Sussex, **invited talk**

Faraday Discussion 108, 1997, University of Sussex, **invited talk**

Symposium on Frontiers of Chemistry, 1997, Hong Kong, **invited talk**

American Chemical Society National Meeting, Anaheim, 1999, **talk**

American Conference on Theoretical Chemistry, Boulder, Colorado, 1999, **posters**

Conference on Dynamics of Molecular Collisions, Split rock, Pennsylvania, 1999, **invited talk**

8th International workshop on DIET, New Jersey, 1999, **talk**

Telluride Conference on Intramolecular Dynamics, 2000, **invited talk**

Third Conference for Worldwide Chinese Young Chemists, 2000, **invited talk**

American Chemical Society National Meeting, Chicago, 2001, **invited talks**

International Workshop on Quantum Dynamical Concepts, Dresden, Germany, 2002, **invited talk**

American Chemical Society National Meeting, New Orleans, 2003, **talks**

NATO Advanced Research Workshop on Dynamics of Elementary Chemical Reactions, Hungary, 2003, **invited talk**

DICP Symposium on Reaction Dynamics, Dalian, 2004, **invited talk**.

International Workshop on Theoretical and Computational Chemistry of Complex Systems, Hong Kong, 2005, **invited talk**.

19th Enzyme Mechanisms Conference, Asilomar, 2005, **poster**

Mesilla Conference, Mesilla, 2005, **invited talk**

XXth Conference on Dynamics of Molecular Collisions, Asilomar, California, 2005, **invited talk**

VIIIth Workshop on Quantum Reactive Scattering, UC Santa Cruz, 2005, **invited talk**

Texas Enzyme Mechanisms Conferences, Austin, 2006, **poster**

53rd Annual Western Spectroscopy Association Conference, Asilomar, California, 2006, **poster**

Fourth Worldwide Chinese Theoretical and Computational Chemistry Conference, Kunming, 2006, **invited talk**

American Chemical Society National Meeting, San Francisco, 2006, **invited talks**

54th Annual Western Spectroscopy Association Conference, Asilomar, California, 2007, **poster**

XXIth Conference on Dynamics of Molecular Collisions, Santa Fe, 2007, **poster**

IXth Workshop on Quantum Reactive Scattering, Cambridge, 2007, **invited talk**

American Chemical Society Southwest Regional Meeting, Lubbock, 2007, **invited talks**

American Chemical Society National Meeting, New Orleans, 2008, **invited talk**

Department of Energy Combustion Meeting, Airlie, VA, 2008, **invited talk**

10th Chinese National Conference on Quantum Chemistry, Nanjing, 2008, **invited plenary talk**

Conference on Computational Molecular Structure and Dynamics, Austin, 2009, **invited talk**

IMA workshop on Chemical Dynamics: Challenges and Approaches, Minneapolis, 2009, **invited talk**

Xth Workshop on Quantum Reactive Scattering, Dalian, China, 2009, **invited talk**

XXIIth Conference on Dynamics of Molecular Collisions, 2009, Snowbird, Utah, **invited talk**

Southwest Theoretical Chemistry Conference, Houston, 2009, **poster**

Telluride Workshop on New Challenges for Theory in Chemical Dynamics, 2010, **invited talk**

Telluride Workshop on Toward Meaningful Analysis of Phosphoryl Transfers and RNA Catalysis: Experiments and Computations, 2010, **invited talk**

American Chemical Society National Meeting, Boston, 2010, **posters**

Department of Energy Combustion Meeting, Airlie, VA, 2011, **invited talk**

NASA/NSF workshop on S mass independent isotope effect, Alexandra, Virginia, **invited talk**

Dynamics of Molecular Collisions, Snowbird, UT, 2011, **invited talk**

The 11th workshop on quantum reactive scattering, Santa Fe, NM, 2011, **posters**

Computational Enzymology Symposium, IUPAC, San Juan, PR, 2011, **invited talk**

International Conference on Theoretical and High Performance Computational Chemistry, Xian, China, 2011, **invited talk**

Telluride Workshop on New Challenges for Theory in Chemical Dynamics, 2012, **invited talk**

Terefe G. Habteyes

Assistant Professor
Department of Chemistry and Chemical Biology
University of New Mexico, Albuquerque, NM 87131
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Education

- Postdoc, University of California at Berkeley, 2008-2012
- Ph.D. in Chemistry, University of Arizona, May 2008
- M.S. in Chemistry, Addis Ababa University, Ethiopia, 2000
- B.S. in Chemistry with Honor and Gold Medal, Addis Ababa University, Ethiopia, 1997

Teaching and Research Experience

- Assistant Professor, Department of Chemistry and Chemical Biology, University of New Mexico (August 2012 -)
- Post Doctoral Fellow, Department of Chemistry, University of California, Berkeley (May 2008 - 2012)
- Teaching/Research Assistant, Department of Chemistry, University of Arizona (2002-2008)
- Lecturer, Department of chemistry, Addis Ababa University, Ethiopia (2000-2002)
- Assistant Lecturer, Department of Chemistry, Addis Ababa University, Ethiopia (1998-2000)
- Graduate Assistant, Department of Chemistry, Addis Ababa University, Ethiopia (1997-1998)

Honors, Awards and Fellowships

- University of California President's Postdoctoral Fellowship (2009 - 2011)
- Promotion to Teaching Assistant (TA) level 3 - the highest award the Department of Chemistry, University of Arizona, offers based on evaluations by the students and supervisors, Spring 2007
- Imaging Fellowship, University of Arizona, 2004-2005
- Exceeds TA expectations, Department of Chemistry, University of Arizona, Spring 2004
- Mid Career Fellowship, Department of Chemistry, University of Arizona, Fall 2003
- The German Academic Exchange Service scholarship, 1998-2000
- Outstanding Student of the Graduating Class Award (Gold Medal), Faculty of Science, Addis Ababa University, 1997

- Academic Excellency Award, Ethiopian Scientists Association in North America, 1997
- Scholastic Achievement Award, Chemical Society of Ethiopia, 1997
- Best Student of the Year Award, Science Faculty, Addis Ababa University, 1996

Courses Taught

- Molecular Structure Theory, Chem. 501, University of New Mexico, Spring 2013
- Physical Chemistry Laboratory, Chem. 411L, University of New Mexico, Fall 2012
- Physical Chemistry Laboratory (*teaching assistant*), University of Arizona, Spring 2007
- Introduction to Quantum Chemistry (*teaching assistant*), University of Arizona, Spring 2004
- General Chemistry Laboratory (*teaching assistant*), University of Arizona, Fall 2002
- Thermodynamics (*taught the full course independently*), Kotebe College of Teacher Education, Summer 2001.
- Introduction to Quantum Chemistry (*taught the full course independently*), Addis Ababa University, Summer 2001.
- Physical Chemistry Laboratory (*coordinator and instructor*), Addis Ababa University, Spring 2001
- General Chemistry (*taught the full course independently*), Addis Ababa University, Fall and Spring semesters of 2000-2002.
- General Chemistry Laboratory (*instructor*), Addis Ababa University, Fall and Spring semesters of 1997-2001.

Publications

1. **T. G. Habteyes**, S. Dhuey, E. Wood, S. Cabrini, P. J. Schuck, A. P. Alivisatos and S. R. Leone, Metallic adhesion layer induced plasmon damping and molecular linkers as a nondamping alternative, *ACS Nano*, 6, 5702, 2012.
2. **T. G. Habteyes**, S. Dhuey, S. Cabrini, P. J. Schuck, and S. R. Leone, Theta-shaped plasmonic nanostructures: bringing “dark” multipole plasmon resonances into action via conductive coupling, *Nano Lett*, 11, 1819, 2011.
3. **T. G. Habteyes**, L. Velarde, and A. Sanov, Effects of isomer coexistence and solvent-induced core switching in the photodissociation of bare and solvated $(CS_2)_2^-$ anions, *J. Chem. Phys.* 130, 124301 (2009).

4. L. Velarde, **T. G. Habteyes**, R. Glass, and A. Sanov, Observation and characterization of the $CH_3S(O)CH^-$ and $CH_3S(O)CH^- \cdot H_2O$ carbene anions by photoelectron imaging and photofragmentation spectroscopy, *J. Phys. Chem.* A 113, 3528 (2009).
5. **T. G. Habteyes** and A. Sanov, Electron Binding Motifs in the $(CS_2)_n^-$ (n> 4) Cluster Anions, *J. Chem. Phys.* 129, 244309 (2008).
6. **T. G. Habteyes**, L. Velarde, and A. Sanov, Relaxation of $(CS_2)_2^-$ to Its Global Minimum Mediated by Water Molecules: A Photoelectron Imaging Study**,** *J. Phys. Chem.* A 112, 10134 - 10140 (2008).
7. **T. G. Habteyes**, L. Velarde, and A. Sanov, Photodissociation of CO_2^- in water clusters via Renner-Teller and conical interactions, *J. Chem. Phys.* 126, 154301 (2007).
8. L. Velarde, **T. G. Habteyes**, E. Grumbling, K. Pichugin, and A. Sanov, Solvent resonance effect on the anisotropy of $NO^-(N_2O)_n$ cluster anion photodetachment, *J. Chem. Phys.* 127, 084302 (2007).
9. L. Velarde, **T. G. Habteyes**, and A. Sanov, Photodetachment and photofragmentation pathways in the $[(CO_2)_2(H_2O)_m]^-$ cluster anions, *J. Chem. Phys.* 125, 114303 (2006).
10. **T. G. Habteyes**, L. Velarde, and A. Sanov, Solvent-enabled photodissociation of CO_2^- in water clusters, *Chem. Phys. Lett.* 424, 268-272 (2006).
11. E. Surber, R. Mabbs, **T. G. Habteyes**, and A. Sanov, Photoelectron imaging of hydrated carbon dioxide cluster anions, *J. Phys. Chem. A* 109, 4452-4458 (2005).

Talks, Posters and Meetings

- *Plasmon Sensitivity and Near-Field Optical Microscopy* (talk), Optical Science and Engineering Program seminar series, University of New Mexico, September 5, 2012
- *Creating Sharp Plasmon Resonances Towards Ultrasensitive Biochemical Sensors* (talk), INCBN IGERT Seminar series, University of New Mexico, September 17, 2012
- *Plasmon Resonance Sensitivity and Apertureless Near-Field Scanning Optical Microscopy* (poster), CINT User Conference, Albuquerque, New Mexico, September 19 - 20
- *Plasmonics and High Resolution Near-Field Optical Microscopy/Spectroscopy* (talk), Chemistry at the Space-Time Limit center, University of California at Irvine, May 19, 2011.
- *Plasmonics and High Resolution Near-Field Optical Microscopy/Spectroscopy* (talk), University of California at Merced, May 6, 2011.
- *Design, Fabrication/Synthesis, Optical Characterization and Coupling/Application of Plasmonic Nanostructures* (talk), Leone Group, November 2, 2010.

- *Investigating Plasmonic and Semiconductor Nanomaterials Applying High Spatial Resolution Optical Microscopy and Spectroscopy* (talk), UC President's Fellowship Program Retreat, UCLA Lake Arrowhead Conference Center, October 30, 2010.
- *Tip-Sample Size Mismatch and Polarization Dependence in Near-Field Interaction of Conical Probe with Gold Nanospheres* (poster), Gordon Research Conference on Plasmonics, Waterville, Maine, June 13-18, 2010
- NIST Nano-Optics Plasmonics Conference (attended), Gaithersburg, MD, April 19-22, 2010
- *Near-Field Microscopy and Metal Nanoparticles* (talk), Leone Group, UC Berkeley, February 23, 2010
- *Near-Field Microscopy and Nanomaterials* (talk), Leone Group, UC Berkeley, July 21, 2009
- *Probing Molecular Dynamics with EUV Laser Pulse* (talk), Leone Group, UC Berkeley, December 2, 2008
- *Switching Anion Structure and Photodissociation Pathways using Solvent Molecules*, Chemistry Department, University of Arizona, October 29, 2007.
- *Gas Phase Photochemistry of CO_2^- in Water Clusters (poster), Gordon Research Conference on Atomic and Molecular Interaction*, New London, NH, July 2006.
- *Gas Phase Photochemistry of CO_2^- in Water Clusters* (talk), Chemistry Department, University of Arizona, March 6, 2006.
- *Study of Cluster Anions Using Photoelectron Imaging Spectroscopy and Tandem Time of Flight Mass Spectroscopy* (poster), ACS 230th National Meeting, Washington, DC, August 2005.
- *Observation of Electronic Structure* (talk), Imaging Fellowship, University of Arizona, April 7, 2005.
- *Electronic States in Quantum Dots: Beyond the Artificial Atom Model* (talk), Chemical Physics After Dark, Chemistry Department, University of Arizona, October 26, 2004.
- *Chemists' Race against Time: Nature on the Femtosecond Time Scale as Revealed by Time Resolved Spectroscopy* (talk), Chemistry Department, University of Arizona, May 5, 2004.

Referee Service

- The Journal of Physical Chemistry

General Services

- Graduate Recruiting Committee, Department of Chemistry & Chemical Biology, University of New Mexico
- Lab. Monitor, Sanov Research Group, Department of Chemistry, University of Arizona, 2006-2008.
- Safety Committee, Department of Chemistry, University of Arizona, 2004-2005.
- Laboratory and office equipment purchasing committee, Science Faculty, Addis Ababa University, Ethiopia.

Membership

- American Chemical Society

Kuangchiu Joseph Ho
Department of Chemistry & Chemical Biology
University of New Mexico
Albuquerque, NM 87131
e-mail: khoj@unm.edu, Phone: 505-277-1385, Fax: 505-277-2609

a. Professional Preparation

- National Taiwan Institute of Technology, Chemical Engineering, B. Science in Engineering,1983
- Minnesota State University Biochemistry M.S., 1989
- University of New Mexico Biophysical Chemistry Ph.D.,1993

b. Appointments

- Director of Chemical Education, Research Professor, 2010-present, Department of Chemistry & Chemical Biology, University of New Mexico
- Director of Chemistry Teaching Laboratories, 1996-present, Department of Chemistry and Chemical Biology, University of New Mexico
- Lecturer III, 1997-present, Department of Chemistry, University of New Mexico

c. Selected Publications

- **FIVE CLOSELY RELATED PUBLICATIONS**

1. K. Joseph Ho, (2013), "Protein Conformation: Engaging Students in Active Learning" in *Teaching Bioanalytical Chemistry*, ACS Symposium Series, edited by Harvey Hou. (in press)
2. K. Joseph Ho, (2013) " A Search of Predicators for Student's Success in the Gateway Chemistry Course", New Mexico Higher Education Assessment and Retention Conference, February 28, 2013
3. K. Joseph Ho, (2013) "Active Learning in General Chemistry: The Mechanics of a Gateway Course Redesign", *Success in the Classroom Conference, February 20.*
4. K. Joseph Ho, "Bioanalytical Chemistry for Teachers", Bioanalytical Chemistry: Analytical Applications in Biological Sciences Symposium, 21th Biennial Chemical Education Conference (BCCE), Bloomington, IN, 2010
5. Ho, K. LaDonna Malone, Justin Marbury, "Integration of Freshman lectures, Laboratories and Bridges", Second Annual NASA-PURSUE Student Conference, Albuquerque, New Mexico, 2001

- **FIVE OTHER SIGNIFICANT PUBLICATIONS**

1. Ho, J., Laboratory Experience I & II, Hayden McNeil Publishing, Inc, 2001-2013
2. Ho, J., Physical Chemistry Laboratory I & II, University of New Mexico, 1997-2008
3. K. Joseph Ho, S. Knottenbelt, "Development of a Parachute Course for College Chemistry", New Mexico Higher Education Assessment and Retention Conference, February 24, 2011

4. J. Wei, Q. Fu, H. Fan, J. Ho, W. Wang, “A highly Selective Fluorescence Probe for Thiophenols”, Angewandte Chemie Int. Ed., v46, 8445-8448, 2007
5. Z. Wang, K.J. Ho, C.J. Medforth, and J.A. Shelnut, “Porphrin Nanofiber Bundles from Phase-transfer Ionic Self-assembly and their Photocatalytic Self-metallization”, Advanced Materials, v18, 255-2560, 2006

d. Synergistic Activities

1. I am serving as the Chair of Undergraduate Study Committee and the Director of Chemical Education, overseeing undergraduate programs of Chemistry at UNM.
2. I serve as the team leader for Gateway Course CHEM 122 and CHEM 121 redesign project. The first project was started in June of 2012 and will be completed in the summer of 2013. The second project will start in June of 2013 and end in August 2014. The assessment of the program is expected to extend into 2015-16.
3. I have developed and taught the on-line chemistry lab that provides training for experimental design and interpretation of experimental data and observations.
4. I have coordinated the development of new upper division, undergraduate lab sequences (instrumental analysis, CHEM 351, physical chemistry lab, 411 and synthesis and characterization lab, 432).
5. The CHEM 123 Lab Manual has been reviewed and selected by Freeman Publishing Co. to be included in the company’s inquiry-based chemistry lab database (LabPartner) for adoption.
6. I served as P.I. for NASA-PURSUE projects in 2000-2002 for a virtual Chemistry lab and have developed an interactive web-site for students to prepare their pre-lab exercises and post-lab calculations.

e. Collaborators & Other Affiliations

1. Professor Vanessa Svihla, University of New Mexico, College of Education, Albuquerque, NM
2. Professor Sushilla Knottenbelt, University of New Mexico, Albuquerque, NM
3. Professor Gary Smith, University of New Mexico, Albuquerque, NM
4. Professor Wei Wang, University of New Mexico, Albuquerque, NM
5. Professor Debra Dunaway Mariano, University of New Mexico, Albuquerque, NM
6. Dr. Shaorong Yang, Central New Mexico Community college, Albuquerque, NM
7. Mrs. Clarrisa Sorensen-Unruh, Central New Mexico Community college, Albuquerque, NM
8. Valerie Varoz, Chair of Science Department & Science teacher, Sandia High School, Albuquerque, NM 87123
9. Dr. Stefi Weisburd, Education & Outreach Manager, School of Engineering Deans Office, University of New Mexico, Albuquerque, NM
10. Professor Amy Reel, Speech & Hearing Sciences, UNM
11. Paul Edmund, Director of Center for English Language & American Culture

Richard W. Holder Chemistry and Chemical Biology 10/5/2012

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1 University of New Mexico
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EDUCATIONAL HISTORY

Ph.D.	1972	Yale University	Organic Chemistry
M.Phil.	1970	Yale University	
M.S.	1966	University of Wyoming	Organic Chemistry
B.S. (Honors)	1964	University of Wyoming	Chemistry

Ph.D. Dissertation: "The Stereochemistry of the Migrating Carbon in Suprafacial 1, 3-Sigmatropic Rearrangements." Advisor: Professor Jerome A. Berson
M.S. Thesis: "Studies of C- and O-Alkylation of Some β-Ketoesters." Advisor: Professor Sara Jane Rhoads.

EMPLOYMENT HISTORY

University of New Mexico (UNM)
- Associate Chair, Department of Chemistry and Chemical Biology, 2012-
- Deputy Provost, 2000-2011
- Provost and Vice President for Academic Affairs (Interim), January-April, 2000
- Associate Provost for Academic Affairs, 1986-2000
- Dean of University College, 1997-2000
- Professor of Chemistry, 1993-present
- Dean of Graduate Studies, 1991-1992
- Chair, Department of Chemistry, 1989-1990
- Associate Professor of Chemistry, 1978-1993
- Assistant Professor of Chemistry, 1974-1978

National Science Foundation (on leave from UNM)
- Program Director, Organic Chemical Dynamics, 1984-1985

Vassar College
- Assistant Professor of Chemistry, 1972-1974

Universidad de Concepcion (Chile)
- Profesor de Quimica Organica (as a Peace Corps Volunteer), 1966-1968

MANAGEMENT EXPERIENCE

As Deputy Provost I supervised seven academic support units with diverse missions.
I also manage most faculty personnel matters at the institutional level, including:
National searches and hiring

- Tenure, promotion, mid-probationary, and post-tenure reviews
- Sabbaticals and other leaves
- Grievances
- Establish and oversee search committees carrying out national searches for Deans, Vice Presidents, and other institutional officers
- Institutional liaison with UNM's four branch campuses regarding faculty matters

- Work with Regents and Faculty Senate to develop and revise faculty policies and procedures
- Work with Internal Audit to address faculty policy compliance issues
- Chair the space allocation committee to support faculty teaching and research

SERVICE, ACADEMIC YEAR 2012-2013

Faculty Senate Policy Committee, Member
Space Allocation Committee, Member
Faculty Senate President-Elect
President, Phi Beta Kappa Alpha of New Mexico (UNM) Chapter
Associate Chair, Department of Chemistry and Chemical Biology
Co-Chair, Tuition and Fee Team
Foundations of Excellence Task Force (Organization Dimension Committee)

SECONDARY APPPOINTMENTS AND HONORS

American Chemical Society Petroleum Research Fund Scholar 1963-1964
Phi Beta Kappa, Phi Kappa Phi, and Sigma Xi, 1964
National Science Foundation Summer Research Fellow, 1965
National Science Foundation Graduate Fellow, Yale University, 1968-1972
Fulbright Senior Lecturer, Bogota and Medillin, Colombia, 1978
Visiting Scientist, Indiana University (on sabbatical leave from UNM), 1982
Visiting Scholar, Harvard University (on sabbatical leave from UNM), 1982

BOOKS EDITED

University of New Mexico Self Study Report for Institutional Accreditation. May, 1989, 619 pages

ARTICLES IN REFEREED JOURNALS

1. "On the '*trans* enol' of Ethyl α-*sec*-butylacetoacetate," Tetrahedron Letters, 669-672 (1963), with S. J. Rhoads, R. W. Hasbrouck, and C. Pryde.
2. "Spectra-Structure Correlations of O-Alkyl Derivatives of β-Ketoesters," J. Colo.-Wyo. Acad. Sci., *V*, 26 (1965), with S. J. Rhoads.
3. "A Comparative Study of C- and O-Alkylation in Cyclic and Acyclic β-Ketoester Systems," Tetrahedron, *25*, 5443-5450 (1969), with S. J. Rhoads.
4. "Forbidden 1,3-Sigmatropic Rearrangements," J. Amer. Chem. Soc., *95*, 2037-2038 (1973), with J. A. Berson.
5. "A Simple Liquid-Liquid Continuous Extractor," J. Chem. Educ., *50*, 639 (1973)
6. "Interpretation of the Pseudocontact Model for Nuclear Magnetic Shift Reagents. VI. Determination of the Stereoisomeric Relationships of Four Structurally Isomeric Methylbicyclooctenols," J. Org. Chem., *40*, 1952-1957 (1975), with M. R. Willcott and R. E. Davis.
7. "Ketene Cycloadditions," J. Chem. Educ., *53*, 81-85 (1976).

8. “Preparation of Vinylketene by 1.4-Elimination. Cycloaddition and Isomerization to form α-Ethylidenecyclobutanones,” J. Org. Chem., *41*, 3303-3307 (1976), with H. S. Freiman and M. F. Stefanchik.
9. “Lithium Triethylborohydride Reduction of Alkyl Methanesulfonate Esters,” J. Org. Chem. *42*, 2166-2168 (1977), with M. G. Matturro.
10. “Geminate-Substituted Cyclopentadienes. 1. Synthesis of 5, 5-Dialkylcyclopentadienes *via* 4, 4-Dialkylcyclopent-2-en-1-ones,” J. Org. Chem., *47*, 1445-1451 (1982), with J. P. Daub, W. E. Baker, R. H. Gilbert III, and N. A. Graf.
11. “Thermal Rearrangements of Encumbered Methylenecyclobutanes. 1. 6-Methylenebicyclo[3.2.0]heptane,” J. Amer. Chem. Soc., *104*, 2926-2927 (1982), with P. A. Leber.
12. “Geminate-Alkylcyclopentadienes. 2. A Secondary Deuterium Kinetic Isotope Effect Study of the Cycloaddition of Diphenylketene and 5, 5-Dimethylcyclopentadiene,” J. Amer. Chem. Soc., *105*, 2929-2931 (1983), with N. A. Graf, E. Duesler, and J. C. Moss.

OTHER WRITINGS

“Chemistry as a Profession,” The Chemist., *XLI*, 436 (1964).

REFEREED PRESENTATIONS TO PROFESSIONAL MEETINGS

1. “A Comparative Study of C- and O-Alkylation in Cyclic *vs*. Acyclic β-Ketoester Systems,” 157th National Meeting, American Chemical Society, Minneapolis, Minnesosta, April 13-18, 1969: ORGN, 156, with S. J. Rhoads.
2. “Preparation of Vinylketene by 1, 4-Elimination,” 170th National Meeting, American Chemical Society, Chicago, Illinois, August 25-29, 1975: ORGN, 99, with H. S. Freiman.
3. “Reduction of Alkyl Sulfonate Esters by Lithium Triethylborohydride,” Rocky Mountain Regional Meeting, American Chemical Society, Laramie, Wyoming, June 17-19, 1976: ORGN, 149, with M. G. Matturro.
4. “Thermal Sigmatropic Reactions of Labeled 7-Methylenebicyclo[4.2.0]oct-2-ene,” 173rd National Meeting, American Chemical Society, New Orleans, Louisiana, March 21-25, 1977: ORGN, 80, with R. E. Voorhees.
5. “Preparation of a Series of 5,5-Dialkylcyclopentadienes,” 175th National Meeting, American Chemical Society, Anaheim, California, March 13-17, 1978: ORGN, 80, with J. P. Daub, W. F. Baker, and R. H. Gilbert, III.
6. “Thermal Reactions of Some Encumbered Methylenecyclobutanes,” 183rd National Meeting, American Chemical Society, Las Vegas, Nevada, March 28-April 2, 1982: ORGN, 141, with P. A. Leber.
7. “Secondary Deuterium Kinetic Isotope Effects in the Cycloaddition of 5, 5-Dimethylcyclopenta-1, 3-diene and Diphenylketene,” 184th National Meeting, American Chemical Society, Kansas City, Missouri, September 12-17, 1982: ORGN, 77, with N. A. Graf.

8. “Ketene Cycloadditions to *geminate*-Alkylcyclopentadienes,” 38th Southwest and 6th Rocky Mountain Combined Regional Meeting, American Chemical Society, El Paso, Texas, December 1-3, 1982; ORGN, 247, with N. A. Graf.
9. “Cycloadditions of Diphenylketene to *geminate*-Alkylcyclopentadienes,” 29th IUPAC Congress, Cologne, June 9, 1983: ORGN, 157, with N. A. Graf, J. C. Moss, and E. M. Duesler.
10. “Kinetic Analysis of the Thermal Interconversion of Four Monomethyl Derivatives of an Encumbered Methylenecyclobutane,” 7th Rocky Mountain Regional Meeting, American Chemical Society, Albuquerque, New Mexico, June 6-8, 1984: ORGN, 78, with C. T. Koch.
11. “The Mechanism of the Thermal Racemization of Encumbered Methylenecyclobutanes,” 7th Rocky Mountain Regional Meeting, American Chemical Society, Albuquerque, New Mexico, June 6-8, 1984: ORGN, 97, with P. A. Leber, P. S. Beauchamp, and D. T. Robertson.
12. “Diels-Alder Reactions of geminate-Alkylcyclopentadienes,” 7th Rocky Mountain Regional Meeting, American Chemical Society, Albuquerque, New Mexico, June 6-8, 1984: ORGN, 98, with G. S. Lichtenstein and K. A. Temple.
13. “Secondary Deuterium Isotope Effects in the Ketene Cycloadditions to 5, 5-Dimethylcyclopentadiene,” 7th Rocky Mountain Regional Meeting, American Chemical Society, Albuquerque, New Mexico, June 6-8, 1984: ORGN, 99, with N. A. Graf, R. W. Irwin, and M. S. McBride.

INVITED LECTURES

1973: Brooklyn College, University of Michigan
1975: University of Wyoming
1981: Indiana University, Harvard University, Boston University, Yale University
1985: Catholic University, University of Wyoming, Vassar College, Franklin & Marshall College, Wellesley College, University of Maryland

RESEARCH GRANTS

July 1, 1973	Vassar College Beadle Fund	$120
Nov. 9, 1973	Vassar College Grant-in-Aid	237
Sept. 1, 1974	Petroleum Research Fund	11,000
Sept. 1, 1974	Research Corporation	6,000
Sept. 17, 1974	UNM Research Allocation Comm.	1,000
Sept. 11, 1975	UNM Research Allocation Comm.	850
June 1, 1976	NSF Undergrad. Research	1,249
Oct. 13, 1976	UNM Research Allocation Comm.	939
Sept. 1, 1977	Petroleum Research Fund	30,000
Sept. 14, 1977	UNM Research Allocation Comm.	1,000
Sept. 1, 1987	Petroleum Research Fund	45,000
Sept. 21, 1982	Petroleum Research Fund Supp.	4,000
Sept. 13, 1991	National Science Foundation	131,600

Curriculum Vitae

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Education:
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1979-84 Ph.D. Chemistry, University of California, Berkeley

Employment History:
1995-present Associate Professor of Chemistry,
University of New Mexico
1989-95 Assistant Professor of Chemistry,
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1988-89 Visiting Research Assistant Professor of Chemistry,
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1987-88 Postdoctoral Assistant, Department of Chemistry,
University of New Mexico
1985-87 Postdoctoral Fellow, Department of Chemistry,
Stanford University
1984-85 Postdoctoral Assistant, Department of Chemistry,
University of New Mexico
1979-84 Research and Teaching Assistant, Department of Chemistry, University of California, Berkeley

Professional Recognitions, Honors, and Memberships:
NIH Postdoctoral Fellow, Stanford University, 1985-87
University Fellow, University of California, Berkeley, 1981-82
Undergraduate Fellow, Department of Chemistry,
Pacific Lutheran University, 1978-79

Current Support
Funded
Controllable Adhesion, Detection, and Release by "Smart" Nanoscale Surfaces- Keller, David J, PI Whitten, D Co-PI, Lopez, G Co-PI, Guo, H Co-PI, Schanze, K Co-PI, Grey, J Co-PI, Ista, L Co-PI Defense Threat Reduction Agency, $1,400,000 Funded July-2011 - Jul-2014
Not Funded
Functional Model for DNA Polymerases Keller, David J PI, Guo, Hua Co-PI, Brozik, James Co-PI National Science Foundation $441,003

Synergistic Activities
NSF Molecular Biophysics Review Panel, 1999-2002
NIH BBCB Study Section, March 2003
NSF Biological Instrumentation Review Panel, Dec 2006
NIH Genome Sequencing Review Panel, April 2007

NSF MCB-Physics Review Panel, November 2009

Collaborators

James Brozik, Department of Chemistry, Washington State University
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Gabriel Lopez, Department of Chemical and Nuclear Engineering, University of New Mexico
Linnae Ista, Department of Chemical and Nuclear Engineering, University of New Mexico
Kirk Schanze, Department of Chemistry, University of Florida

Publications

1. I. Tinoco Jr. and D. Keller Scattering of Circularly Polarized Radiation *J. Phys. Chem.* **87**, 2915 (1983).

2. D. Keller, C. Bustamante, and I. Tinoco Jr. Quantum Mechanical Treatment of Circular Intensity Differential Scattering: The Elastic Process *J. Chem. Phys.* **81**, 1643 (1984).

3. C. Bustamante, M. F. Maestre, D. Keller, and I. Tinoco Jr. Differential Scattering (CIDS) of Circularly Polarized Light by Dense Particles *J. Chem. Phys.* **80,** 4817 (1984).

4. C. Bustamante, K. S. Wells, D. Keller, B. Samori, M. F. Maestre, and I. Tinoco Jr. The Circular Intensity Differential Scattering (CIDS) of Cholesteric and Blue Mesophases *Mol. Cryst. Liq. Cryst.* **111**, 79-102 (1984).

5. I. Tinoco Jr., M. F. Maestre, C. Bustamante, and D. Keller Use of Circularly Polarized Light to Study Biological Macromolecules *Pure and Appl. Chem.* **56**, 1423 (1984).

6. D. Keller, C. Bustamante, M. F. Maestre, and I. Tinoco Jr. Imaging of Optically Active Biological Structures Using Circularly Polarized Light *Proc. Natl. Acad. Sci. USA* **82**, 401 (1985).

7. D. Keller, C. Bustamante, M. F. Maestre, and I. Tinoco Jr. Model Computations on the Differential Scattering of Circularly Polarized Light (CIDS) by Dense Macromolecular Structures *Biopolymers* **24**, 783 (1985).

8. C. Bustamante, M. F. Maestre, and D. Keller Simplified Expressions for the Circular Intensity Differential Scattering of Chiral Aggregates *Biopolymers* **24**, 1595 (1985).

9. K. Hall, K. S. Wells, D. Keller, B. Samori, M. F. Maestre, I. Tinoco Jr., and C. Bustamante Circular Intensity Differential Scattering Measurements of Planar and Focal Conic Orientations of Cholesteric Liquid Crystals in "Applications of Circularly Polarized Radiation" F. S. Allen and C. Bustamante eds., Plenum Press, N. Y. (1985).

10. D. Keller and C. Bustamante CIDS Calculations on Quartz at Hard X-ray Wavelengths in "Applications of Circularly Polarized Radiation" F. S. Allen and C. Bustamante, eds., Plenum Press, N. Y. (1985).

11. M. F. Maestre, D. Keller, C. Bustamante, and I. Tinoco Jr. Circular Differential Microscopy in "Applications of Circularly Polarized Radiation" F. S. Allen and C. Bustamante, eds., Plenum Press, N. Y. (1985).

12. D. Keller and C. Bustamante Theory of the Interaction of Light with Large Inhomogeneous Molecular Aggregates: I. Absorption *J. Chem. Phys.* **84**, 2961 (1986).

13. D. Keller and C. Bustamante Theory of the Interaction of Light with Large Inhomogeneous Molecular Aggregates: II. Psi-Type Circular Dichroism *J. Chem. Phys.* **84**, 2972 (1986).

14. M. Kim, L. Ulibarri, D. Keller, M. F. Maestre, and C. Bustamante Theory of the Interaction of Light with Large Inhomogeneous Molecular Aggregates: III. Calculations *J. Chem. Phys.* **84**, 2981 (1986).

15. K. S. Wells, D. Beach, D. Keller, and C. Bustamante The measurement of the Circular Intensity Differential Scattering of Chiral Aggregates: Studies on the Sperm Cell of Eledone Cirrhosa *Biopolymers* **25**, 2043 (1986).

16. H. M. McConnell, D. J. Keller, and H. E. Gaub Thermodynamic Models for the Shapes of Monolayer Phospholipid Crystals *J. Phys. Chem.* **90**, 1717 (1986).

17. V. T. Moy, D. J. Keller, H. E. Gaub, and H. M. McConnell Long-Range Molecular Orientational Order in Monolayer Solid Domains of Phospholipid *J. Phys. Chem.* **90**, 3198 (1986).

18. D. Keller, H. M. McConnell, and V. Moy Theory of Super- structures in Lipid Monolayer Phase Transitions *J. Phys. Chem.* **90**, 2311 (1986).

19. D. J. Keller , J. P. Korb, and H. M. McConnell Theory of Shape Transitions in Two Dimensional Phospholipid Domains. *J. Phys. Chem.* **91**, 6417 (1987).

20. C. Bustamante and D. Keller Theory of Absorption and Circular Dichroism of Large Inhomogeneous Molecular Aggregates. in "New Developments of Polarized Spectroscopy of Ordered Systems", NATO Advanced Studies Institute Series (1988).

21. R. Garcia, D. Keller, J. A. Panitz, and C. Bustamante Imaging of Metal Coated Biological Samples by Scanning Tunneling Microscopy, *Ultramicroscopy* **27**, 367 (1989).

22. D. Keller, C. Bustamante, and R.Keller Imaging of Single DNA Molecules by Scanning Tunneling Microscopy *Proc. Natl. Acad. Sci. U.S.A.* **86**, 5356 (1989).

23. R. W. Keller, D. D. Dunlap, C. Bustamante, D. J. Keller, R. G. Garcia, C. Gray, and M. F. Maestre STM Images of Metal Coated Bacteriophages and Uncoated Double Stranded DNA *J. Vac. Sci. Technol.*, **A8**, 706 (1989).

24. D. Keller, Reconstruction of STM and AFM Images Distorted by Finite Size Tips, *Surface Science* **253**, 353 (1991).

25. D. Keller and C. C. Chou Imaging Steep, High Structures by Atomic Force Microscopy Using Electron Beam Deposited Tips, *Surface Science*, **268**, 333 (1992).

26. S. Singh and D. Keller Atomic Force Microscopy of Supported Planar Membrane Bilayers, *Biophys. J.*, **60**, 1401 (1991).

27. Jiang Yuqiu, Juang Ching-Bo, David Keller, Carlos Bustamante, David Beach, Tim Houseal, Eduardo Builes, and Marcos Maestre, Mechanical, Electrical, and Chemical Manipulation of Single DNA Molecules, *Nanotechnology*, **1**, 5 (1991).

28. David Keller, Dan Deputy, Andrew Alduino, and Ke Luo Sharp, Vertical-Walled Tips for Scanning Force Microscopy of Steep or Soft Samples *Ultramicroscopy*, **42-44**, 1481 (1992).

29. J. Vasenka, M. Guthold, C. L. Tang, D. Keller, R. Keller, E. Delain, and C. Bustamante Substrate Preparation for Reliable Imaging of DNA Molecules with the Scanning Force Microscope, *Ultramicroscopy*, **42-44**, 1243(1992).

30. Keller, R.W., Keller, D.J., Bear, D., Vasenka, J., and Bustamante, C., "Electrodeposition procedure of *E.coli* RNA polymerase onto gold and deposition of *E. coli* RNA polymerase onto mica for observation with scanning force microscopy" *Ultramicroscopy* **42-44**,1173-1180 (1992).

31. D. Keller, L. Chang, Ke Luo, Seema Singh, and M. Yorgancioglu Scanning Force Microscopy of Cells and Membrane Proteins *Proc. SPIE*, **1639**, 91 (1992).

32. L. Chang, D. Keller, T. Kious, M. Yorgancioglu, J. Pfeiffer, and J. Oliver Living, Unstained Cells Imaged by Scanning Force Microscopy, *Biophys J.*, **64**, 1282 (1993).

33. D. Keller and C. Bustamante Attaching Molecules to Surfaces for Scanning Probe Microscopy, *Biophys. J.*, **64**, 896-897 (1993).

34. C. Bustamante, D. Keller, and G. Yang Scanning Force Microscopy of Nucleic Acids and Nucleoprotein Assemblies, *Current Opinion in Structural Biology*, **3**, 363 - 372 (1993).

35. K. Luo, M. Yorgancioglu, and D. Keller Scanning Force Microscopy at -25°C, *Ultramicroscopy*, **50**, 147-155 (1993).

36. F. Franke and D. Keller Toward High Resolution Imaging of DNA, *Proc. SPIE*, **1891**, 78-84 (1993).

37. D. Keller and F. Franke Envelope Reconstruction of Scanning Probe Microscope Images, *Surface Science*, **294**, 409-419 (1993).

38. R. H. Krukar, S. S. H. Naqvi, J. R. McNeil, D. R. Hush, J. E. Franke, T. M. Niemczyk, D. Keller, R. A. Gottscho, and Avi Kornblit Analyzing Simulated andMeasured Optical Scatter

for Semiconductor Process Verification, Proc. SPIE-Int. Soc. Opt. Eng. 1907, 238-249 (1993).

39. C. Bustamante, D. Erie, and D. Keller Biomolecular Imaging by Scanning Force Microscopy, *Current Opinion in Structural Biology*, **4**, 750-760 (1994).

40. Leda Chang, Fransiska S. Franke, Paula Flicker, and David Keller Left and Right Topography of F-Actin Filaments, *Proc. SPIE-Int. Soc. Opt. Eng.* **2040, 223-226** (1995).

41. Carlos Bustamante and David Keller Imaging Applications of Scanning Force Microscopy in Biology, *Physics Today* **48**, 32-38 (1995).

42. David Keller, Theory of Circular Dichroism of DNA, in Circular Dichroism and The Conformational Analysis of Biomolecules, Gerald D. Fasman, editor, Plenum Press, New York (1996), pp413-431.

43. David Keller A Nanotube Molecular Tool (News & Views article), Nature **384**, 111 (1996).

44. Seema Singh, Paola Turina, Carlos J. Bustamante, David J. Keller, and Roderick Capaldi Topographical Structure of E. Coli F1Fo ATP Synthase in Aqueous Buffer by Scanning Force Microscopy FEBS Letters **397**, 30-34 (1996).

45. Carlos Bustamante, Claudio Rivetti, and David Keller Scanning Force Microscopy Under Aqueous Solutions Current Opinion in Structural Biology, **7**, 709-716 (1997).

46. David Keller Making Movies of Molecular Motions Biophys J. **74**, 2743-2744 (1998).

47. David Keller Scanning Force Microscopy in Biology, in Physical Chemistry of Biological Interfaces, Adam Baszkin and Willem Norde, eds, Marcel Dekker, NY, pp769-797 (1999).

48. David Keller and Carlos Bustamante, The Mechanochemistry of Molecular Motors. Biophys. J. **78**, 541-556 (2000).

49. Wuite GJL, Smith SB, Young M, Keller D, Bustamante C Single-molecule studies of the effect of template tension on T7 DNA polymerase activity Nature **404**, 103-106 (2000)

50. Carlos Bustamante, David Keller, and George Oster The Physics of Molecular Motors Accounts of Chemical Research **34**, 412-420 (2001).

51. Solomon B. Basame, Diana Habel-Rodriquez, and David Keller Morphology and Surface Reconstruction on RuO_2 Single Crystals Applied Surface Science **183**, 62-67 (2001).

52. David Keller, David Swigon, and Carlos Bustamante Relating Single-Molecule Measurements to Thermodynamics Biophys. J. **84**, 733-738 (2003).

53. Sandra L. Martin, Dan Branciforte, David Keller and David L. Bain Novel trimeric structure for an essential protein in LINE-1 retrotransposition. Proc. Nat. Acad. Sci. **100**, 13815-13820 (2003).

54. Hailong Lu, Jed Macosko, Diana Habel-Rodriquez, Rebecca W. Keller, James A. Brozik, and David J. Keller Closing of the Fingers Domain Generates Motor Forces in the HIV Reverse Transcriptase J. Biol. Chem. **279**, 54529-54532 (2004).

55. Qiang Fu, G. V. Rama Rao, Solomon B. Basame, David J. Keller, Kateryna Artyushkova, Julia E. Fulghum, and Gabriel P. Lopez Reversible Control of Free Energy and Topography of Nanostructured Surfaces J. Am. Chem. Soc.**126**, 8904-8905 (2004)

56. Ryan W. Davis, Elizabeth L. Patrick, Lauren A. Meyer, Theodore P. Ortiz, Jason A. Marshall, David J. Keller, Susan M. Brozik, and James A. Brozik* "The Thermodynamic Properties of Single Ion Channel Formation: Gramicidin". *Journal of Physical Chemistry B,* **108**, 15364-15369 (2004).

57. David J. Keller and James A. Brozik Framework Model for DNA Polymerases Biochemistry **44**, 6877-6888 (2005)

58. Theodore P. Ortiz, Jason A. Marshall, Lauren A. Meyer, Ryan W. Davis, Jed C. Macosko, Jeremy Hatch, David J. Keller, and James A. Brozik "Stepping Statistics of Single HIV-1 Reverse Transcriptase Molecules During DNA Polymerization", J. Phys. Chem. B **109**, 16127-16131 (2005).

59. Solomon Basame, Patrick Wai-lun Li, Grant Howard, Dan Branciforte David Keller and Sandra L. Martin Spatial Assembly and RNA Binding Stoichiometry of a LINE-1 Protein Essential for Retrotransposition J. Mol. Biol. **357**, 351-357 (2006)

60. S. Mendez, B. P. Andrzejewski, H. E. Canavan,D. J. Keller, J. D. McCoy, G. P. Lopez, and J. G. Curro Understanding the Force-vs-Distance Profiles of Terminally Attached Poly(N-isopropyl acrylamide) Thin Films Langmuir **25**, 10624 (2009)

61. Kumud Poudel, David Keller, and James Brozik Single-Particle Tracking Reveals Corralling of a Transmembrane Protein in a Double-Cushioned Lipid Bilayer Assembly Lanmuir **27**, 320-327 (2011)

62. Lance Edens, James Brozik, and David Keller Coarse-Grained Model DNA: Structure, Sequences, Stems, Circles, Hairpins J. Phys. Chem. Accepted with revision March 2012

63. Kumud R. Poudel†, David J. Keller, and James A. Brozik* "The Effect of a Phase Transition on Single Molecule Tracks of Annexin V in Cushioned DMPC Assemblies", Submitted to Soft Matter, May 2012

Abstracts and Presentations

1. Carlos Bustamante, Rebecca Keller, David Keller, and David Dunlap STM Imaging of Single Uncoated DNA Molecules 4th International Conference on Scanning Tunneling Microscopy/Spectroscopy, Oarai, Japan (1989).

2. David Keller, Scanning Probe Microscopy of Biological Molecules, recruiting trip to Adam State College, Alamosa, CO, Nov. 1990.

3. D. J. Keller, J. Pfeiffer, and J. M. Oliver STM Imaging of Immune Receptors on Metal Coated Cell Surfaces 34th Annual Meeting of the Biophysical Society, Baltimore (1990).

4. David Keller and Ching-Bo Juang Legendre Transform STM and AFM Image Reconstruction 5th International Conference on Scanning Tunneling Microscopy/Spectroscopy, Baltimore (1990).

5. David Keller, Jan Pfeiffer, and Janet Oliver STM Imaging of Metal Coated Cell Surfaces and Antibody Molecules 5th International Conference on Scanning Tunneling Microscopy/Spectroscopy, Baltimore (1990).

6. Jiang Yuqiu, Juang Ching-Bo, David Keller, Carlos Bustamante, David Beach, Tim Houseal, Eduardo Builes, and Marcos Maestre Mechanical, Electrical, and Chemical Manipulation of Single DNA Molecules, Micro 90: Proceedings of the Royal Microscopical Society, London (1990).

7. Rebecca Keller, Jiang Yuqiu, David Keller, and Carlos Bustamante Imaging and Manipulation of Biomolecules by Scanning Tunneling Microscopy 5th International Conference on Scanning Tunneling Microscopy/Spectroscopy, Baltimore (1990).

8. David Keller, Scanning Tunneling Microscopy and Atomic Force Microscopy of Biological Materials, recruiting trip to University of Colorado, Colorado Springs, Feb. 1991

9. D. Keller Probe Tips for Scanning Probe Microscopy: Effects of Probe Geometry on Images, Fabrication, and Applications to High Resolution Force Microscopy SEMATECH Scanning Probe Microscopy Meeting, Austin 1991.

10. David Keller and Chou Chih-Chung, Hard, Vertical-Walled Tips for Scanning Force Microscopy of Steep Structures, 6th International Conference on Scanning Tunneling Microscopy/Spectroscopy, Interlaken, Switzerland, August (1991).

11. David Keller and Seema Singh, Scanning Force Microscopy of Model Membranes, 6th International Conference on Scanning Tunneling Microscopy/Spectroscopy, Interlaken, Switzerland, August (1991).

12. L. Chang, T. Kious, M. Yorgancioglu, D. Keller, J. Pfeiffer, and J. Oliver Cytoskeletal Elements Imaged by Scanning Force Microscopy, 6th International Conference on Scanning Tunneling Microscopy/Spectroscopy, Interlaken, Switzerland, August (1991).

13. Rebecca W. Keller, David J. Keller, and Carlos Bustamante, Atomic Force Microscopy of RNA Polymerase on Gold Substrates, 6th International Conference on Scanning Tunneling Microscopy/Spectroscopy, Interlaken, Switzerland, August (1991).

14. J. Vasenka, M. Guthold, E. Delain, R. Keller, D. Keller, and C. Bustamante, Substrate Preparation for Imaging Biomolecules with Scanning Force Microscopy, 6th International Conference on Scanning Tunneling Microscopy/Spectroscopy, Interlaken, Switzerland, August (1991).

15. David Keller, Leda Chang, Ke Luo, and Maxim Yorgancioglu Scanning Force Microscopy of Cells and Cell Membranes Lasers, Sensors, and Spectroscopy, SPIE OE LASE „92, Los Angeles, January 1992.

16. D. Keller Progress on Scanning Force Microscopy of Biological Materials, Los Alamos National Labs, Jan. 1992.

17. D. Keller and Andrew Alduino Deposition and Growth of Small Structures by Focused Electron Beams, 182nd Meeting of the Electrochemical Society, Toronto, Canada, Oct. 15, 1992.

18. Leda Chang and David Keller Probing Cytoskeleton of Fixed and Living Cells With Scanning Force Microscopy 39th National Symposium of the American Vacuum Society, Chicago, Nov. 13, 1992.

19. David Keller Imaging Biological Molecules by Scanning Force Microscopy University of Colorado, Colorado Springs, Nov. 1992.

20. David Keller Imaging Biological Molecules by Scanning Force Microscopy Colorado College, Colorado Springs, Nov. 1992.

21. D. Keller, F. Franke, and L. Chang Envelope Reconstruction, Second Fourmentin Society Workshop on STM-AFM and Biological Objects, Abbey Royaumont, France, Nov. 13, 1992.

22. David Keller and Andrew Alduino Mechanisms of Electron Beam Deposition and Growth 39th National Symposium of the American Vacuum Society, Chicago, Nov. 13, 1992.

23. David Keller and Andrew Alduino Probe Tips and Other Structures Fabricated with a Focused Electron Beam, in Scanning Probe Microscopies II, S. P. I. E. conference O. E. Lase „93, Los Angeles, Jan., 1993.

24. D. Keller, Seema Singh, and Ke Luo Imaging Respiratory Proteins by Scanning Force Microscopy, in Scanning Probe Microscopies II, S. P. I. E. conference O. E. Lase „93, Los Angeles, Jan. 18, 1993.

25. D. Keller, A. Alduino, Ke Luo, and F. Franke Toward High Resolution Imaging of DNA by Scanning Force Microscopy, in Advances in DNA Sequencing Technology, S. P. I. E. conference O. E. Lase „93, Jan. 21, 1993

26. David Keller, Short Course on Scanning Probe Microscopy (8 lectures), University of Calabria, Arcavacata di Rende, Calabria, Italy, May 13-23 (1993).

27. Leda Chang, Fransiska Franke, Ke Luo, Maxim Yorgancioglu, and David Keller, Scanning Force Microscopy of Actin and Myosin, 7th International Conference on Scanning Tunneling Microscopy/Spectroscopy, Beijing, Aug. 1993.

28. Ke Luo, Fransiska Franke, and David Keller, Sharp Tips Fabricated by Oxygen Etching of E-Beam Carbon Spikes, 7th International Conference on Scanning Tunneling Microscopy/Spectroscopy, Beijing, Aug. 1993.

29. Ke Luo, Fransiska Franke, and David Keller, Semiconductor Metrology by SFM, Topometrix, Santa Clara, Sept. 1993.

30. Fransiska S. Franke and David J. Keller, Envelope Reconstruction of SFM Images for Semiconductor Device Metrology, TECHON „93, Atlanta, Sept. 1993.

31. Ke Luo, Fransiska Franke, and David Keller, Electron Beam Growth of High Aspect Ratio Structures, TECHON „93, Atlanta, Sept. 1993.

32. Leda Chang, Fransiska Franke, and David Keller, Can Actin Be Left Handed?, American Society for Cell Biology, New Orleans, Dec. 1993.

33. David Keller, Leda Chang, and Fransiska Franke, Investigating Cytoskeleton by SFM, tutorial session at the American Society for Cell Biology, New Orleans, Dec. 1993.

34. D. Keller, Ke Luo, and Fransiska Franke Sharp Probe Tips and Probe Image Interpretation, American Chemical Society, San Diego, March 1994.

35. D. Keller and Fransiska Franke. Analysis of Probe Microscope Images. National Institute of Standards and Technology, May 1994

36. David Keller, Scanning Probe Microscopy, 3 hr tutorial session at Scanning/SEEMS „94, Charleston, May 1994

37. D. Keller, Left and Right Handed F-Actin / Tapping Force Microscopy. Topometrix Inc., Santa Clara, July 1994

38. D. Keller, Leda Chang, and Fransiska Franke, Actin Can Adopt Left and Right Handed Helical Conformations. NATO Conference on Advances in Scanning Probe Microscopy, Schloß Ringberg, Germany, June 1994.

39. W. Wriggers, R. Jones, K. Schulten and D. Keller Conformational Differences in ATP- and ADP-bound G-Actin, 7th Annual Biophysical Discussions, New Orleans, Aug. 1994.

40. D. Keller, Leda Chang, Fransiska Franke, and Robert Jones, Right and Left Handed Actin Filaments, Scanning Probe Microscopies III, Photonics West, SPIE San Jose, Feb 6, 1995.

41. Leda Chang, Fransiska Franke, Paula Flicker, and David Keller. Atomic Force Microscopy of F-Actin Shows Apparent Left Handed Filaments, Biophysical Society Meeting, San Fransisco, Feb. 1995.

42. Seema Singh, Sean Quigley, Katherine G. Vogel, and David Keller. Atomic Force Microscopy of Collagen and Proteoglycan, Biophysical Society Meeting, San Fransisco, Feb. 1995.

43. Seema Singh, Paola Turina, David Keller, Carlos Bustamante, and Roderick Capaldi. Stucture of the F_1F_o ATP Synthase of E. coli. 8th International Conference in Scanning Tunneling Microscopy/Spectroscopy, Denver, CO, July 1995.

44. D. Keller, Seema Singh, Paola Turina, Carlos Bustamante, and Roderick Capaldi. Subunit Structure of ATP Synthase by SFM and Single Particle Image Analysis. Microscopy Society of America, 53rd Annual Meeting, Kansas City, MO, Aug. 1995.

45. David Keller, Seema Singh, Paola Turina, Roderick Capaldi, and Carlos Bustamante Structure of E. coli F1Fo ATP Synthase in Aqueous Buffer. Gordon Conference on Biopolymers, Newport, RI, June 1996.

46. D. Keller and C. Bustamante Kinetic/Stochastic Theory of Molecular Machines. Gordon Conference on Biopolymers, Newport, RI, June 1998.

47. David Keller, Gys Wuite, and Carlos Bustamante Single-Molecule Mechanochemistry and Molecular Motors, Conference on Single Molecule Biophysics, Tours, France, July 1999.

48. David Keller, David Swigon, and Carlos Bustamante Measurement and Non-Thermodynamic Behavior in the Single Molecule Limit. Conference on Single Molecule Biophysics, Tours, France, July 1999.

49. David Keller, Gijs Wuite, Steve Smith, and Carlos Bustamante Motions, Forces, and Mechanisms of Single Polymerase Molecules Los Alamos National Lab, Los Alamos NM, September 1999

50. David Keller Mechanochemistry of Molecular Motors and Machines Program on Mathematics and Molecular Biology Conference, Santa Fe NM, December 1999.

51. David Keller Single Molecule Physics Consortium of the Americas for Interdisciplinary Science Conference, Center for Advanced Studies, Albuquerque, NM, June 2000

52. David Keller Mechanochemistry of T7 DNA Polymerase Sandia National Labs, Albuquerque NM, July 2000

53. David Keller Single Molecular Motors Department of Physics, University of New Mexico, Albuquerque NM, May 2000

54. David Keller Single Molecule Theory and Modeling NIH Symposium on Single Molecule Biophysics, Bethesda, MD, April 2000

55. David Keller Single Molecular Machines Center for High Technology Materials MURI Program, Albuquerque NM, October 2000

56. David Keller Single Molecular Machines Department of Biology, University of New Mexico, Albuquerque NM, August 2000

57. David Keller Biological Nanomachines 2 Lectures, Nanotechnology Course, Center for High Technology Materials, Albuquerque NM, April 2001

58. David Keller Theory of Molecular Motors 1 Lecture, Biophysics Course, Department of Molecular and Cellular Biology, UC Berkeley, May 2002

59. David Keller and Hailong Lu Forces and Motions of HIV Reverse Transcriptase NIH National Institute on Drug Abuse Symposium, Bethesda MD, December 2002

60. Sandra Martin, David Bain, Dan Branciforte, David Keller, and Patrick Li Structural and Functional Analyses of the ORF1 Protein from Mouse LINE-1: Implications for Retrotransposition, February 2003

61. David Keller and Hailong Lu Single Molecule Studies on HIV Reverse Transcriptase Aspen Conference on Single Molecule Biophysics, Aspen Center for Physics, Aspen CO, January 2003.

62. J. A. Brozik, J. A. Marshall, T. P. Ortiz, L. A. Meyer, R. W. Davis, J. C. Macosko, and D. J. Keller "Single-Molecule Kinetic Analysis of DNA Polymerization by HIV-1 Reverse Transcriptase" 59th Southwest Regional American Chemical Society Meeting, Oklahoma City, OK, October 2003.

63. R. W. Davis, E. L. Patrick, T. P. Ortiz, L. A. Meyer, S. M. Brozik, D. J. Keller, and J. A. Brozik "Thermodynamics of Single Gramicidin Ion Channel Formation" 59th Southwest Regional American Chemical Society Meeting, Oklahoma City, OK, October 2003.

64. Hailong Lu, Solomon Basame, Diana Habel-Rodriguez, and David Keller Motor Forces of HIV Reverse Transcriptase, Southwest Regional ACS Meeting, Logan Utah, June, 2004

65. David Keller Molecular Machines Physics Colloquium, UNM. Aug. 2004

66. Solomon Basame, Grant Howard, Jed Macosko, Sandra Martin, and David Keller ORF1p: Structure and Binding Specificity to RNA, Southwest Regional ACS Meeting, Logan Utah, June, 2004

67. R. W. Davis, E. L. Patrick, T. P. Ortiz, L. A. Meyer, S. M. Brozik, D. J. Keller, and J. A. Brozik "The Thermodynamic Properties of Single Ion Channel Formation: Gramicidin" Joint Northwest / Rocky Mountain Regional American Chemical Society Meeting, Logan, UT, June 2004.

68. T. P. Ortiz, J. A. Marshall, L. A. Meyer, R. W. Davis, J. C. Macosko, D. J. Keller, and J. A. Brozik "Stepping Statistics of Single HIV-1 Reverse Transcriptase Molecules During DNA Polymerization" Joint Northwest / Rocky Mountain Regional American Chemical Society Meeting, Logan, UT, June 2004.

69. David Keller and Jim Brozik Framework Model for DNA Polymerases Southwest Regional ACS Meeting, Logan Utah, June, 2004

70. Theodore P. Ortiz, M. Schulze, J. A. Marshall, L. A. Meyer, D. Latham, R. W. Davis, D. J. Keller, and J. A. Brozik "Kinetic Rates of Nucleotide Incoporation and Stepping Statistics of HIV-1 Reverse Transcriptase During DNA Polymerization", 50th Annual Biophysical Society Meeting, Salt Lake City, UT Feb 18th – 22nd 2006.

71. David Keller, Jim Brozik, Ted Ortiz, and Hailong Lu Mechanics of DNA Polymerases Gordon Conference on Single Molecule Methods in Biology, Colby-Sawyer College, NH, June 2006

72. J. A. Brozik, R.W. Davis, T.P. Ortiz, and D.J. Keller "Dynamic Single Molecule Fluorescence Imaging and Fluorescence Correlation of Membrane Bound Proteins on New Optically and Electrochemically Addressable Platforms" Gordon Research Conference, *Single Molecule Approaches to Biology*, Colby-Sawyer College, NH June 18th – 23rd 2006.

73. David Keller Machines that Replicate Genetic Information Department of Physics, University of Pittsburgh, March 2006

74. David Keller and Jim Brozik Machines that Replicate Genetic Information Los Alamos National Laboratory, July 2006

75. David Keller Mechanochemistry of DNA Polymerases Department of Chemistry, Wake Forest University, Aug. 2006

76. David Keller and Kirk Schanze Control of Biological Surface Adhesion CBDIF/DTRA Initial Review Conference, Washington DC, Nov. 2007

77. David Keller, David Whitten, Gabriel Lopez, Linnea Ista, John McCoy, John Grey Functional Polymer Surfaces for Binding, Sensing, and Destruction of Bioagents DTRA Site Visit, NM Tech/U. New Mexico Jan. 16 2008.

78. J. A. Brozik, A.O. Barden, K.R. Poudel, and D.J. Keller “Following Submonolayer Bioadhesion One Molecule at a Time” Chemical and Biological Defense Physical Science and Technology Conference, New Orleans, LA, February 2008

79. David Keller and David Whitten Biocidal Surfaces and Bacterial Adhesion Annual DTRA Review Meeting, Washington DC, June 2008

80. David Keller, David Whitten, Gabriel Lopez, Linnae Ista, and John Grey Control of Biological Surface Adhesion DTRA Site Visit Review, U. New Mexico, Dec. 2008

81. Keenan Dotson, John McCoy, Daniel McCoy, Sergio Mendez, John Curro, Brett Andrzejewski, Comparison of AFM and Density Functional Theory Force Profiles Gabriel Lopez, David Keller APS Meeting, March 10-14 2008

82. David Keller and David Whitten Controlled Capture, Destruction, and Release of CBW Agents Presentation for DTRA Site Visit/Review July 2008.

83. L Edens, D Keller, S McQuate, K Ogawa, X Zhao, L Ista, G Lopez, K Schanze, D Whitten Microscopic Interaction Energies on Biocidal Surfaces Chemical and Biological Defense Physical Science and Technology Conference, New Orleans November 2008

84. Brett Andrzejewski, Sarah McQuate, Lance Edens, Linnea Ista, David Whitten, Gabriel Lopez, and David Keller Surface Forces on Thermally Switchable Polymer Layers Chemical and Biological Defense Physical Science and Technology Conference, New Orleans November 2008

85. David Keller, David Whitten, Gabriel Lopez, Linnae Ista, and John Grey Multifunctional Biocidal Materials and Surfaces DTRA Site Visit/Review May 2009

86. David Keller, David Whitten, Gabriel Lopez, Linnea Ista, John McCoy, John Grey Control of Biological Surface Adhesion_ DTRA Site Visit, NM Tech/U. New Mexico Feb. 13 2009.

87. David Keller and Lance Edens A Residue-by-Residue Coarse-Grained Model for DNA Workshop on Multi-Scale Modeling of Biological Molecules, Mesilla, NM Feb.4 2009.

88. Brett Andrzejewski, Lance Edens, David Whitten, Gabriel Lopez, and David Keller Protein adhesion on the thermally responsive mixed self assembled monolayer of hexa(ethylene glycol) and dodecane thiolates Chemical and Biological Defense Physical Science and Technology Conference, Dallas, November 2009

89. David Keller, Lance Edens, and Brett Andrzejewski PWA Model for Bacterial and Particle Adhesion to Complex Surfaces Chemical and Biological Defense Physical Science and Technology Conference, Dallas, November 2009

90. Lance Edens and David Keller Adhesion and Elasticity of Biocidal Films by Atomic Force Microscopy Chemical and Biological Defense Physical Science and Technology Conference, Dallas, November 2009

91. J. A. Brozik, A.O. Barden, and D.J. Keller "Following Bioadhesion of Single Molecules onto Specific Receptor Sites" Chemical and Biological Defense Physical Science and Technology Conference, Dallas, TX, November 2009

92. L. Edens, J. A. Brozik, D. J. Keller "Simulating Bacterial Adhesion to Complex Surfaces" Chemical and Biological Defense Physical Science and Technology Conference, Orlando, FL, November 2010.

93. Kumud Poudel, David Keller, and James Brozik In Vitro Coralling of a Transmembrane Protein in a Double Cushioned Lipid Bilayer Assembly Biophysical Society Meeting, Baltimore, March 2011

94. David Keller "Switchable "Smart" Surfaces for Controlling Biological Adhesion and Release" DTRA Annual Review Meeting, Springfield VA, July 2012

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Education

Ph.D. in Inorganic Chemistry (1981), The University of Texas at Austin, Austin, Texas
Major Professor: Dr. Alan H. Cowley, *FRS*
Dissertation: "Cationic, Anionic, and Free Radical Chemistry of Low-Coordinate Phosphorus"
B.S. in Chemistry (1978), Texas Tech University, Lubbock, Texas
Undergraduate Research Advisors: Dr. John N. Marx (Organic) and Dr. Jerry L. Mills (Inorganic)

Professional Experience

Sandia National Laboratories/University of New Mexico, Albuquerque, New Mexico
2001-present: Principal Member of the Technical Staff, Full Professor of Chemistry

- Research Into New Nanomaterials for Catalytic Applications (DOE)
- Synthesis of New Homogeneous and Heterogeneous Olefin Polymerization Catalysts (ACS-PRF)
- Synthesis of New Catalysts for CO_2 Fixation and Sequestration (NSF, DOE)
- Homogeneous Catalyst Research into Direct Oxidation of Olefins (DOE-BES)

Union Carbide Corporation/Dow Chemical Company, Westhollow Research Center, Houston, Texas
1996-2001: Senior Research Scientist

- Co-Invented SHAC®330 High Selectivity Catalyst for Manufacture of Impact Co-Polymers
- Research Into Controlled Morphology Magnesium Alkoxide Catalyst Precursors (*with Sandia*)
- Developed and Commercialized SHAC®207 Controlled Morphology Polypropylene Catalyst
- R&D Into New Ligand Systems for Single-Site Polypropylene Catalysts
- Discovered Several New Donor Systems Useful for Ziegler-Natta Polypropylene Catalysts

Notes: *Shell Polypropylene Company Sold to Union Carbide Corporation in January, 1996*
Union Carbide Corporation Sold to Dow Chemical Company in February, 2001

Shell Development/Shell Polypropylene Companies, Westhollow Research Center, Houston, Texas
1990-1995: Senior Research Chemist

- Lab R&D Into New Super High Activity Catalysts (SHAC®) Polypropylene Catalysts
- Invented, Developed, and Commercialized S-880 and S-882 High Selectivity Catalysts for Ethylene Oxide Production Which Currently Produce >40% of the World's Ethylene Oxide
- Discovered a New Class of Ligands for the Oligomerization of Ethylene to Produce α-Olefins

1985-1990: Research Chemist

- Research Leading to a New Catalyst System for the Selective Oxidation of Alcohols to Acids
- Invented and Helped Commercialize Two Novel Catalyst Systems for the Production of Narrow Range Ethoxylates (*One Commercialized in U.S., One Commercialized in Europe*)
- Co-Invented New Olefin Metathesis Catalyst Useful in the Shell Higher Olefins Process

Richard Alan Kemp, Ph.D.

Shell Development/Shell Polypropylene Companies, Westhollow Research Center, Houston, Texas
1983-1985: Associate Research Chemist

- Invented a Novel One-Step Synthesis of Hydroprocessing Catalysts by an Aqueous Sol-Gel Process

Gulf Oil Chemicals Company, Polymer Research Center, Houston, Texas
1981-1983: Research Chemist

- Invented and Developed at Pilot Plant Scale a Novel Single-Component Ziegler-Natta Catalyst for Polyethylene with a Unique Hydrogen Sensitivity Response

Principal Scientific Interests

Heterogeneous Catalysis
Olefin Polymerization, Isomerization, Metathesis, Hydrotreating, Oxidation, Ethoxylation, Hydrogenation, Rare Earths
Homogeneous Catalysis
Olefin Polymerization, Oligomerization, Depolymerization, Hydrogenation

Synthetic Main Group Chemistry
Organo-Phosphorus Chemistry
Silicon Chemistry
Weakly Coordinating Anions
Organometallic Chemistry
Sol-Gel Chemistry
Polymer Chemistry and Properties

Miscellaneous Information and Service Record

- Fourth Highest Total of U.S. Patents in Shell Oil Company Among U.S. Inventors (*upon leaving Shell*)
- Winner of Two Shell Special Recognition Awards for Technical Achievement
- 1992 Winner of Shell's Highest Corporate Award for Teamwork (*President's Award*)
- Ph.D. Recruiter for Shell Development Company *(Texas, Wisconsin, Berkeley),* 1988-1994
- Led Implementation of Technical Training Course Program for Technicians at Shell Development (1992)
- Participated in IRI Visiting Industrial Scientist/Engineer Program for Shell Development (1988-1993)
- Chairman of the Southwest Catalysis Society Local Section of North American Catalysis Society (1996-7)
- Local Southwest Section Representative to National North American Catalysis Society (1998-2001)
- Began Postdoc Program in Shell/Union Carbide and Supervised Five Post-Doctoral Students in Industry
- Adjunct Professor, Department of Chemistry, University of Houston, Houston, Texas (1999–2001)
- Vice-Chairman, Gordon Research Conference on Inorganic Chemistry, 2001
- Inaugural Speaker in Los Alamos Postdoctoral Staff Seminar Series, 2002
- Invited Participant, DOE Basic Energy Sciences Workshop, Catalysis, Washington, DC, 2002
- Invited Participant, DOE Basic Energy Sciences Workshop, Catalysis, Chicago, IL, 2002
- Co-Organizer, DOE National Laboratory Catalysis Conference, Richland, WA, 2002
- Chairman, Gordon Research Conference on Inorganic Chemistry, 2002
- Organizer, "Modern Aspects of Main Group Chemistry" Symposium, 227th National Meeting of the American Chemical Society, Anaheim, CA March 2004
- Chairman and Organizer, National Science Foundation Workshops on Inorganic Chemistry, 2004-6
- Advisory Panel, National Academy of Science Associateships Program, 2005-10
- Advisory Panel, Los Alamos Neutron Science Center, 2004-10
- Advisory Panel for 2006 Gordon Research Conference on Inorganic Chemistry, 2005
- Advisory Panel for 2007 Gordon Research Conference on Inorganic Chemistry, 2006
- Advisory Panel for 2008 Gordon Research Conference on Inorganic Chemistry, 2007
- Advisory/Selection Panel, National Science Foundation Workshops on Inorganic Chemistry, 2007-9
- Organizer, DOE-BES Contractor's Workshop on Catalysis, June 2010

PUBLICATION, OUTSIDE TALKS, PATENT, AND CURRENT FUNDING LIST

Published Papers

1. A.H. Cowley, R.A. Kemp, and J.C. Wilburn, "Reaction of (Chlorophosphine)iron Tetracarbonyl Complexes with Aluminum Chloride. Iron Tetracarbonyl Complexes of Two-coordinate Phosphorus Cations", *Inorg. Chem.*, **20**(12), 4289 (1981).

2. A.H. Cowley, R.A. Kemp, M. Lattman, and M.L. McKee, "Lewis Base Behavior of Methylated and Fluorinated Phosphines. A Photoelectron Spectroscopic Investigation", *Inorg. Chem.*, **21**(1), 85 (1982).

3. A.H. Cowley, R.A. Kemp, and J.C. Wilburn, "Phosphinyl Radicals as Ligands: Preparation of Novel Paramagnetic Organometallic Compounds", *J. Am. Chem. Soc.*, **104**(1), 331 (1982).

4. A.H. Cowley and R.A. Kemp, "An Improved Synthesis of Bis(trimethylsilyl)chloromethane", *Synth. React. Inorg. Met.-Org. Chem.*, **11**(6), 591 (1981).

5. S.G. Baxter, A.H. Cowley, R.A. Kemp, S.K. Mehrotra, and J.C. Wilburn, "Recent Developments in the Chemistry of Dicoordinated Phosphorus Radicals and Cations", *ACS Symp. Ser.*, **171** (Phosphorus Chem.), 391 (1981).

6. A.H. Cowley, R.A. Kemp, and C.A. Stewart, "Reaction of Stannocene and Plumbocene with Phosphenium Ions: Oxidative Addition of Carbon-Hydrogen Bonds to Low-coordination Number Main Group Species", *J. Am. Chem. Soc.*, **104**(11), 3239 (1982).

7. A.H. Cowley and R.A. Kemp, "Structures and Reactions of Iminophosphoranide Anions", *Chem. Comm.*, 319 (1982).

8. R.A. Kemp, "Cationic, Free-radical, and Anionic Chemistry of Low-Coordinate Phosphorus", *Diss. Abstr. Int. B*, 1982, **43**(3), 718-19.

9. A.H. Cowley, E.A.V. Ebsworth, R.A. Kemp, D.W.H. Rankin, and C.A. Stewart, "Two-coordinate Phosphorus Compounds with Bis(trimethylsilyl)methyl Ligands: Phosphaalkene and Phosphide Anion", *Organometallics*, **1**(12), 1720 (1982).

10. A.H. Cowley and R.A. Kemp, "Preparation and Properties of Bulky Secondary Phosphines", *Inorg. Chem.*, **22**(3), 547 (1983).

11. A.H. Cowley, R.A. Kemp, J.G. Lasch, N.C. Norman, and C.A. Stewart, "Reaction of Phosphenium Ions with 1,3-Dienes: A Rapid Synthesis of Phosphorus-containing Five-membered Rings", *J. Am. Chem. Soc.*, **105**(25), 7444 (1983).

12. A.H. Cowley, R.A. Kemp, E.A.V. Ebsworth, D.W.H. Rankin, and M.D. Walkinshaw, "Structure/reactivity Relationships for Cationic (Phosphenium)iron Tetracarbonyl Complexes", *J. Organomet. Chem.*, **265**(2), C19 (1984).

13. A.H. Cowley and R.A. Kemp., "Synthesis and Reaction Chemistry of Stable Two-Coordinate Phosphorus Cations (Phosphenium Ions)", *Chem. Rev.*, **85**(5), 367 (1985).

14. A.H. Cowley, R.A. Kemp, J.G. Lasch, N.C. Norman, C.A. Stewart, B.R. Whittlesey, and T.C. Wright, "Reactivity of Phosphenium Ions Toward 1,3- and 1,4-Dienes", *Inorg. Chem.*, **25**(6), 740 (1986).

15. R.A. Kemp, R.C. Ryan, and J.A. Smegal, "Stacking of Molybdenum Disulfide in Hydrotreating Catalysts", *Proc. 9th International Congress on Catalysis*, M.J. Phillips and M. Ternan, Eds., **Vol. 1**, 128 (1988).

16. R.C. Ryan, R.A. Kemp, J.A. Smegal, D.R. Denley, and G.E. Spinnler, "Stacking of Molybdenum Disulfide in Hydrotreating Catalysts", *Advances in Hydrotreating Catalysts*, M. L. Ocelli and R. Anthony, Eds., Elsevier Scientific Publishing, 21 (1989).

17. N. Yao, G.E. Spinnler, R.A. Kemp, D.C. Guthrie, R.D. Cates, and C.M. Bolinger, "Environmental-Cell TEM Studies of Catalyst Particle Behavior", *Proceedings of the 49th Annual Meeting of the Electron Microscopy Society of America*, G.W. Bailey, Ed., San Francisco Press (1991).

18. R.A. Kemp, "Phosphoranes Containing P-H Bonds", *Phosphorus, Sulfur, and Silicon*, **Vol. 87**, 83 (1994).

19. R.A. Kemp and C.T. Adams, "Hydrogel-Derived Catalysts. Laboratory Results on Nickel-Molybdenum and Cobalt-Molybdenum Hydrotreating Catalysts", *Applied Catalysis, A:General*, **134**, 299 (1996).

20. R.A. Kemp and A.H. Cowley, "Improved Synthesis of Bis(trimethylsilyl)chloromethane", *Inorganic Syntheses*, Vol. **31**, A.H. Cowley, Ed., 101-2, John Wiley (1997).

21. R.A. Kemp, D.S. Brown, M. Lattman, and J. Li, "Calixarenes as a New Class of External Donors in Ziegler-Natta Polypropylene Catalysts", *J. of Molecular Catalysis*, A: Chemical, **149**, 125 (1999).

22. R.A. Kemp, L. Chen, I. Guzei, and A.L. Rheingold, "Synthesis and Structural Characterization of Group 14 Complexes Containing Two {9-[2-(Dimethylamino)ethyl]fluorenyl-} Ligands and a Unique Coupling Product", *J. of Organomet.Chem.,* **596**, 70 (2000).

23. R.A. Kemp, D.S. Brown, and K.A. Gonzalez, "Guaiacol-Substituted Silanes as Selectivity Control Agents for Ziegler-Natta Polypropylene Catalysts", *Main Group Metal Chemistry*, **23**(11), 655 (2000).

24. C.A. Zechmann, T.J. Boyle, M.A. Rodriguez, and R.A. Kemp, "Solvent Influences on the Molecular Aggregation of Magnesium Aryloxides", *Polyhedron*, **19**, 2557 (2000).

25. C.A. Zechmann, T.J. Boyle, M.A. Rodriguez, and R.A. Kemp, "Solvent Influences on the Molecular Aggregation of Magnesium Aryloxides", *Inorg. Chim. Acta*, **319**, 137 (2001).

26. T.J. Boyle, E.N. Coker, C.A. Zechmann, J.A. Voigt, M.A. Rodriguez, R.A. Kemp, and M.P. Zum Mallen, "Precipitation of Spherical Magnesium(II) Cresolate Particles", *Chem. of Mater.*, **15**(1), 309 (2003).

27. Y. Tang, L.N. Zakharov, A.L. Rheingold, and R.A. Kemp, "Insertion of Carbon Dioxide into Mg-N Bonds. Structural Characterization of a Previously Unknown η^2 Chelation Mode to Mg in Magnesium Carbamates", *Organometallics*, **23**, 4788 (2004).

28. Y. Tang, A. M. Felix, L.N. Zakharov, A.L. Rheingold, and R.A. Kemp, "Syntheses and Structural Characterization of a Monomeric Tin(II) Diamide and a Novel Chlorotin(II) Amide Trimer", *Inorg. Chem*., **43**, 7239 (2004).

29. Y. Tang, D.R. Dunphy, and R.A. Kemp, "Low Temperature Preparation of Crystalline Barium Sulfide", *Appl. Organometal. Chem*., **19**, 803 (2005).

30. Y. Tang, W.S. Kassel, L.N. Zakharov, A.L. Rheingold, and R.A. Kemp, "Insertion Reactions of Carbon Dioxide into Zn-N Bonds. Syntheses and Structures of Tetrameric and Dimeric Alkylzinc Carbamato Complexes", *Inorg. Chem*., **44**, 359 (2005).

31. Y. Tang, L.N. Zakharov, A.L. Rheingold, and R.A. Kemp, "Synthesis and Structural Characterization of Magnesium Amide Complexes Containing –N[(R)($SiMe_3$)] Ligands", *Organometallics*, **24**, 836 (2005).

32. Y. Tang, A. M. Felix, L.N. Zakharov, W.S. Kassel, A.L. Rheingold, and R.A. Kemp, "Syntheses and Structural Characterizations of Solvated Calcium Amides Containing Silylamide Ligands: $Ca[N(R)(SiMe_3)]_2(Solvent)_x$ (R = $SiMe_2$*t*-Bu, $SiPh_2$*t*-Bu, and $SiPh_3$)", *Inorg. Chim. Acta*, **358**, 2014 (2005).

33. Y. Tang, A. M. Felix, V. Manner, L.N. Zakharov, A.L. Rheingold, B. Moasser, and R.A. Kemp, "Synthesis and Characterization of Divalent Main Group Diamides and Reactions with CO_2", *ACS Symposium Series*, **917**, 409 (2005).

34. Y. Tang, A.M. Felix, B.J. Boro, L.N. Zakharov, A.L. Rheingold, and R.A. Kemp, "Syntheses and X-ray structures of monomeric zinc and mercury bis(silylamides)", *Polyhedron*, **24**, 1093 (2005).

35. Z. Yinghuai, S.L.P. Sia, F. Cooli, K. Carpenter, and R.A. Kemp, "Another Example of Carborane Based Trianionic Ligand: Syntheses and Catalytic Activities of Cyclohexylamino Tailed *ortho*-Carboranyl Zirconium and Titanium Dicarbollides", *J. Organometal. Chem*., **690**, 6284 (2005).

36. Y. Tang, L.N. Zakharov, A.L. Rheingold, and R.A. Kemp, "Synthesis and structure of lithium amides and solvated derivatives containing bulky silylamide ligands", *Polyhedron*, **24**, 1739 (2005).

37. M.C. Denney, N.A. Smythe, K.L. Cetto, R.A. Kemp, and K.I. Goldberg, "Insertion of Molecular Oxygen into a Palladium(II) Hydride Bond", *J. Amer. Chem. Soc.*, **128***,* 2508 (2006).

38. Z. Yinghuai, S.L.P. Sia, K. Carpenter, F. Cooli, and R.A. Kemp, "Syntheses and Catalytic Activities of Single-Wall Carbon Nanotubes-Supported Nickel (II) Metallacarboranes for Olefin Polymerization", *J. Phys. Chem. Solid.*, **67**, 1218 (2006).

39. J.A. Saria, B.J. Boro, B. Moasser, and R.A. Kemp, "Insertion of Carbon Dioxide in Main Group Amido Complexes", *Proceedings, East and Southern Africa Environmental Chemistry Workshop*, Namibia AFRICA (2006).

40. Y. Tang, L.N. Zakharov, A.L. Rheingold, and R.A. Kemp, "Two new bulky amido ligands useful for the preparation of metal complexes and examples of their reactivity", *Inorg. Chim. Acta*, **359**, 775 (2006).

41. J.M. Keith, R.P Muller, R.A. Kemp, K.I. Goldberg, W.A. Goddard III, and J. Oxgaard, "Mechanism of Direct Molecular Insertion in a Palladium(II) Hydride Bond", *Inorg. Chem*, **45**, 9631 (2006).

42. Z. Yinghuai, S. C. Peng, A. Emi, Z. Su, Monalisa, and R.A. Kemp, "Supported Ultra Small Palladium on Magnetic Nanoparticles Used as Catalysts for Suzuki Cross-Coupling and Heck Reactions", *Advanced Synthesis and Catalysis*, **349**, 1917 (2007).

43. Z. Yinghuai, C.N. Lee, R.A. Kemp, N.S. Hosmane, and J.A. Maguire, "Latest Developments in the Catalytic Application of Nanoscaled Neutral Group 8-10 Metals", *Chemistry –Asian J.*, 3, 650 (2008).

44. G.R. Fulmer, R.P. Muller, R.A. Kemp, and K.I. Goldberg, "The Hydrogenolyses of Palladium(II) Hydroxide and Methoxide Pincer Complexes". *J. Am. Chem. Soc.*, **131**, 1346 (2008).

45. D.A. Dickie and R.A. Kemp, "P,P-Diphenyl-N-(1,1,2,2-tetraphenyl-1λ5-diphosphanylidene)phosphinous amide", *Acta Cryst.* **E64**, o1449 (2008).

46. B.J. Boro, D.A. Dickie, K.I. Goldberg, and R.A. Kemp,"{2,6-Bis[(di-tert-butylphosphino)methyl]phenyl}chloronickel", *Acta Cryst.* **E64**, m1304 (2008).

46. D.A. Dickie, M.V. Parkes, and R.A. Kemp, "Insertion of Carbon Dioxide Into Main Group Complexes: Unprecedented Reaction to Form the $[N(CO_2)_3]^{3-}$ Ligand", *Angew. Chem. Int. Ed*., **47**, 9955 (2008). (article highlighted in *C&EN*, November 10, 2008 issue)

47. B.J. Boro, E.N. Duesler, K.I. Goldberg, and R.A. Kemp, "An Unprecedented Bonding Mode for Potassium within a PCP-Pincer Palladium Hydride – K-Selectride® Complex", *Inorg. Chem. Comm.,* **11**, 1426 (2008).

48. G.R. Fulmer, R.P. Muller, R.A. Kemp, and K.I. Goldberg, "The Hydrogenolysis of Palladium(II) Hydroxide and Methoxide Pincer Complexes", *J. Amer. Chem. Soc*., **131**, 1346 (2009).

49. B.J. Boro, E.N. Duesler, K.I. Goldberg, and R.A. Kemp, "Synthesis, Characterization, and Reactivity of Nickel Hydride Complexes Containing PCP Pincer Ligands", *Inorg. Chem*., **48**, 5081 (2009).

50. C.A. Henao, C.T. Maravelias, J.E. Miller, and R.A. Kemp, "Synthetic Production of Methanol Using Solar Power", *Proceedings: 7th International Conference on Foundations of Computer-aided Process Design*, June 7-12, 2009, Breckenridge, Colorado (2009).

51. C.A. Stewart, D.A. Dickie, and R.A. Kemp, "1,3-Bis(phenylthiomethyl)benzene", *Acta Cryst.,* **E66**, o677 (2010).

52. G. Page, A.M. Felix, D.A. Dickie, L. Chen, and R.A. Kemp, "Yellow and Blue Make Green: The Importance of Stoichiometry in the Reaction of 1,4-bis(2,6-diisopropylphenyl)-1,4,-diazabutadiene with Dimethylgallium Chloride", *Main Group Chem.*, **9**, 11 (2010) (cover article highlighted in *C&EN*, April 20, 2009 issue)

53. A. Mrutu, K.I. Goldberg, and R.A. Kemp, "Synthesis and Characterization of a Dinuclear Ni Complex Containing a Bridging CNC Pincer Ligand", *Inorg. Chim. Acta,* **364**, 115 (2010).

54. C.A. Stewart, D.A. Dickie, M.V. Parkes, J.A. Saria, and R.A. Kemp, "Reactivity of Bis(2,2,5,5-tetramethyl-2,5-disila-1-azacyclopent-1-yl)tin with CO_2, OCS, and CS_2 and Comparison to That of Bis[bis(trimethylsilyl)amido]tin", *Inorg. Chem.,* **49**, 11133 (2010).

55. A. Mrutu, D.A. Dickie, K.I. Goldberg, and R.A. Kemp, "A Unique Three-Dimensional Coordination Cluster Based on a Silver Carbene Complex", *Inorg. Chem.,* **50**, 2729 (2011).

56. B.J. Boro, R. Lansing, K.I. Goldberg, and R.A. Kemp, "Reaction of a Monomeric Titanium Hydride with Dioxygen Does Not Produce a Stable Titanium Hydroperoxide", *Inorg. Chem. Comm.,* **14**, 531 (2011).

57. G.R. Fulmer, W. Kaminsky, R.A. Kemp, and K.I. Goldberg, "Syntheses and Characterization of Palladium Complexes with Hemilabile "PCO" Ligands", *Organometallics*, **30**, 1627 (2011).

58. R. Lansing, K.I. Goldberg, and R.A. Kemp, "Unsymmetrical $^{R}PNP^{R'}$ Pincer Ligands and Their Group 10 Complexes", *Dalton Trans*., **40**, 8950 (2011).

59. C.A. Stewart, D.A. Dickie, Y. Tang, and R.A. Kemp, "Insertion Reactions of CO_2, OCS, and CS_2 Into the Sn-N bonds of $(Me_2N)_2Sn$: NMR and X-ray Structural Characterization of the Products", *Inorg. Chim. Acta,* **376**, 73 (2011).

60. D.A. Dickie, E.N. Coker, and R.A. Kemp, "Formation of an Intramolecular Main Group-CO_2 Adduct", *Inorg. Chem.*, **50**, 11288 (2011).

61. G.R. Fulmer, A.N. Herndon, R.A. Kemp, and K.I. Goldberg, "Hydrogenolysis of Pd(II)-OR Complexes", *J. Am. Chem. Soc.*, **133**, 17713 (2011).

62. C.A. Stewart, D.A. Dickie, B. Moasser, and R.A. Kemp, "Reactions of CO_2 and Related Heterollenes with CF_3-Substituted Aromatic Silylamines of Tin", *Polyhedron,* **32**, 14 (2012).

63. B.M. Barry, D.A. Dickie, A.E. Wetherby Jr., W.E. Barker IV, C.A. Larsen, R. Waterman, W.E. Geiger, and R.A. Kemp, "CO_2 Interactions with Main Group Compounds Directed Towards Preparing Useful Organic Compounds", *Prepr. Pap. - Am. Chem. Soc. - Fuel Chem*., **57**, 294 (2012).

64. D.A. Dickie, K.B. Gislason, and R.A. Kemp, "Formation of Phosphino-substituted Isocyanate by Reaction of CO_2 with Group 2 Complexes Based on the $(Me_3Si)(i\text{-}Pr_2P)NH$ Ligand", *Inorg. Chem*., **51**, 1162 (2012).

65. A. Mrutu, W. William, and R.A. Kemp, "Synthesis and Characterization of Molybdenum and Tungsten Complexes Containing Tris(diphenylphosphino)methane", *Inorg. Chem. Comm.,* **18**, 110 (2012).

66. A.M. Felix, D.A. Dickie, Giang Page, Ian S. Horne, and R.A. Kemp, "Addition of Aluminum and Gallium Species to Aromatic and Alkyl-substituted 1,4-Diaza-1,3-butadiene Ligands", *Inorg. Chem*., **51**, 4650 (2012).

67. A.M. Felix, B.J. Boro, D.A. Dickie, Y. Tang, J.A. Saria, B. Moasser, C.A. Stewart, B.J. Frost, and R.A. Kemp, "Insertion of CO_2 into Divalent Group 2 and 12 Amides", *Main Group Chem.*, **11**, 13 (2012).

68. C.A. Stewart, D.A. Dickie, and R.A. Kemp, "Investigation of Metal Cyclam Complexes as Potential Catalysts for the Production of Dimethylcarbonate", *Inorg. Chim. Acta*, **392**, 268 (2012).

69. L.A. Steele, R.A. Kemp, and T.J. Boyle, "Lanthanide Alkoxides with CO_2", *Polyhedron*, **42**, 258 (2012).

70. D.A. Dickie, R.P. Ulibarri-Sanchez, P.J. Jarman, and R.A. Kemp, "Activation of CO_2 and CS_2 by $(Me_3Si)(i\text{-}Pr_2P)NH$ and its zinc complex", *Polyhedron*, accepted (2012).

71. H.-W. Suh, T.J. Schmeier, N. Hazari, R.A. Kemp, and M.K. Takase, "Experimental and Computational Studies of the Reaction of Carbon Dioxide with Pincer-Supported Nickel and Palladium Hydrides", *Organometallics*, **31**, 8225 (2012).

72. M.V. Parkes, K.I. Goldberg, and R.A. Kemp, "Mechanistic Insights into the Reaction of Pd-OH with H_2 and the Effect of Hemilabile Ligands on Hydrogenolysis", *Organometalllics*, submitted (2012).

Outside Presentations (partial listing)

* 9th International Conference on the Chemistry of Phosphorus, 1981
* Southwest Catalysis Society, 1988, 1996 (invited)
* 49th Annual Meeting of the Electron Microscopy Society of America, 1991
* 1993 Southwest Regional ACS Meeting, Austin, TX (invited)
* 1996 National Science Foundation Organometallic Chemistry Workshop, Orcas Island, WA (participant)
* 1996 Inorganic Gordon Research Conference (invited speaker)
* 1997 National Science Foundation Inorganometallic Chemistry Workshop, Santa Fe, NM (participant)
* 1998 Conference on Main Group Chemistry, Fargo, ND (invited speaker)
* 2002 Mountain Regional ACS Meeting, Albuquerque, NM (invited)
* 2002 Southwest Regional ACS Meeting, Symposium on Main Group Chemistry, Austin, TX (invited)
* 2003 North American Catalysis Society, Cancun, MEX
* 2004 American Chemical Society Meeting, Anaheim, CA (invited)
* 2005 American Chemical Society Meeting, San Diego, CA
* 2005 Materials Research Meeting, San Francisco, CA
* 2005 American Chemical Society Meeting, Washington, DC (invited)
* 2006 DOE Workshop on Catalysis, Cambridge, MD
* 2009 General Electric Whitney Symposium, Niskayuna, NY (invited)
* 2010 DOE Workshop on Catalysis, Annapolis, MD (invited)
* 2010 Singapore Catalysis Society, Singapore (invited)
* 2010 A*STAR ICES Symposium, Singapore (invited)
* 2010 American Chemical Society Meeting, New Orleans, LA (invited)
* 2011 American Chemical Society Meeting, Anaheim, CA (invited)
* 2011 American Chemical Society Meeting, Austin, TX (invited)
* 2012 American Chemical Society Meeting, San Diego, CA (invited)

* Invited University/National Laboratory Talks

Southern Methodist University (2)
Texas Tech University (2)
University of Texas, Austin (2)
Sandia National Laboratory (4)
University of New Mexico (2)
University of Houston
New Mexico State University
Tennessee State University
University of California, San Diego
Brigham Young University
Yale University
Mercer University
Missouri Western State College
Florida State University
Los Alamos National Laboratory (2)
Texas Christian University
University of Minnesota
University of Dar es Salaam, Tanzania
University of Texas, Arlington
Northern Arizona University
University of Nevada, Reno
University of Texas, Dallas
Texas Lutheran College
University of Washington, Seattle (2)
Rice University (2)
Colorado State University
University of Kentucky
University of Vermont
Georgetown University
Texas Tech University
Mississippi State University

Issued and Applied United States Patents (does not include World Patents)

1. W.J. Heilman and R.A. Kemp, *"Catalyst and Process for the Polymerization of Ethylene"*, USP 4525557.
2. R.A. Kemp, *"Process for Producing Wide-Pore Catalyst Supports"*, USP 4624938.
3. R.A. Kemp, *"Process for Producing Narrow Pore Catalyst Supports"*, USP 4629716.
4. R.A. Kemp, *"Hydrotreating Catalysts Prepared From Hydrogels"*, USP 4716140.
5. R.A. Kemp, *"Hydrotreating Catalysts Prepared From Hydrogels"*, USP 4716141.
6. R.A. Kemp, *"Hydrotreating Catalysts Prepared From Hydrogels"*, USP 4717698.
7. R.A. Kemp, *"Hydrotreating Catalysts Prepared From Hydrogels"*, USP 4717704.
8. R.A. Kemp, *"Hydrotreating Catalysts Prepared From Hydrogels"*, USP 4717705.
9. R.A. Kemp, *"Hydrotreating Catalysts Prepared From Hydrogels"*, USP 4717706.
10. R.A. Kemp, *"Hydrotreating Catalysts Prepared From Hydrogels"*, USP 4717707.
11. R.A. Kemp, *"Hydrotreating Catalysts Prepared From Hydrogels"*, USP 4738945.
12. R.A. Kemp and D.M. Hamilton, *"Disproportionation of Olefins"*, USP 4754099.
13. R.Q. Kluttz, R.A. Kemp, and R.C. Ryan, *"Stabilized Crystalline Polymers"*, USP 4761448.
14. R.A. Kemp, *"Process for Hydrotreating Hydrocarbon Feed"*, USP 4786403.
15. R.A. Kemp, *"Process for Hydrotreating Hydrocarbon Feed"*, USP 4786404.
16. R.A. Kemp, *"Hydrotreating Catalysts Prepared From Hydrogels"*, USP 4810684.
17. R.A. Kemp, *"Hydrotreating Catalysts Prepared From Hydrogels"*, USP 4810686.
18. R.A. Kemp, *"Hydrotreating Catalysts Prepared From Hydrogels"*, USP 4810687.
19. R.A. Kemp, *"Hydrotreating Catalysts Prepared From Hydrogels"*, USP 4820679.
20. R.A. Kemp, *"Hydrotreating Catalysts Prepared From Hydrogels"*, USP 4820680.
21. R.A. Kemp, *"Hydrotreating Catalysts Prepared From Hydrogels"*, USP 4832826.
22. R.A. Kemp, *"Hydrotreating Catalysts Prepared From Hydrogels"*, USP 4832827.
23. R.A. Kemp, *"Hydrotreating Catalysts Prepared From Hydrogels"*, USP 4832828.
24. R.A. Kemp, *"Hydrotreating Catalysts Prepared From Hydrogels"*, USP 4839028.
25. R.A. Kemp, *"Process for Hydrotreating Hydrocarbon Feeds"*, USP 4853108.
26. R.A. Kemp, *"Hydrotreating With Wide-Pore Hydrogel-Derived Catalysts"*, USP 4861460.
27. R.A. Kemp, *"Process for Hydrotreating Hydrocarbon Feeds"*, USP 4880522.
28. R.A. Kemp, *"Process for Hydrotreating Hydrocarbon Feeds"*, USP 4880523.
29. R.A. Kemp, *"Process for Hydrotreating Hydrocarbon Feeds"*, USP 4880524.
30. R.A. Kemp, *"Process for Hydrotreating Hydrocarbon Feeds"*, USP 4880525.
31. R.A. Kemp, *"Hydrotreating Catalysts Prepared From Hydrogels"*, USP 4880526.
32. D.M. Hamilton and R.A. Kemp, *"Olefin Isomerization Process"*, USP 4895997.
33. D.M. Hamilton and R.A. Kemp, *"Disproportionation of Olefins"*, USP 4956516.
34. R.A. Kemp, *"Alkoxylation Process Catalyzed by Lanthanum Silicates and Metasilicates"*, USP 4960952.
35. D.M. Hamilton and R.A. Kemp, *"Disproportionation of Olefins"*, USP 4962263.
36. R.A. Kemp, *"Alkoxylation Process Catalyzed by Barium Phosphate"*, USP 4967016.
37. D.M. Hamilton and R.A. Kemp, *"Concurrent Isomerization and Disproportionation of Olefins"*, USP 4996386.
38. R.A. Kemp, *"Sulfiding of Hydrogel Derived Catalysts"*, USP 5001101.
39. R.A. Kemp, *"Alkoxylation Process Catalyzed by Lanthanum Silicates and Metasilicates"*, USP 5023224.
40. R.A. Kemp, *"Alkoxylation Process Catalyzed by Borate Salts of the Rare Earth Elements"*, USP 5026923.
41. C.L. Edwards and R.A. Kemp, *"Alkoxylation Process Catalyzed by Compounds of the Rare Earth Elements"*, USP 5057628.
42. R.A. Kemp, *"Sulfiding of Hydrogel Derived Catalysts"*, USP 5062947.
43. R.A. Kemp and P.R. Weider, *"Supported Rare Earth and Phosphorus Catalyst"*, USP 5102849.
44. R.A. Kemp, *"Alkoxylation Process Catalyzed by Rare Earth and Phosphorus-Containing Xerogels"*, USP 5118870.
45. R.A. Kemp and D.M. Hamilton, *"Concurrent Isomerization and Disproportionation of Olefins"*, USP 5120896.
46. L.R. Chamberlain, C.J. Gibler, R.A. Kemp, and S.E. Wilson, *"Selective Hydrogenation of Conjugated Diolefin Polymers"*, USP 5141997.
47. C.J. Gibler, L.R. Chamberlain, R.A. Kemp, and S.E. Wilson, *"Depolymerization of Conjugated Diene Polymers"*, USP 5162446.
48. L.R. Chamberlain, C.J. Gibler, R.A. Kemp, and S.E. Wilson, *"Selective Hydrogenation of Conjugated Diolefin Polymers with Rare Earth Catalysts"*, USP 5177155.
49. R.A. Kemp, *"Alkoxylation Process Catalyzed by Rare Earth and Phosphorus-Containing Xerogels"*, USP 5208199.
50. R.A. Kemp and P.R. Weider, *"Supported Rare Earth and Phosphorus Catalyst"*, USP 5210325.
51. R.A. Kemp, *"Process for Preparing Ethylene Oxide Catalysts"*, USP 5364826.
52. R.A. Kemp, *"Process for Preparing Ethylene Oxide Catalysts"*, USP 5380885.
53. S.E. Wilson and R.A. Kemp, *"Olefin Polymerization Catalyst"*, USP 5411926.
54. R.A. Kemp, *"Oligomerization Catalyst and Process"*, USP 5439862.
55. R.A. Kemp, *"Ethylene Oxide Catalyst and Process"*, USP 5447897.
56. R.A. Kemp, *"Ethylene Oxide Catalyst and Process"*, USP 5486628.
57. S.E. Wilson and R.A. Kemp, *"Olefin Polymerization Catalyst"*, USP 5498676.
58. R.A. Kemp, *"Process for Preparing Ethylene Oxide Catalysts"*, USP 5545603.
59. R.A. Kemp, *"Oligomerization Catalyst and Process"*, USP 5557027.
60. R.A. Kemp, *"Ethylene Oxide Catalyst and Process"*, USP 5663385.
61. R.A. Kemp and L. Chen, "*Olefin Polymerization Catalyst Compositions and Method of Preparation*", published, 20050003953.
62. L. Chen, R.A. Kemp, and T.L. Nemzek, "*Olefin Polymerization Catalyst Compositions and Method of Preparation*", USP 7601664.

<u>Current Academic Funding (Sandia Funding Not Included)</u>

Heteroallenes as Building Blocks for Synthesis and Sequestration	NSF	9/09-6/13	$435,000
Direct Partial Oxidations Using Molecular Oxygen *(co-PI Karen Goldberg, Washington)*	DOE-BES	4/09-5/13	$750,000
New Earth-Abundant Metal Complexes for CO_2 Conversion and Reduction	NSF	9/12-12/15	$390,000

<u>Pending</u>

Direct Partial Oxidations Using Molecular Oxygen *(renewal - co-PI Karen Goldberg, Washington)*	DOE-BES	6/13-5/16	$750,000

Martin L. Kirk
Department of Chemistry
The University of New Mexico

Curriculum Vitae and Selected Publications

Curriculum Vitae

Martin L. Kirk
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MSC03 2060
1 University of New Mexico
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Educational History

Postdoctoral, 7/90-9/93, National Science Foundation Postdoctoral Fellow, Stanford University, Stanford, CA 94305. (Prof. Edward. I. Solomon)

Ph.D., 8/90, The University of North Carolina at Chapel Hill, Chapel Hill, NC, Inorganic Chemistry, Dissertation Title: "Unusual Linear Chain Magnetism" Prof. William E. Hatfield, advisor.

B.S. 6/85, West Virginia University, Morgantown, WV, Chemistry. *Cum Laude.*

Research Interests

Metallobiochemistry. Mechanisms of electron and atom transfer in pyranopterin Mo and W enzymes. Spectroscopic studies on pyranopterin molybdenum enzyme active sites coupled with parallel studies on small molecule analogs. Electronic structure contributions to reactivity in bioinorganic chemistry. I have more than 25 years of experience in physical inorganic chemistry and more that 20 years experience in bioinorganic chemistry. I have a strong track record of sustained federally funded grant support from NIH and NSF. Our research program is involved in spectroscopic, synthetic, biochemical and computational studies of pyranopterion molybdenum enzymes and models, as well as other enzyme systems. We are especially focused on molybdoenzymes, NO synthase, and LuxS. Our spectroscopic approach employs a combination of magnetic circular dichroism, low-temperature electronic absorption, variable frequency EPR, and resonance Raman. All of these capabilities are available in the PIs laboratories at The University of New Mexico.

Molecular Electronics. Spectroscopic, magnetic, and computational studies of molecular systems related to molecular electron transport and quantum interference effects. Understanding the electronic origins of molecular bistability in thermal charge transfer and valence-tautomeric materials. Developing new molecule-based systems as models of solid-state inorganic spin electronic (spintronic) systems. Magnetic molecules on surfaces. Polymeric valence tautomers, novel thermal charge transfer materials, and high-spin hybrid metal-organic systems as potential components of spintronic devices including hybrid inorganic/organic magnetic semiconductors, molecular switches, beyond binary information storage registers, and optical limiters.

Magnetochemistry. New single-molecule magnets. Lanthanide and Actinide magnetic properties. Excited state contributions to ground state exchange coupling. Magnetostructural correlations.

Employment History-Principal Positions Since the Bachelor's Degree

Associate Chair, 8/09 – 8/12, Department of Chemistry and Chemical Biology, The University of New Mexico, Albuquerque, NM 87131.

Interim Chair, 8/08 – 8/09, Department of Chemistry and Chemical Biology, The University of New Mexico, Albuquerque, NM 87131.

Associated Faculty, Nanoscience and Microsystems Graduate Program, The University of New Mexico, Albuquerque, NM 87131.

Professor, 7/04 – present, Department of Chemistry and Chemical Biology, The University of New Mexico, Albuquerque, NM 87131.

Associate Professor, 7/99 – 7/04, Department of Chemistry, The University of New Mexico, Albuquerque, NM 87131.

Research Fellow (Sabbatical Leave), 7/03-1/04, Glenn T. Seaborg Institute Los Alamos National Laboratories, Los Alamos, NM

Assistant Professor, 9/93 - 6/99, Department of Chemistry, The University of New Mexico, Albuquerque, NM 87131.

National Science Foundation Postdoctoral Fellow, 7/90-9/93, Stanford University, Stanford, CA 94305.
with Prof. Edward I. Solomon.

Graduate Research Assistant,1986-1990, The University of North Carolina at Chapel Hill, Chapel Hill, NC.

Undergraduate Chemistry Tutoring Program, 1988 -1990, The University of North Carolina at Chapel Hill, Chapel Hill, NC.

Laboratory Teaching Assistant, 1985 - 1986, The University of North Carolina at Chapel Hill, Chapel Hill, NC.

Professional Recognitions, Honors, and Memberships

Editorial Advisory Board, *Inorganic Chemistry*, 2013 - present

Former ACS Inorganic Division; Chair, Bioinorganic Subdivision.

Chair, Molybdenum and Tungsten Enzyme Gordon Conference, Barga, Italy.

National Science Foundation Postdoctoral Fellowship in Chemistry, 7/90-9/93, Stanford University.

National Science Foundation Summer Institute Grant, 1989, Pittsburgh Supercomputing Center.

B.S. *cum laude* , Chemistry, West Virginia University 1985.

Inducted Phi Lambda Upsilon National Chemistry Honorary, 1984.

Phillips Scholar, 1983 - 1985, West Virginia University.

Member of the American Chemical Society 1990 - present.

Member of the Society of Bioinorganic Chemistry (SBIC)

Articles in Refereed Journals

106. M. L. Kirk, D. A. Shultz, Donor Acceptor Biradicals. *Coord. Chem. Rev.* **2012**, *In Press*.

105. M. L. Kirk, D. A. Shultz, E. C. Depperman, D. Habel-Rodriguez, and R. D. Schmidt. Spectroscopic Studies of Bridge Contributions to Electronic Coupling in a Donor-Bridge-Acceptor Biradical System, *J. Am. Chem. Soc.* **2012**, *134,* 7812-7819. DOI: 10.1021/ja300233a

104. R. A. Rothery, B. Stein, M. Solomonson, M. L. Kirk, J. H. Weiner, Pyranopterin Conformation Defines the Function of Molybdenum and Tungsten Enzymes. *PNAS.* **2012**, *109 (37)* 14773-14778. doi:10.1073/pnas.1200671109.

103. K. P. O'Halloran, C. C. Zhao, N. S. Ando, A. J. Schultz, T. F. Koetzle, P. M. B. Piccoli, B. Hedman, K. O. Hodgson, E. Bobyr, M. L. Kirk, S. Knottenbelt, E. C. Depperman, B. Stein, T. M. Anderson, R. Cao, Y. V. Geletii, K. I. Hardcastle, D. G. Musaev, W. A. Neiwert, X. K. Fang, K. Morokuma, S. X. Wu, P. Koegerler, C. L. Hill, Revisiting the Polyoxometalate-Based Late-Transition-Metal-Oxo Complexes: The "Oxo Wall" Stands. *Inorg. Chem.* **2012**, *51*, 7025-7031. DOI: 10.1021/ic2008914.

102. M. L. Kirk, B. Stein, The Molybdenum Enzymes. *Encyclopedia of Inorganic Chemistry. In Press* **2012**.

101. H. Zhang, D. Dunphy, X. Jiang, H. Meng, B. Sun, D. Tarn, M. Xue, X. Wang, S. Lin, Z. Ji, R. Li, F. Garcia, J. Yang, M. L. Kirk, T. Xia, J. Zink, A. Nel, C. J. Brinker, Processing Pathway Dependence of Amorphous Silica Nanoparticle Toxicity - Colloidal Versus Pyrolytic. *J. Am. Chem. Soc.* **2012**, *in Press*.

100. M. L. Kirk, A. Berhane, Correlating C-H Bond Cleavage and Molybdenum Reduction in Xanthine Oxidase. *Chemistry and Biodiversity,* **2012**, *9*, 1756-1760. doi: 10.1002/cbdv.201200073.

99. J. Sempombe, B. Stein, and M. L. Kirk. Spectroscopic and Electronic Structure Studies Probing Covalency Contributions to C-H Bond Activation and Transition State Stabilization in Xanthine Oxidase, *Inorg. Chem.* **2011**, *50*, 10919-10928.

98. A. Williams, J. Yang, M. L. Kirk. "Oxomolybdenum Diselenolene Chemistry Related to Pyranopterin Molybdenum Enzymes: Synthesis, Structure and Spectroscopic Properties of $[HB(Me_2C_3N_2H)_3]MoO(Se_2C_6H_4)$ *Submitted Inorg. Chem.* **2011**.

97. R. P. Mtei, E. Perera, B. Mogeesa, P. Basu, and M. L. Kirk. A Valence Bond Description of Dizwitterionic Dithiolene Character in an Oxomolybdenum-bis(dithiolene), *European Journal of Inorganic Chemistry, EuroJIC,* **2011**, *36,* 5467-5470.

96. J. Sempombe, M. G. I. Galinato, B. O. Elmore, W. Fan, J. G. Guillemette, N. Lehnert, M. L. Kirk, C. Feng, Mutation in the Flavin Mononucleotide Domain Modulates Magnetic Circular Dichroism Spectra of the iNOS Ferric Cyano Complex in a Substrate-Specific Manner. *Inorg. Chem.* **2011**, *50*, 6859-6861. DOI: 10.1021/ic200952c

95. C. M. Zaleski, S. Tricard, E. C. Depperman, W. Wernsdorfer, T. Mallah, M. L. Kirk, V. L. Pecoraro. Single Molecule Magnet Behavior of a Pentanuclear Mn-based Metallacrown Complex: Solid State and Solution Magnetic Studies. *Inorg. Chem.* **2011**, *50,* 11348-11352.

94. K. G. Matz, R. Mtei, R. Rothstein, M. L. Kirk, and S. J. Nieter Burgmayer. A Study of Mo(4+)(Quinoxalyl-Dithiolenes) as Models for the Non-Innocent Pyranopterin in the Molybdenum Cofactor. *Inorg. Chem.* **2011**, *50,* 9804-9815.

93. R. P. Mtei, G. Lyashenko, B. Stein, N. Rubie, R. Hille, and M. L. Kirk. Spectroscopic and Electronic Structure Studies of a DMSO Reductase Caltalytic Intermediate: Implications for Electron and Atom Transfer Reactivity, *J. Am. Chem. Soc.* **2011**. *133*, 9762–9774. **DOI:** 10.1021/ja109178q

92. H. Sugimoto, H. Tano, K. Suyama, T. Kobayashi, H. Miyake, S. Itoh, R. P. Mtei, and M. L. Kirk, Chalcogenidobis(ene–1,2–dithiolate)molybdenum(IV) Complexes (Chalcogenide E = S, Se): Probing Mo≡E and Ene–1,2–dithiolate Substituent Effects on Geometric and Electronic Structure*, Dalton Trans.,* **2011***, 40*, 1119-1131. DOI: 10.1039/c0dt00871k

91. Hideki Sugimoto, Susumu Tatemoto, Koichiro Suyama, Hiroyuki Miyake, Regina P. Mtei, Shinobu Itoh, and Martin L. Kirk. Monooxo Molybdenum(VI) Complexes Possessing Olefinic Dithiolene Ligands: Probing Mo-S Covalency Contributions to Electron Transfer in DMSO Reductase Family Molybdoenzymes. *Inorg. Chem.* **2010**, *49*, 5368-5370.

90. M. L. Kirk, D. A. Shultz, D. Habel-Rodriguez, R. D. Schmidt, U. Sullivan. Hyperfine Interaction, Spin Polarization, and Spin Delocalization as Probes of Donor-Bridge-Acceptor Interactions in Exchange Coupled Biradicals, *J. Phys. Chem. B* **2010**, *114*, 14712-14716. DOI: 10.1021/jp102955j

89. K. G. Matz, R. P. Mtei, B. Leung, S. J. Nieter Burgmayer, and M. L. Kirk. Non-Innocent Dithiolene Ligands: A New Oxomolybdenum Complex Possessing a Donor-Acceptor Dithiolene Ligand. *J. Am. Chem. Soc.* **2010** *132*, 7830-7832.

88. J. Sempombe, B.O. Elmore, X. Sun, A. Dupont, D. K. Ghosh, J. G. Guillemette, M. L. Kirk, C. Feng. Mutations in the FMN Domain Modulate MCD Spectra of the Heme Site in the Oxygenase Domain of Inducible Nitric Oxide Synthase, *J. Am. Chem. Soc*., **2009**, *131*, 6940-6941. DOI: 10.1021/ja902141v

87. H. Sugimoto, K. Suyama, S. Tatemoto, H. Miyake, S. Itoh, J. Yang, C. Dong, M. L. Kirk. Dioxo–Molybdenum(VI) Complexes with Ene–1,2– dithiolate Ligand: Synthesis, Characterization, Reactivity in Oxygen Atom Transfer to AsO_2^-, and Electronic Structure Description. *Inorg. Chem.,* **2009**, *48.* 10581-10590.

86. M. L. Kirk, D. A. Shultz, R. D. Schmidt, D. Habel-Rodriguez, H. Lee, J. Lee. Ferromagnetic Nanoscale Electron Correlation Promoted by Organic Spin-Dependent Delocalization, *J. Am. Chem. Soc.* **2009**, *131*, 18304-18313.

85. J. Yang, R. Rothery, J. Sempombe, J. H. Weiner, M. L. Kirk. Spectroscopic Characterization of YedY: The Role of Sulfur Coordination in a Mo(V) Sulfite Oxidase Family Enzyme Form, *J. Am. Chem. Soc.,* **2009**, *131*, 15612-15614.

84. M. L. Kirk, S. Knottenbelt, A. Habtegabre. The Reaction Coordinate of Pyranopterin Molybdenum Enzymes, *Computational Inorganic and Bioinorganic Chemistry*, Wiley, **2009**. *Published Online: 15 SEP 2009,* DOI: 10.1002/0470862106.ia621

83. T. M. Anderson, R. Cao, E. Slonkina, Hedman, K. O. Hodgson, Hardcastle, B. B. B., W. A. Neiwert, S. X. Wu, M. L. Kirk, S. Knottenbelt, E. C. Depperman, B. Keita, L. Nadjo, D. G. Musaev, K. Morokuma, C. L. Hill. A Palladium-Oxo Complex. Stabilization fo this proposed Catalytic Intermediate by an Encapsulating Polytungstate Ligand (vol. 127, pg. 11948, 2005). Correction. *J. Am. Chem. Soc.,* **2008**, *130*, 2877-2877.

82. R. Cao, J. W. Han, T. M. Anderson, D. A. Hillesheim, K. I. Hardcastle, E. Slonkina, B. B. B. Hedman, K. O. Hodgson, M. L. Kirk, D. G. Musaev, K. Morokuma, Y. V. Geletii, C. L. Hill. Late Transition Metal-Oxo Compounds and Open-Framework Materials that Catalyze Aerobic Oxidations. *Advances in Inorganic Chemistry,* **2008**, *60,* 245-272.

81. J. J. Scepaniak, M. D. Fulton, R. P. Bontchev, E. N. Duesler, M. L. Kirk, J. M. Smith. Structural and Spectroscopic Characterization of an Electrophilic Iron Nitrido Complex. *J. Am. Chem. Soc.,* **2008**, *130*, 10515-10517. PMID: 18630913

80. R. L. McNaughton, B. S. Lim, S. Z. Knottenbelt, R. H. Holm, M. L. Kirk. Spectroscopic and Electronic Structure Studies of Symmetrized Models for Reduced Members of the Dimethylsulfoxide Reductase Enzyme Family. *J. Am. Chem. Soc.,* **2008**, *130*, 4628-4636. PMID: 18341333

79. C. J. Doonan, R. D. Rubie, K. Peariso, H. H. Harris, S. Z. Knottenbelt, G. N. George, C. G. Young, M. L. Kirk. Electronic Structure Description of the cis-MoOS unit in Models for Molybdenum Hydroxylases. *J. Am. Chem. Soc.,* **2008**, *130*, 55-65. PMID: 18062689

78. S. J. Nieter Burgmayer, M. Kim, R. Petit, A. Rothkopf, A. Kim, S. BelHamdounia, Y. Hou, A. Somogyi, D. Habel-Rodriguez, A. Williams, M. L. Kirk. Synthesis, Characterization, and Spectroscopy of Model Molybdopterin Complexes, *J. Inorg. Biochem.*, **2007**, *101*, 1601-1616.

77. R Cao, T. M. Anderson, P. M. B. Piccoli, A. J. Schultz, T. F. Koetzle, Y. V. Geletii, E. Slonkina, B. Hedman, K. O. Hodgson, K. I. Hardcastle, X. Fang, M. L. Kirk, S. Knottenbelt, P. Kögerler, D. G. Musaev, K. Morokuma, M. Takahashi, C. L. Hill. Terminal Gold-Oxo Complexes. *J. Am. Chem. Soc.,* **2007**, *129*, 11118-11133.

76. M. L. Kirk, D. A. Shultz, E. C. Depperman, C. L. Brannen, Donor-Acceptor Biradicals as Ground State Analogues of Photoinduced Charge Separated States. *J. Am. Chem. Soc.* **2007**, *129*, 1937-1943. DOI: 10.1021/ja065384t

75. C. M. Zaleski, J. W. Kampf, T. Mallah M. L. Kirk, Vincent L. Pecoraro. Assessing the Slow Magnetic Relaxation Behaviour of LnIII4MnIII6. *Inorg. Chem.,* **2007**, *46*, 1954-1956.

74. C. M. Zaleski, E. C. Depperman, J. W. Kampf, M. L. Kirk, V. L. Pecoraro. Using $Ln^{III}[15\text{-}MC_{CuII(N)S\text{-}pheHA}\text{-}5]^{3+}$ Complexes to Construct Chiral Single-Molecule Magnets and Chains of Single-Molecule Magnets. *Inorg. Chem,* **2006**, *45*, 10022-10024. DOI: 10.1021/ic061326x

73. C. N. Carlson, C. J. Kuehl, L. Ogallo, D. A. Shultz, J. D. Thompson, M. L. Kirk, K. D. John, D. E. Morris. Influence of Ligand Geometry in Bimetallic Ytterbocene Complexes of Bridging bis(Bipyridyl) Ligands. *Organometallics.* **2007**, *26*, 4234-4242.

72. J. Zhu, S. Z. Knottenbelt, M. L. Kirk, D. Pei. Catalytic Mechanism of *S*-Ribosylhomocysteinase (LuxS): Ionization State of Active Site Residues. *Biochemistry,* **2006**, *45,* 12195-12203. DOI: 10.1021/bi061434v

71. S. Bin-Salamon, S. H. Brewer, E. C. Depperman, S. Franzen, J. W. Kampf, M. L. Kirk, R. K. Kumar, S. Lappi, K. Peariso, K. A. Preuss, D. A. Shultz, Testing Bridge Mediated Differences in Valence Tautomeric Behavior. *Inorg. Chem*., **2006**, *45*, 4461-4467. DOI: 10.1021/ic060170y

70. C. Gourlay, D. J. Nielsen, J. M. White, S. Z. Knottenbelt, M. L. Kirk, and C. G. Young, Paramagnetic Active Site Models for the Molybdenum-Copper Carbon Monoxide Dehydrogenase. *J. Am. Chem. Soc.,* **2006**, *128,* 2164-2165.

69. F. E. Inscore, S. Knottenbelt, N. D. Rubie, H. K. Joshi, M. L. Kirk, J. H. Enemark. Understanding the Origin of Metal-Sulfur Vibrations in an Oxo-Molybdenum Dithiolene Complex: Relevance to Sulfite Oxidase. *Inorg. Chem.* **2006**; *45*, 967-976. DOI: 10.1021/ic0506815

68. Hemann, C. Hood, B. L., M. Fulton, E. Riebeseel, G. Schwarz, R. R. Mendel, M. L. Kirk, R. Hille. Spectroscopic and Kinetic Studies of *Arabidopsis thaliana* Sulfite Oxidase: Nature of the Redox-active Orbital and Electronic Structure Contributions to Catalysis. *J. Am. Chem. Soc.* **2005**, *127,* 16567-16577.

67. K. Peariso, M. E. Helton, E. N. Duesler, S. E. Shadle, M. L. Kirk. Sulfur K-edge Spectroscopic Investigation of Second Coordination Sphere Effects in Oxomolybdenum-Thiolates: Relationship to Molybdenum-Cysteine Covalency and Electron Transfer in Sulfite Oxidase. *Inorg. Chem.* **2007**, *46*, 1259-1267. DOI: 10.1021/ic061150z

66. T. M. Anderson, R. Cao, K. I. Hardcastle, B. Hedman, K. O. Hodgeson, M. L. Kirk, S. Knottenbelt, E. C. Depperman, C. L. Hill. A Palladium-Oxo Complex. Simultaneous Electronic and Steric Stabilization of this Proposed Catalytic Intermediate by a Polytungstate Ligand. *Journal of the American Chemical Society,* **2005**, *127,* 11948-11949.

65. R. L. McNaughton, S. Mondal, V. N. Nemykin, P. Basu, M. L. Kirk. Oxomolybdenum Tetrathiolates with Sterically Encumbering Ligands: Modeling the Effect of a Protein Matrix on Electronic Structure and Reduction Potentials. *Inorganic Chemistry,* **2005**, *44,* 8216-8222.

64. M. L. Kirk, D. A. Shultz, E. C. Depperman. Beyond the Active Electron Approximation: Origin of Ferromagnetic Exchange Coupling in Donor-Acceptor Biradicals. *Polyhedron,* **2005**, *24*, 2880-2884.

63. D. A. Shultz, R. K. Kumar, S. Bin-Salamon, M. L. Kirk. Valence Tautomerization and Exchange Coupling in a Cobalt-Nitronylnitroxide-Semiquinone Complex. *Polyhedron,* **2005**, *24*, 2876-2879.

62. C. M. Zaleski, E. C. Depperman, C. Dendrinou-Samara, M. Alexiou, J. W. Kampf, D. P. Kessissoglou, M. L. Kirk, Vincent L. Pecoraro, Metallacryptate Single-Molecule Magnets: The Effect of Lower Molecular Symmetry on Blocking Temperature, *Journal of the American Chemical Society*, **2005**, *127,* 12862-12872.

61. C. M. Zaleski, E. C. Depperman, J. W. Kampf, M. L. Kirk, V. L. Pecoraro, Synthesis, Structure, and Magnetic Properties of a Large Lanthanide-Transition-Metal Single-Molecule Magnet. *Angew. Chem. Int. Ed***. 2004**, *43*, 3912-3914.

60. R. L. McNaughton, M. E. Helton, M. M. Cosper, J. H. Enemark, M. L. Kirk, Nature of the Oxomolybdenum-Thiolate p-bond: Implications for Mo-S Bonding in Sulfite Oxidase and Xanthine Oxidase. *Inorg. Chem*., **2004**, *43*, 1625-1637.

59. M. L. Kirk, K. Peariso. Ground and Excited State Spectral Comparisons of First and Second Generation Models for Sulfite Oxidase *Polyhedron*, **2004**, *23* 499-506.

58. T. M. Anderson, W. A. Neiwert, M. L. Kirk, P. M. B. Piccoli, A. J. Schultz, T. F. Koetzle, D. G. Musaev, K. Morokuma, R. Cao, C. L. Hill, A Late-Transition Metal-Oxo Complex, $O{=}Pt^{IV}(H_2O)L_2$, L = $[PW_9O_{34}]^{9-}$. *Science,* **2004**, *306,* 2074-2076.

57. K. Peariso, C. Carrano, M. L. Kirk. Synthesis and EPR Characterization of New Models for the One-Electron Reduced Molybdenum Site of Sulfite Oxidase. *Inorg. Chem.*, **2003**, *42*, 6194-6203.

56. M. L. Kirk. MCD Spectroscopic Studies on Molybdenum Enzymes and Models. *ACS Symposium Series*, No. 858, **2003**, 340-357. Paramagnetic Resonance of Biomolecules.

55. M. L. Kirk, M. E. Helton, R. L. McNaughton, The Electronic Structure and Spectroscopy of Metallo-Dithiolene Complexes. *Progress in Inorganic Chemisty*, **2003**, *52*, 111-212.

54. T. M. Rajendiran, T. Caudle, M. L. Kirk, J. I. Setyawati, W. Kampf, V. L. Pecoraro. Evaluating Hydrogen Bond Interactions in Enzymes Containing Mn(III)-histidine Complexation Using Manganese-imidazole Complexes. *J. Biol. Inorg. Chem. JBIC* **2003**; *8*, 283-293.

53. M. L. Kirk. Metal Ions in Biological Systems. Volume 39. Molybdenum and Tungsten: Their Roles in Biological Processes. Book Review, *J. Am. Chem. Soc.* **2003**, *125*, 305-306.

52. M. L. Kirk, K. Peariso. Recent Applications of MCD Spectroscopy to Metalloenzymes. *Curr. Op. Chem. Biol.* **2003**, *7*, 220-227.

51. T. M. Rajendiran, M. L. Kirk, I. A. Setyawati, M. T. Caudle, J. W. Kampf, V. L. Pecoraro. Isolation of the First Ferromagnetically Coupled Mn(III/IV) Complex. *Chem. Comm*. **2003**; *7*, 824-825.

50. C. Dendrinou-Samara, M. Alexiou, C. M. Zaleski, J. W. Kampf, M. L. Kirk, D. P. Kessissoglou, V. L. Pecoraro, Synthesis and Magnetic Properties of a Metallacryptate that Behaves as a Single-Molecule Magnet. *Angew. Chem. Int. Ed.* **2003**, *42*, 3763-3766.

49. T. M. Rajendiran, T. Caudle, M. L. Kirk, J. I. Setyawati, W. Kampf, V. L. Pecoraro. Evaluating Hydrogen Bond Interactions in Enzymes Containing Mn(III)-histidine Complexation Using Manganese-imidazole Complexes. *J. Biol. Inorg. Chem. JBIC* **2003**; *8*, 283-293.

48. D. A. Shultz, D. E. Vostrikova, S. H. Bodnar, H.-J. Koo, M.-H. Whangbo, E. C. Depperman, J. W. Kampf, P. D. Boyle, M. L. Kirk. Trends in Metal-Biradical Exchange Interaction for First-Row M^{II}(Nitronyl Nitroxide-Semiquinone) Complexes. *Journal of the American Chemical Society,* **2003**, *125*, 1607-1617.

47. S. Mukhopadhyay, B. A. Gandhi, M. L Kirk, W H. Armstrong. A New Class of Oxo-Bridged High-Valent Hexamanganese Clusters Supported by Sterically Hindered Carboxylate Ligands. *Inorg. Chem.* **2003**, *42,* 8171-8180.

46. V. N. Nemykin, S. R. Davie, S. Mondal, N. Rubie, M. L. Kirk, A. Somogyi, P. Basu, An Analogue System Displaying All the Important Processes of the Catalytic Cycles Involving Monooxomolybdenum(VI) and Desoxomolybdenum(IV)Centers. *J. Am. Chem. Soc.,* **2002**, *124, 756-757*.

45. K. Peariso, R. L. McNaughton, M. L. Kirk, Active Site Stereochemical Control of Oxygen Atom Transfer Reactivity in Sulfite Oxidase. submitted, *Journal of the American Chemical Society,* **2002**, *124, 9006-9007*.

44. E. Depperman, S. H. Bodnar, D. E. Vostrikova, D. A. Shultz, M. L. Kirk, Spin Robustness of a New Hybrid Inorganic-Organic High-Spin Molecule. *Journal of the American Chemical Society,* **2001**, *123,* 3133-3134.

43. M. L. Kirk, N. D. Rubie, L. Hybl, Magnetic Circular Dichroism Studies of $Mn[Mn(CN)_6]$. *Polyhedron,* **2001**, *20,* 1741-1743.

42. M. E. Helton, N. L. Gebhart, E. S. Davies, J. McMaster, C. D. Garner, M. L. Kirk, Thermally Driven Intramolecular Charge Transfer in an Oxo-Molybdenum Dithiolate Complex. *Journal of the American Chemical Society,* **2001**, *123,* 10389-10390.

41. S. R. Davie, N. D. Rubie, B. S. Hammes, C. J. Carrano, M. L. Kirk, P. Basu, Geometric Contol of Reduction Potentials in Oxomolybdenum Centers: Implications for the Serine Coordination in DMSO Reductase. *Inorganic Chemistry,* **2001** *40*, 2632-2633.

40. R. L. McNaughton, M. E. Helton, N. D. Rubie, M. L. Kirk, The Oxo-gate Hypothesis and DMSO Reductase: Implications for a Psuedo-s Bonding Interaction Involved in Enzymatic Electron Transfer. *Inorg. Chem.* **2000**, *39,* 4386-4387.

39. R. L. McNaughton , A. A. Tipton, R. R. Conry, M. L. Kirk, Electronic Structure Studies of Oxomolybdenum Tetrathiolates: Origin of Reduction Potentials and Relationship to Cysteine-Oxomolybdenum Bonding in Enzymes. *Inorg. Chem.* **2000,** ***39,*** 5697-5706.

38. M. E. Helton, A. Pacheco, J. McMaster, J. H. Enemark, M. L. Kirk, An MCD Spectroscopic Study of the Molybdenum Active Site in Sulfite Oxidase: Insight into the Role of Coordinated Cysteine. *J. Inorg. Biochem.* **2000**, *80,* 227-233.

37. M. E. Helton, N. Gruhn, R. McNaughton, M. L. Kirk, Control of Oxo-Molybdenum Reduction and Ionization Potentials by Dithiolate Donors. *Inorg. Chem*. **2000**, *39,* 2273-2278.

36. M. E. Helton, M. L. Kirk, A Model for Ferricyanide Inhibited Sulfite Oxidase. *Inorg. Chem.* **1999**, *38,* 4384-4385.

35. A. J. Stemmler, J. W. Kampf, M. L. Kirk, B. H. Atasi, V. L. Pecoraro, The Preparation, Characterization, and Magnetism of Copper 15-Metallacrown-5 Lanthanide Complexes. *Inorg. Chem.* **1999**, *38,* 2807-2817.

34. F. E. Inscore, R. McNaughton, B. Westcott, M. E. Helton, R. Jones, J. H. Enemark, M. L. Kirk, Spectroscopic Evidence for a Unique Bonding Interaction in Oxo-Molybdenum Dithiolate Complexes: Implications for σ Electron Transfer Pathways in the Pyranopterin Dithiolate Centers of Enzymes. *Inorg. Chem.* **1999**, *38,* 1401-1410.

33. R. M. Jones, F. E. Inscore, R. Hille, M. L. Kirk, Freeze-Quench Magnetic Circular Dichroism Spectroscopic Study of an Intermediate in the Reaction Mechanism of Xanthine Oxidase. *Inorg. Chem.* **1999**, *38*, 4963-4970.

32. A. J. Stemmler, B. R. Gibney, J. W. Kampf, M. L. Kirk, V. L. Pecoraro, Synthesis and Characterization of a Dimer, Trimer and Pentamer or Metallacrown formed from Hydroximate Ligands and Nickel. submitted to *Inorg. Chem.*

31. R. Jones, K. Jayaraj, A. Gold, M. L. Kirk, Ground and Excited State Spectroscopic Probes of [FeIV=O(TMP)]+: The First Magnetic Circular Dichroism Study of a Model Peroxidase Compound I Intermediate. *Inorg. Chem.* **1998**,*37,* 2842-2843.

30. R. Jones, J. Dewitt, M. L. Kirk**,** X-ray Absorption Spectroscopic Determination of s and p Contributions to Fe(IV)=O Bonding in a Model Peroxidase Compound I Intermediate. *SSRL 1996 Act. Rep.* **1997**, A15-A17.

29. A. Gelasco, M. L. Kirk, J. W. Kampf, V. L. Pecoraro, The [Mn2(2-OHsalpn)2]2-,1-,0 1+ System: I. Synthesis, Structure, Spectroscopy, and Magnetism of the First Structurally Characterized Dinuclear Manganese Series Containing Four Distinct Oxidation States. *Inorg. Chem.* **1997**, *36*, 1829-1837.

28. M. T. Caudle, J. W. Kampf, M. L. Kirk, P. G. Rasmussen, V. L. Pecoraro, The First Binuclear Mn(IV) Complex Containing a Bridging Imidazolate Ligand Exhibits Unique EPR Spectral Features. *J. Am. Chem. Soc*. **1997**, *119,* 9297-9298.

27. A. J. Stemmler, J. W. Kampf, M. L. Kirk, V. L. Pecoraro, A Model for the Inhibition of Urease by Hydroxamates. *J. Am. Chem. Soc.* **1995**, *117*, 6368-6369.

26. D. A. Malamatari, P. Hitou, A. G. Hatzidimitriou, A. Gourdon, F. E. Inscore, M. L. Kirk, D. P. Kessissoglou, The Crystal Structure of [Mn3(saladhp)2(acetato)2(5-Cl-salicylato)2]n; The First Example of a Mixed Valence Mn(III)Mn(II)Mn(III) Schiff-Base Polymeric Complex Containing a Trimeric Repeat Unit. *Inorg. Chem.* **1995**, *34*, 2493-2494.

25. M. H. Wall Jr., P. Basu, B. Wicks, T. Buranda, E. Findsen, J. H. Enemark, M. Ondrias, M. L. Kirk, Photoinduced Electron Transfer in Covalently Linked Oxo-Molybdenum(V)-Porphyrin Systems. *Inorg. Chem.* **1997**, *36*, 5676-5677.

24. D. R. Gamelin, E. Bominaar, C. Mathoniere, M. L. Kirk, K. Wieghardt, J.-J. Girerd, E. I. Solomon, Excited State Distortions and Electron Delocalization in Mixed-Valence Dimers: Vibronic Analysis of the Near-IR Absorption and Resonance Raman Profiles of [Fe2(OH)3(tmtacn)2]2+. *Inorg. Chem.* **1996**, *35,* 4323-4335.

23. D. R. Gamelin, E. Bominaar, M. L. Kirk, K. Wieghardt, E. I. Solomon, Excited State Contributions to Ground State Properties of Mixed-Valence Dimers: Spectral and Electronic Structural Studies of Fe2(OH)3(tacn)2 Related to the [Fe2S2]+Actives Sites of Plant Type Ferridoxins. *J. Am. Chem. Soc.* **1996**, *118,* 8085-8097.

22**.** M. J. Baldwin, T. L. Stemmler, P. J. Reggs-Gelasco, M. L. Kirk, J. E. Penner-Hahn, V. L. Pecoraro, Structural and Magnetic Effects of Successive Protonations of Oxo Bridges in High Valent Manganese Dimers. *J. Am. Chem. Soc.* **1994**, *116*, 11349-11356.

21**.** M. J. Baldwin, J. W. Kampf, M. L. Kirk, V. L. Pecoraro, Structural and Magnetic Studies of Mn(II) Complexes of the Imidazole-Containing Ligand 5-NO2-salimH[5-NO2-salimH2 = 4-(2-(5-nitrosalicylideneamino)ethyl)imidazole] With Varying Nuclearity. *Inorg. Chem*. **1995**, *34*, 5252-5260.

20. E. I. Solomon, M. L. Kirk, D.R. Gamelin, S. Pulver, "Bioinorganic Spectroscopy"; *Methods in Enzymology*. Vol **246**, p 271, 1995.

19. D. R. Gamelin, M. L. Kirk, T. L. Stemmler, S. Pal, W. H. Armstrong, J. E. Penner-Hahn, E. I. Solomon, Magnetic Circular Dichroism Spectroscopic Comparison of [Mn(III)Mn(IV)] Model Complexes and Manganese Catalase. *J. Am. Chem. Soc.* **1994**,*116*, 2392-2399.

18. M. L. Kirk, M. K. Chan, W. H. Armstrong, E. I. Solomon, Ground State Electronic Structure of the Dimer of Dimers Complex [(Mn2O2)2(tphpn)2]4+: Potential Relevance to the Photosystem II Water Oxidation Catalyst, *J. Am. Chem. Soc.* **1992**, *114*, 10432-10440.

17. D. P. Kessissoglou, M. L. Kirk, M. S. Lah, X. Li, C. Raptopoulou, W. E. Hatfield, V. L. Pecoraro, Models for the Manganese Clusters in Photosynthesis: Structural and Magnetic Characterization of Trinuclear, Mixed-Valence Manganese Acetates, *Inorg. Chem*, **1992**, *31*, 5425.

16. E. Larson, A. Haddy, M. L. Kirk, R. Sands, W. E. Hatfield, V. L. Pecoraro, The Highly Asymmetric Mixed Valent Dimer {[Mn(2-O-SALPN]2(THF)}ClO4 Shows a Temperature Dependent Interconversion Between g=2 Multiline and g=4 EPR Signals, *J. Am. Chem. Soc.* **1992**, *114*, 6263.

15. M. L. Kirk, M. S. Lah, C. Raptopoulou, D. P. Kessissoglou, W. E. Hatfield, V. L. Pecoraro, Cationic Control of Spin Diminsionality in Infinite Chains of (Cation)2[Mn(III)(Salicylate)2(CH3OH)2, *Inorg. Chem*,

1991, *30,* 3900.

14. M. L. Kirk, W. E. Hatfield, M. S. Lah, D. P. Kessissoglou, V. L. Pecoraro, L. W. Morgan, J. D. Petersen, Effects of Alternation in Some Quasi-One-Dimensional Magnetic Materials, *J. Appl. Phys.*, **1991**, *69*, 6013.

13. K. L. Trojan, W. E. Hatfield, K. D. Kepler, M. L. Kirk, Strong Exchange Coupling in Lanthanide bis-(phthalocynainato) Sandwich Compounds, *J. Appl. Phys.*, **1991**, *69*, 6007.

12. K. L. Trojan, W. E. Hatfield, K. D. Kepler, M. L. Kirk, Bis(phthalocynainato) Lanthanide Sandwich Compounds Exhibiting Mixed Valence Ligands, in *Mixed Valency Systems: Applications in Chemistry, Physics and Biology*, K. Prassides, Ed.; Dluwer Academic Publishers: Dordrect, 1991.

11. D. A. Tucker, P. S. White, K. L. Trojan, M. L. Kirk, W. E. Hatfield, Identification of a Novel Tetragonally Compressed Six-Coordinate Copper(II) Complex: Preparation and Characterization of a 3-Chloroanilinium Copper Chloride Complex, (3-chloroanilinium)8[CuCl6]Cl4, *Inorg. Chem*, **1991**, *30*, 823.

10. M. S. Lah, V. L. Pecoraro, M. L. Kirk, W. E. Hatfield, Transition Metal Encapsulation by "Metallocrown" Ethers, in *Biosensor Technology*, R. P. Buck, W. E. Hatfield, M. Umana, Eds.; Marcel Dekker, Inc.: New York, 1990.

9. E. Bill, X. Ding, E. L. Bominaar, A. X. Trautwein, H. Winkler, D. Mandon, R. Weiss, A. Gold, K. Jayaraj, W. E. Hatfield and M. L. Kirk, Evidence for Variable Metal-Radical Spin Coupling in Oxoferryl Porphyrin Cation Radical Complexes, *Eur. J. Biochem.*, **1990**, *188*, 665.

8. T. Garber, S. Van Wallendael, D. P. Rillema, M. L. Kirk, W. E. Hatfield, J. H. Welch and P. Singh, A Novel Copper(II) Complex Containing the Ligand 1,2-bis(2,2'-bipyridyl-6-yl)ethane: Structural, Magnetic, Redox and Spectral Properties, *Inorg. Chem*., **1990**, *29*, 2863.

7. M. S. Lah, M. L. Kirk, W. E. Hatfield and V. L. Pecoraro, The Tetranuclear Cluster Fe(III)[Fe(III)(salicylhydroximato)(CH_3OH)(Acetate)]$_3$ is an Analogue of M3+(9-crown-3), *J. Chem. Soc. Chem. Comm.*, **1989**, 1606.

6. J. H. Welch, R. D. Bereman, P. Singh, D. Haase, W. E. Hatfield and M. L. Kirk, Effect of Cation on the Structures, Magnetic Properties and Specific Heats of Salts of Bis(5,6-dihydro-1,4-dithiin-2,3-dithiolato)nickelate(III): The Crystal Structure of [(CH3)4N][Ni(DDDT)2], *Inorg. Chim. Acta*, **1989**, 162, 89.

5. J. A. Bonadies, M. L. Kirk, M. S. Lah, D. P. Kessissoglou, W. E. Hatfield and V. L. Pecoraro, Structurally Diverse Manganese (III) Schiff Base Complexes: Chains, Dimers, and Cages, *Inorg. Chem.*, **1989**, 28, 2037.

4. J. H. Miller Jr., W. E. Hatfield, B. R. Rohrs, M. L. Kirk, J. L. Perkinson, K. L. Trojan, J. D. Hunn, Z. H. Zhang and W. J. Riley, Synthesis and Characterization of BiCaSrCuO and BiSnCaSrCuO Superconducting Ceramics, in *High Temperature Superconductivity: The First Two Years* R.M. Metzger ed.; Gordon and Breach Science Publishers: New York, 1989.

3. D. P. Kessissoglou, M. L. Kirk, C. A. Bender, M. S. Lah and V. L. Pecoraro, A Bent Mixed-Valence Manganese (III/II/III) Complex: A New Class of Trinuclear, Acetate Bridged Schiff Base Compounds Exhibiting a g=2 Multiline Signal, *J. Chem. Soc. Chem. Comm.*, **1989**, 84.

2. W. E. Hatfield, B. R. Rohrs, M. L. Kirk, J. H. Helms, H. Ro and E. J. Williamsen, Magnetic Anomalies in the Rare Earth Oxide Superconductors GdBa2Cu3O7-x, in *High Temperature Superconducting Materials: Preparations, Properties, and Processing* W.E. Hatfield and J.H. Miller eds.; Marcel Dekker, Inc.: New York, 1988.

1. X. Li, D. P. Kessissoglou, M. L. Kirk, C. Bender and V. L. Pecoraro, Isolation of a Mixed-Valence

Trinuclear Complex Potentially Relevant to the Photosynthetic Oxygen-Evolving Center, *Inorg. Chem.*, **1988**, 27, 1.

Support

Research Support

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"Spectroscopic Studies of Molybdoenzymes and Models"
R01 GM57378 Kirk (PI)
2.0 Academic Months and 1 Summer Month
NIH/NIGMS 08/02/2011 – 03/31/2015
The specific aims of this project are i) determine the reaction coordinate for the molybdenum hydroxylases, ii) develop a comprehensive understanding of active site contributions to catalysis in the SO family enzymes YedY and mARC, and iii) identify key molybdenum-sulfur covalency contributions to electron transfer (ET) and redox potential modulation in DMSOR family enzymes.
Total: $1,218,597

"Nanoscale Electron Correlation and Ferromagnetic Exchange in Donor-Acceptor Biradical Systems: Relationship to Molecular Electronics"
Kirk (PI) 8/1/10 – 7/31/13
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The major goals of this project are to (1) understand excited state contributions of new acceptor fragments to the enhancement of electronic coupling (H_{ab}) and ferromagnetic exchange in donor-acceptor biradicals, (2) Increase the dimensionality of current metallo-bis(dioxolene) systems by incorporating spin or emissive centers at axial positions on the central metal ion, and (3) Understand how d-electron configuration and M-dioxolene orbital overlap influence the nature of electron delocalization and long-range ferromagnetic coupling of localized radical spin centers.
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Kirk (co-PI) 8/1/13 – 7/31/18
EPSCoR
The goals of this proposal are to improve the research, cyberinfrastructure (CI), and human resources required to enable NM to achieve its energy, education and workforce development potential. These goals will be accomplished via successful completion of the following objectives: (1) invest in critical research equipment, facilities, and faculty hires that strengthen New Mexico's ability to compete for large, interdisciplinary grants; (2) increase the size and diversity of the STEM workforce, emphasize community colleges, Tribal colleges, and Hispanic-serving institutions; (3) build new interdisciplinary and inter-institutional collaborations; and (4) develop a culture of innovation and entrepreneurship.
Total: $20,000,000

"Donor-Acceptor Interactions, Long-Range Electron Correlation, and Dynamic Spin Manipulation: Relationship to Molecular Electronics
Kirk (PI) 8/1/13 – 7/31/16

National Science Foundation
The primary goals of the proposed project are to understand excited state contributions to bridge mediated electronic coupling (H_{ab}), understand how open-shell excited state singlet configurations promote long-range electron correlation, and develop new platforms for spin control of excited state dynamics in photoexcited donor-acceptor (D-A) molecules. The research plan will achieve these long-term goals by adding to the electron/spin transport knowledge base through completion of key project objectives.
Total: $531,038

"Combinatorial Studies of Novel Spin-Crossover Complexes on Surfaces"
Kirk (co-PI) 7/1/13 – 6/30/17
National Science Foundation
The primary goals of the proposed project are to synthesize and characterize new magnetic active layer materials for molecular spintronics applications. These active layer materials will possess switchable magnetic properties that will be employed as switchable molecular-level components in spintronic device applications. A detailed characterization of these systems is critical to fully understanding the behavior of the active layer components and will assist in the rational design of newer generations of active layer materials that are optimized for desired performance characteristics.
Total: $288,503

Previous Funding

Electronic Structure Studies of Magnetic Donor-Acceptor Biradical Systems Related to Molecular Electronics
Kirk (PI) 8/15/06 – 7/31/10
National Science Foundation (CHE-0616190)
$500,000
This grant focuses on understanding excited state contributions to electron transfer/transport, spin-polarized electron transfer/transport, and rectification behavior in molecular conduits.

Spectroscopic Studies of Molybdoenzymes and Models
Martin L. Kirk, P. I.
NIH/NIGMS Public Health Service Grant, National Institutes of Health
2/1/07 - 1/31/11, $1,300,000

MCD and EPR Studies of S-ribosylhomocysteinase (LuxS) Kirk (PI) 1/01/06 – 12/31/06
NIH/The Ohio State University
$75,000

LANL Laboratory Directed Research & Development Kirk (PI) 2/01/04 – 1/31/07
Los Alamos National Laboratories – DOE
Role: co-PI
$35,000

Joint Science and Technology Laboratory (JSTL) – Collaborative Research Program Kirk (PI) 2/01/05 – 1/31/06
LANL and The University of New Mexico
Role: PI
$75,000

Metal-Ligand Redox Interplay and Molecular Bistability in
Quinoxaline-Based Complexes
Martin L. Kirk, P. I.
Petroleum Research Fund
6/1/02 - 5/31/04, $80,000

Spectroscopic Studies of Thiolate Donors in Mo Enzymes
National Institutes of Health
$38,000 / yr. 3 years – NIH Postdoctoral Fellowship Grant

XAS Studies of High-Valent Mo-oxo Sites
Martin L. Kirk P. I.
Stanford Synchrotron Radiation Laboratory

Purchase and Acquisition of a 35GHz EPR/ENDOR Spectrometer
Martin L. Kirk, P. I.
National Science Foundation
8/1/02 - 7/30/04, $450,000

Spectroscopic Studies of Molybdoenzymes and Models
Martin L. Kirk, P. I.
Public Health Service Grant, National Institutes of Health
4/1/98 - 3/31/02, $663,189

Electronic Structure Contributions to Reactivity in Oxotungsten Dithiolene Compounds.
Martin L. Kirk, P.I.
Petroleum Research Fund - Type AC
6/1/98 - 8/31/00, $60,000

Electronic Structure Studies of Molybdenum Oxotransferases.
Martin L. Kirk, P. I.
Sandia-University Research Program, Sandia National Laboratories
10/94 - 9/95; $35,000

Electronic Structure Studies of Molybdenum Oxotransferases.
Martin L. Kirk, P. I.
NSF Starter Grant, National Science Foundation
9/94 - 10/96, $32,000

Research Experience for Chemistry Undergraduates
Martin L. Kirk co - P. I.
National Science Foundation
6/1/99 - 5/31/02, $154,080

Selected Invited Talks at International Meetings

243rd National ACS Meeting, *Donor-Acceptor Ligands in Inorganic Chemistry: The Influence of Excited States on Ground State Properties* – San Diego, CA 3/2012.

2012 Mesilla Workshop, *New Insights into Ligand Control of (Spin) Delocalization* – Mesilla, NM 2/12.

Fourth "North America-Greece-Cyprus Workshop on Paramagnetic Materials" (NAGC 2011), *Donor-Acceptor Ligands in Inorganic Chemistry: The Influence of Excited States on Ground State Properties* – Patras, Greece. 6/2011.

International Conference on Bioinorganic Chemistry ICBIC, *Electronic Structure Contributions to Reactivity in Pyranopterin Molybdenum Enzymes* - Vancouver, Canada. 8/2011.

Molybdenum and Tungsten Enzymes Conference, *Spectroscopic and Electronic Structure Probes of Electron and Atom Transfer in DMSOR* – Edmonton, Canada. 8/2011.

Metals in Biology Gordon Conference – *Spectroscopic and Electronic Structure Studies of Pyranopterin Molybdenum Enzymes and Models* – Oxnard, California. 2/2011

242nd National ACS Meeting - *Magnetic Spectroscopic Studies of Pyranopterin Molybdenum Enzymes and Models* – Anaheim, California. 5/2011.

241st National ACS Meeting - *Spectroscopic and Electronic Structure Studies of Pyranopterin Molybdenum Enzymes and Models* – Boston, Massachusetts. 8/2010.

NSF Workshop on Inorganic Chemistry - *Donor-Acceptor Ligands in Inorganic Chemistry: The Influence of Excited States on Ground State Properties* – Santa Fe, New Mexico. 5/2010.

52nd Annual Rocky Mountain Conference on Analytical Chemistry - *EPR Spectroscopy as Part of a Combined Spectroscopic Approach to Understand ElectronicStructure Contributions to Reactivity in Pyranopterin Molybdenum Enzymes and Models* – Snowmass, Colorado. 8/2010.

International Conference on Bioinorganic Chemistry ICBIC, *Spectroscopic and Electronic Structure Studies of Probing the Reaction Coordinate of the Molybdenum Hydroxylases* - Nagoya, Japan 7/09.

239th National ACS Meeting - *Spectroscopic and Electronic Structure Studies Probing the Reaction Coordinate of Molybdenum Hydroxylases* – Washington, DC. 8/2009.

Metals in Biology Gordon Conference – *Electronic Structure Contributions to Reactivity in Sulfite Oxidase.* Oxnard, California, 1/08.

International Conference on Bioinorganic Chemistry ICBIC, *Spectroscopic and Electronic Structure Studies of the Mlybdenum Hydroxylases* - Vienna, Austria 7/07.

Metals in Biology Gordon Conference – *Electronic Structure Contributions to Catalysis in Xanthine Oxidase and CO Dehydrogenase*. Oxnard, California, 1/06.

International Conference on Bioinorganic Chemistry ICBIC, *Session Chair* - Ann Arbor, Michigan, 7/05.

Molybdenum and Tungsten Enzymes Gordon Conference – *Spectrosocpic and Computational Probes of Xanthine Oxidase and CO Dehydrogenase Reactivity*. Queen's College, Oxford, UK 7/05.

International Conference on Molecular Magnetism – *Metallobiradicals: Origin of Ferromagnetic Exchange and Implications for Molecular Wires*. Tsukuba, Japan 10/04.

Excited State Processes in Electronic and Bio Nano-Materials, *Low-Dimensional Materials: New Paradigms for Molecular Bistability* – Los Alamos, New Mexico 8/03

International Conference on Bioinorganic Chemistry ICBIC, *The Oxo-Gate Hypothesis in the Pterin-Containing Mo Enzymes* - Cairns, Queensland, Australia 7/03.

National Conference of the Inorganic Chemistry Division of the Royal Australian Chemical Institute - *An Electronic Structure Description of the cis-MoOS Unit in Models for Molybdenum Hydroxylase Active Sites.* Melbourne, Victoria, Australia 2/03.

ACS National Meeting - Pyrazolylborate Symposium - *Small Molecule Analogues of Sulfite Oxidase and Xanthine Oxidase: Spectroscopy, Bonding, and Electronic Structure.* New Orleans, Louisiana, 4/03.

Molybdenum and Tungsten Enzymes Gordon Conference - *The Mechanism of Sulfite Oxidase: From Biomimetic Compounds to Plant SO*. New Hampshire, 7/03

National Science Foundation Inorganic Chemistry Workshop - *Metal-Ligand Redox Interplay and Molecular Bistability: Toward Multi-Property Magnetic Materials.* Santa Fe, New Mexico 4/02.

International Coordination Chemistry Conference - *Mo-S p-Bonding Contributions to Electron and Atom Transfer Reactivity in Pyranopterin Molybdenum Enzymes.* Heidelberg, Germany 7/02.

Inorganic Gordon Conference - *Mo-S p-Bonding Contributions to Electron and Atom Transfer Reactivity in Pyranopterin Molybdenum Enzymes.* Newport, Rhode Island 7/02.

Molybdenum and Tungsten Enzymes Gordon Conference - *Spectroscopically Derived Mechanism of the Reductive Half-reaction in Xanthine Oxidase*. Queen's College, Oxford, UK 7/01.

ACS National Meeting - Tutorial on Paramagnetic Resonance Techniques for Biomolecules - *MCD Spectroscopy as a Probe of Ground and Excited State Electronic Structure.* Orlando, Florida, 4/02.

International Conference on Molecular Magnetism - *Thermally Driven Intramolecular Charge Transfer in New Paramagnetic Metal Complexes*, San Antonio, Texas 4/16/00

National Meeting of the American Chemical Society, *A Molecular Level Description of Electron and Atom Transfer in the Pyranopterin Molybdenum Enzymes* , San Francisco, California 4/00.

Metals in Biology Gordon Conference, *A Molecular Level Description of Electron and Atom Transfer in the Pyranopterin Molybdenum enzymes* - Oxnard, California 1/00.

International Conference on Bioinorganic Chemistry ICBIC, *The Oxo-Gate Hypothesis in the Pterin-Containing Mo Enzymes* - Minneapolis, Minnesota 6/99.

Recent Highlights in Personnel Development

Current Group Members and Projects

Dr. Jing Yang – Ph.D. (The University of New Mexico)
Sulfite Oxidizing Enzymes

Dr. Logan Giles – Ph.D. (Montana State University)
Charge Transfer Complexes and Spectroscopic Studies of Molybdoproteins

Antonio Williams - BS (Alcorn State)
Modeling Mo Enzymes

Diana Habel-Rodriquez – BS (New Mexico)
VBCI Studies of Molecular Wires and Rectifiers. Mixed-Valency and Electron Delocalization

Ben Stein – BS (University of Northern Colorado)
Electron Delocalization; Mechanistic Bioinorganic Chemistry; Electronic Structure

Chao Dong – BS (BS, PRC)
Molybdenum Model Chemistry, Enzyme Studies, and Electronic Structure Studies

Dominic Kersi – MS (University of Minnesota - Duluth)
Inorganic Synthesis and Spectroscopy

Michael Williams – BS (The University of New Mexico)
Spectroscopic Studies of Molybdoenzymes and Models

Past Doctoral Associates

Dr. Mark Wall - PhD 1997 (New Mexico) Postdoctoral (Univ. of Idaho)
PhD Research: Spectroscopic Studies of Peripherally Elaborated Tetraarylporphyrins.
Senior Scientist - Instruments SA, Newark, New Jersey

Dr. Robert Jones - PhD 1998 (New Mexico) Postdoctoral (University of California)
PhD Research: Spectroscopic Probes of High-Valent Transition Metal-Oxygen Intermediates.
Senior Staff Scientist - QTL Biosystems, Santa Fe, New Mexico

Dr. Frank Inscore - PhD 1999 (New Mexico) Postdoctoral (University of Arizona)
PhD Research: Electronic Structure Studies of Oxo-Molybdenum (V) Complexes: Relationship to Pterin-Containing Oxomolybdenum Enzyme Active Sites.

Dr. Matthew Helton - PhD 2000 (New Mexico) NIH postdoctoral fellow - Johns Hopkins
PhD Research: Electronic Structure Studies of oxo-Molybdenum Model Complexes and Proteins.
Unilever Corporation

Dr. Rebecca McNaughton - PhD 2002 (New Mexico) UNM Dissertation Fellow
NIH Postdoctoral Fellow - Northwestern University
PhD Research: Synthetic, Spectroscopic, and Theoretical Studies of Mo and W Catalytic Centers

Nouvelle Gebhart - BS (New Mexico) DOE Predoctoral Fellow - New Mexico
PhD Research: Studies of Thermally Induced Charge Transfer

Dr. Nick Rubie – PhD 2003 (New Mexico)
Postdoctoral Fellow – Oregon Graduate Institute
PhD Research: Electronic Structure Contributions to Reactivity in Molybdenum Hydroxylases
Instructor – The University of New Mexico

Dr. Ezra Depperman – PhD 2005 (New Mexico)
PhD Research: High-Spin Metal Organic Magnetic Materials
Chemistry Teacher – Albuquerque Academy

Dr. Abebe Habtegabre – PhD 2010 (New Mexico)
PhD Research: Mechanistic Studies of Xanthine Oxidase

Dr. Joseph Sempombe – BS (University of Dar Es Salaam), PhD 2011 (New Mexico)
PhD Research: Spectroscopic Studies of Metalloenzymes

Dr. Regina Mtei – BS (University of Dar Es Salaam), PhD 2011 (New Mexico)
PhD Research: Spectroscopic Studies of DMSO Reductase and Models

Past Masters Students

Meita Fulton – BS (Texas A&M)
The Reductive Half-Reaction in Sulfite Oxidase

Surhabi Sharma – BS
Spectroscopic Studies of Sulfite Oxidase Models
Los Alamos National Laboratory

Raphael Malisa – BS (University of Dar Es Salaam)
Molybdenum Models

Ellen Yuzhi Li – BS
Long Range Electronic Coupling, Molecular Bistability, and Organic Mixed-Valency

Past Postdoctoral Associates

Dr. Katrina Peariso - PhD 2000 (Michigan) NIH postdoctoral fellow - New Mexico
Spectroscopy and Mechanism of Sulfite Oxidase
Medical Student, The University of New Mexico
University of Cincinnati School of Medicine

Dr. Sushilla Knottenbelt – PhD 2003 (University of York)
Electronic Structure of Xanthine Oxidase and CO dehydrogenase
Instructor – The University of New Mexico

Dr. Nick Rubie – PhD 2003 (New Mexico)
Xanthine Oxidase Model Chemistry
Instructor – The University of New Mexico

DR SUSHILLA KNOTTENBELT

PERSONAL DETAILS

Address:	1699 Quail Run Ct NE, Albuquerque, NM 87122
Email address :	sknottenbelt@gmail.com
Cell phone number:	505-620-7786
Date of birth:	03/18/1977
Citizenship:	US citizenship pending
Marital Status:	Married

EXPERIENCE

Fall 2011 – present: Visiting Assistant Professor at the University of New Mexico

Teaching responsibilities

General Chemistry I and II, Instructor: taught large sections employing active learning pedagogies and an 'inverted' classroom approach. Implemented a new course design involving team-based learning in the new UNM collaborative learning classroom for a small section of pre-health science students. Developed group work activities with an emphasis on applications of general chemistry to the health sciences.

Foundations of Chemistry: Coordinator: designed to save students enrolled in and failing in their first semester of General Chemistry. Implemented a new course design integrating learning skills and chemistry concepts aimed to build students' metacognition as well as their chemistry background.

Teaching development workshops facilitated by OSET

September 2011	ENGAGE with Proven Pedagogical Strategies for Student Success in Engineering, Science, and Mathematics
November 2011	Effective Classroom Teaching and Learning with Student Groups
January 2012	Pathway to Transforming Student Learning and Persistence in Gateway Science and Math Courses
February 2012	Interactive Engagement Techniques, Assessments, and Their Research Basis
May 2012	Designing Courses for Effective Student Learning
September 2012	Using Cooperative Group Structures and Related Approaches to Promote Your and Your Students' Active Teaching and Learning in Mathematics
September 2012	Pulling It All Together and Getting Real Students to Really Discuss.
January 2013	Designing Courses for Effective Student Learning (attended as facilitator)

Conference presentations

7th Annual Success in the Classroom-Sharing Practices that Work, UNM (02/15/2012)

New Mexico Higher Education Assessment and Retention Conference (02/23/2012)

Oral Presentation at both conferences (with Dr Joseph Ho): Can a Parachute Class Prepare Students to Succeed upon Returning to General Chemistry?

Biennial Conference on Chemical Education (BCCE) (07/29/2013 – 08/02/2013) Poster presentation: 'Can a Parachute Class prepare students to succeed?'

Proposals

December 2011: Teaching Allocation Grant Proposal (with Dr. Lisa Whalen): Using molecular orbital model kits to enhance learning of crucial concepts in chemical bonding by bringing activity-based learning into the classroom in General Chemistry and Organic Chemistry **(Fully funded)**

March 2012: 2012-2013 Gateway Science and Math Course Reform Projects (with Dr Joseph Ho, Dr Stephen Cabaniss, Ms Clarissa Sorensen-Unruh and Dr Shaorong Yang): Develop engaging interdisciplinary exercises and resources to support active learning in the classroom in CHEM 122 (**Accepted)**

Service

Member of Search Committee for Assistant Professor in the area of energy, materials or catalysis

Member of the BA/MD Committee for Curriculum and Student Progress (CCSP)

Chair of the BA/MD Basic Sciences subgroup of the CCSP

Member of the Undergraduate Committee

Worked with General Chemistry groups for CHEM 121 and 122 to develop and standardize learning outcomes, homework and exams between sections. Provided support for part-time instructors.

Recognized by the Accessibility Resource Center as an Outstanding Faculty Member.

Fall 2009-May 2011 Part-time instructor at the University of New Mexico teaching General Chemistry 1st and 2nd semester classes.

Fall 2010: Extensive course redesign of CHEM 121 to incorporate active and collaborative learning into a large enrollment setting, resulting in improved student success and achievement, as well as better student evaluations.

Teaching development workshops taken through OSET

April 2010	Designing Effective Multiple Choice Tests
June 2010	Course Design Institute
September 2010	Defining, Assessing, and Using Learning Outcomes for Your Course
February 2011	Designing Deep Learning Experiences for Fractal Brains
March 2011	Active Learning and Critical Thinking
July 2011	Course Design Institute

2004-2007 Postdoctoral Fellowship, University of New Mexico, in the group of Professor Martin Kirk, investigating problems in bio-inorganic chemistry using advanced spectroscopic techniques and computational chemistry.

2000-2003 Graduate Teaching Assistant, Department of Chemistry, University of York, UK.

EDUCATION

2000 – 2003 **PhD in Computational Chemistry**, University of York.

Thesis title: Investigation of electronic structure in inorganic and bioinorganic chemistry, using Density Functional Theory.

1996 – 2000 **MChem First Class (Honors) in Chemistry, Resources and the Environment,** University of York, UK. (analogous to MSc, magna cum laude in the U.S).

Prizes and Scholarships

2001-2003	University of York Overseas Research Students' Award
2002	Shell Award for the best 2nd year graduate student poster on research work
2000	Twycross Prize, for personal development, academic progress, future plans
1999	Castrol Prize, for the best final year undergraduate research project.
1999	Margaret Bishop Prize, for best student specializing in Environmental Chemistry.
1998	ICI scholarship
1996-2003	University of York International Students' Scholarship

REFERENCES

Dr. Gary Smith, Special Assistant to the Provost, Faculty Development.
Office of Support for Effective Teaching, 250 Scholes Hall, MSC053400, UNM, 87131
(505) 277-2297 gsmith@unm.edu

Postdoctoral advisor: Dr. Martin Kirk, Professor of Inorganic Chemistry,

Department of Chemistry and Chemical Biology, MSC03 2060, UNM, 87131
(505) 277 5992, mkirk@unm.edu.

Doctoral advisor: Dr. John McGrady, Professor of Computational Inorganic Chemistry, Chemistry Department, Oxford University, UK,
(011) 44 1865 272 645, john.mcgrady@chem.ox.ac.uk.

PUBLICATIONS

1. Reaction Coordinate of Pyranopterin Molybdenum Enzymes, Encyclopedia of Inorganic Chemistry, 2009. Kirk, M. L., Knottenbelt, S., & Habtegabre, A.
2. Spectroscopic and electronic structure studies of symmetrized models for reduced members of the dimethylsulfoxide reductase enzyme family. Journal of the American Chemical Society 2008;130(14):4628-36. McNaughton R. L; Lim B. S; Knottenbelt S Z; Holm R. H; Kirk M. L.
3. Electronic structure description of the cis-MoOS unit in models for molybdenum hydroxylases.
Journal of the American Chemical Society 2008;130(1):55-65. Doonan C. J; Rubie N. D; Peariso K; Harris H. H; Knottenbelt S. Z; George G. N; Young C. G; Kirk M. L
4. Terminal gold-oxo complexes. Journal of the American Chemical Society 2007;129(36):11118-33. Cao R; Anderson T. M; Piccoli P. M B; Schultz A. J; Koetzle T. F; Geletii Y. V; Slonkina E; Hedman B; Hodgson K. O; Hardcastle K. I; Fang X; Kirk M. L; Knottenbelt S. Z; Kögerler P; Musaev D. G; Morokuma K; Takahashi M; Hill C. L.
5. Catalytic mechanism of S-ribosylhomocysteinase: ionization state of active-site residues. Biochemistry 2006;45(40):12195-203.Zhu J; Knottenbelt S; Kirk M L; Pei D.
6. Paramagnetic active site models for the molybdenum-copper carbon monoxide dehydrogenase. Journal of the American Chemical Society 2006;128(7):2164-5. Gourlay C; Nielsen D. J; White J. M; Knottenbelt S Z; Kirk M L; Young C. G.
7. Understanding the origin of metal-sulfur vibrations in an oxo-molybdenum dithiolene complex: relevance to sulfite oxidase. Inorganic chemistry 2006;45(3):967-76. Inscore F. E; Knottenbelt S. Z; Rubie N. D; Joshi H. K; Kirk M. L; Enemark J. H
8. A palladium-oxo complex. Stabilization of this proposed catalytic intermediate by an encapsulating polytungstate ligand. Journal of the American Chemical Society 2005;127(34):11948-9.Anderson T. M; Cao R.; Slonkina E; Hedman B; Hodgson K. O; Hardcastle K. I; Neiwert W. A; Wu S; Kirk M. L; Knottenbelt S; Depperman E. C; Keita B; Nadjo L; Musaev D G; Morokuma K; Hill C L
9. On the electronic origins of structural isomerism in the iron-sulfur cubane, $[(C_5H_5)_4Fe_4S_4]^{2+}$. Journal of the American Chemical Society 2003;125(32):9846-52.Knottenbelt S Z; McGrady J E
10. Stable formally zerovalent and diamagnetic monovalent niobium and tantalum complexes based on diazadiene ligands. Journal of the American Chemical Society (Communication) 2002;124(15):3818-3819. Daff P J; Etienne M; Donnadieu B; Knottenbelt S Z; McGrady J E.
11. The interplay between steric repulsions and metal-metal bonding in $[Ru_2(\mu Cl)_3(PR_3)_6]^{z+}$, R=H, Me, Et, z = 1, 2, 3: a hybrid QM/MM study. Dalton Transactions, 2003; 227-232.Knottenbelt, S. Z.; McGrady, J. E. and Heath, G.A

FU-SEN LIANG, Ph.D.

Assistant Professor

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1 University of New Mexico, Albuquerque, NM 87131
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Education

2005 Ph.D., Bioorganic Chemistry, *The Scripps Research Institute*, La Jolla, CA, USA
1996 M.S., Organic Chemistry, *National Chiao Tung University*, Hsinchu, Taiwan
1994 B.S., Chemistry, *National Taiwan University*, Taipei, Taiwan

Experience

2012-Present Assistant Professor, Department of Chemistry & Chemical Biology, University of New Mexico
Developing methods for spatiotemporal controls of miRNA and translation activity in neurons; Developing methods for cellular protein modification by small molecules.

2005-2011 Post-doctoral fellow (Gerald Crabtree lab), Department of Pathology, Stanford Medical School
Engineered small molecule-inducible system to control cellular processes; Epigenetic studies of BAF45 PHD domains in BAF chromatin remodeling complex.

2001-2005 Ph.D. research (Chi-Huey Wong lab), Department of Chemistry, The Scripps Research Institute
Tobramycin and HIV-PR library synthesis; RNA targeting and specificity studies and assay development.

2000-2001 Ph.D. research (Peter Schultz lab), Department of Chemistry, The Scripps Research Institute
Purine library synthesis; Small molecule screening for directing mesenchymal stem cell differentiation.

1999-2000 Research assistant (Henry Sun lab), Institute of Molecular Biology, Academia Sinica
Dissecting the regulatory element of the eyg gene in Drosophila.

1994-1996 M.S. research (Tse-Lok Ho lab), Department of Chemistry, National Chiao Tung University
Total synthesis of (-)-herbasolide.

1993-1994 Undergraduate research (Shiuh-Tzung Liu lab), Department of Chemistry, National Taiwan University
Synthetic studies of spirocyclic natural products.

Positions and Services

2012-present Assistant Professor of Chemistry and Chemical Biology, University of New Mexico
2012-present Member, New Mexico Cancer Nanotechnology Training Center
2012-present Member, University of New Mexico Nanoscience and Microsystems Program
2012-present Editorial Board Member, Organic Chemistry: Current Research Journal
2012-present Editorial Board Member, International Journal of Bioorganic Chemistry & Molecular Biology
2012-present Grant Reviewer, Medical Research Council (MRC), UK

Awards and Funding

2012-2013 American Cancer Society Institutional Research Grant (IRG-92-024)
2001-2005 Skaggs Predoctoral Fellowship
1994-1995 Chung Hwa Rotary Educational Foundation Scholar

Patents

<u>Liang, F. -S.</u> & Crabtree, G. R. "Alkenyl Substituted Cycloaliphatic Compounds as Chemical Inducers of Proximity." *International patent WO 2011/163029.*

<u>Liang, F. -S.</u> "Modular miRNA Regulators and Methods." *US Provisional Patent 61/712,598* filed October **2012**.

Publications

1. **<u>Liang, F. -S.</u>** & Crabtree, G. R. "Small Molecule Induced Proximity" *Chembiomolecular Science: at the Frontier of Chemistry and Biology*, **2012**, 115.
2. **<u>Liang, F. -S.</u>**, Ho, W. Q. & Crabtree, G. R. "Engineering the ABA Plant Stress Pathway for Regulation of Induced Proximity" *Sci. Signal.* **2011**, *4*, rs2.
   Highlighted in: *Sci. Signal.* **2011**, *4*, pe13. and *Nat. Struct. Mol. Biol.* **2011**, *18*, 403.
3. **<u>Liang, F. -S.</u>** & Crabtree, G. R. "Developmental Biology: The Early Heart Remodelled" *Nature* **2009**, *459*, 654.
4. **<u>Liang, F. -S.</u>**, Greenberg, W. A.; Hammond, J. A., Hoffmann, J, Head, S. R. & Wong, C. -H. "Evaluation of RNA Binding Specificity of Aminoglycosides with DNA Microarrays" *Proc. Natl. Acad. Sci. U.S.A.* **2006**, *103*, 12311.
5. **<u>Liang, F. -S.</u>**, Brik, A., Lin, Y.-C., Elder, J. H. & Wong, C. -H. "Epoxide Opening in Water for Rapid Inhibitor Discovery in Microtiter Plate and in situ Screening" *Bioorg. Med. Chem.* **2006**, *14*, 1058.
6. Fridman, M., Belakhov, V., Lee, L. V., **<u>Liang, F. -S.</u>**, Wong, C. -H. & Baasov, T. "Dual Effect of Synthetic Aminoglycosides: Antibacterial Activity Against *Bacillus anthracis* and Inhibition of Anthrax Lethal Factor" *Angew. Chem. Int. Ed.* **2005**, *44*, 447.
7. **<u>Liang, F. -S.</u>**, Wang, S.-K., Nakatani, T. & Wong, C. -H. "Targeting RNAs by Tobramycin Analogs" *Angew. Chem. Int. Ed.* **2004**, *43*, 6496.
8. Wu, C. -Y., Jan, J. -T., Ma, S. -H., Kuo, C. -J., Juan, H. -F., Cheng, Y. -S. E., Hsu, H. -H., Huang, H. -C., Wu, D., Brik, A., **<u>Liang, F. -S.</u>**, Liu, R. -S., Fang, J. -M., Chen, S. -T., Liang, P. H. & Wong, C. -H. "Small Molecules Targeting Severe Acute Respiratory Syndrome Human Coronavirus" *Proc. Natl. Acad. Sci. U.S.A.* **2004**, *101*, 10012.
9. Lee, L. V., Bower, K. E., **<u>Liang, F. -S.</u>**, Shi, J., Wu, D., Sucheck, S. J., Vogt, P. K. & Wong, C. -H. "Inhibition of the Proteolytic Activity of Anthrax Lethal Factor by Aminoglycosides" *J. Am. Soc. Chem.* **2004**, *126*, 4774.
10. Agnelli, F., Sucheck, S. J., Marby, K. A., Rabuka, D., Yao, S. -L., Sears, P. S., **<u>Liang, F. -S.</u>** & Wong, C. -H. "Dimeric Aminoglycosides as Antibiotics" *Angew. Chem. Int. Ed.* **2004**, *43*, 1562.
11. Wong, C. -H. & **<u>Liang, F. -S.</u>** "Surface Plasmon Resonance Study of RNA-Aminoglycoside Interactions" *Methods Enzymol* **2003**, *362*, 340.
12. Ho, T. -L. & **<u>Liang, F. -S.</u>** "Synthesis of ent-Herbasolide" *Chem. Commun.* **1996**, 1887.

Invited Presentations

2013.4	Department of Neurosciences, University of New Mexico
2012.11	Department of Biochemistry and Molecular Biology, University of New Mexico
2012.6	Center for Molecular Discovery, University of New Mexico
2012.5	Spatiotemporal Modeling Center, University of New Mexico
2012.1	IGERT Integrating Nanotechnology with Cell Biology and Neuroscience, University of New Mexico
2012.1	Department of Chemistry and Chemical Biology, University of New Mexico

Patrick S. Mariano
Department of Chemistry and Chemical Biology
University of New Mexico
Albuquerque, NM 87131-1096
Tel. No. 505-277-6390
<mariano@unm.edu>

EDUCATION

B.S., Fairleigh Dickinson University, 1964
Ph.D., University of Wisconsin, 1969; Professor H.E. Zimmerman
Postdoctoral, Yale University, 1968-1970; Professor H.H. Wasserman

POSITIONS HELD

1964; Instructor of Chemistry, Fairleigh Dickinson University
1966-1968; NIH Predoctoral Fellow, University of Wisconsin
1968-1970; NIH Postdoctoral Research Fellow, Yale University
1970-1976; Assistant Professor, Texas A&M University
1976-1979; Associate Professor, Texas A&M University
1978; Visiting Professor of Chemistry, Cornell University
1979-1997; Professor of Chemistry, University of Maryland
1997-present; Professor of Chemistry, University of New Mexico

PROFESSIONAL HONORS

Camille and Henry Dreyfus Foundation Teacher-Scholar Award, 1975-1980;
Phi-Lambda Upsilon Fresenius Award for Outstanding Contributions to Chemistry, 1978
University of Maryland Life Science's Award for Outstanding Research, 1990

RESEARCH INTERESTS

Organic Photochemistry
Bioorganic and Medicinal Chemistry
Mechanistic Enzymology
Synthetic Methodology Development
Natural Product Synthesis

CURRENT AND FORMER STUDENTS

Professor Mariano currently directs the research work of 2 doctoral, 4 undergraduate and 1 postdoctoral student. Seven students have received MS degrees, 76 PhD degrees, and 14 postdoctoral training under his direction since he began his academic career.

CURRENT RESEARCH GRANTS

• Enzymes: Structure, Mechanism, Function and Inhibition (Co-PI) NIH 09/01/08-08/31/1 $2,266,578

PUBLICATIONS

1968-1970

1. "The Stereochemistry of Protonation," H.E. Zimmerman and P.S. Mariano, *J. Am. Chem. Soc.*, **90**, 6091-6096 (1968).
2. "The Di-π-Methane Rearrangement. Interaction of Electronically Excited Vinyl Chromophores," H.E. Zimmerman and P.S. Mariano, *J. Am. Chem. Soc.*, **91**, 1718-1727 (1969).
3. "Photooxidation of Hexamethylbenzene and Related Aromatic Systems," H.H. Wasserman, P.S. Mariano, and P.M. Keehn, *J. Org. Chem.*, **36**, 1765-1767 (1970).

4. "On the Biosynthesis of Mycotoxins, Metabolites of Streptomyces Ruber," H.H. Wasserman, P.A. Zoretic, and P.S. Mariano, *J. Chem. Soc. Chem. Commun.*, 1634-1635 (1970).

1972

5. "The Stereochemistry of Excited State Atom Reorganization Processes. Di-π-Methane Rearrangement," P.S. Mariano and J.K. Ko, *J. Am. Chem., Soc.*, **94**, 1766-1767 (1972).
6. "Lanthanide Induced Shift Differences of Diastereotopic Protons," P.S. Mariano and R. McElroy, *Tetrahedron Lett.*, 5305-5308 (1972).
7. "Stereochemical Aspects of the Di-π-Methane Rearrangement," P.S. Mariano, R.B. Steitle, and J.K. Ko, Manuscript of papers, IV IUPAC Symposium on Photochemistry, 156-159 (1972).

1973

8. "Highlights of the Fourth IUPAC Symposium on Organic Photochemistry," P. Lichten, N.J. Turro, P.S. Mariano, and R.S. Givens, *Molecular Photochem.*, **5**, 235-249 (1973).
9. "Di-π-Methane Stereochemistry. The Effect of Structural Limitations Which Preclude Preferred Modes," P.S. Mariano and R.B. Steitle, *J. Am. Chem. Soc.*, **95**, 6114-6115 (1973).
10. "The Di-π-Methane and Oxa-Di-π-Methane Rearrangements," S. S. Hixson, P.S. Mariano, and H.E. Zimmerman, *Chem. Rev.*, **73**, 532-557 (1973).
11. "The Di-π-Methane Rearrangement. Stereochemistry," P.S. Mariano and J.K. Ko, *J. Am. Chem. Soc.*, **95**, 8670-8678 (1973).

1974

12. "Photofragmentation and Photoaffinity Labeling of Phenacyl and Naphthacyl-σ-Chymotrypsins," P.S. Mariano, G.I. Glover, T. Wilkinson, R.A. Hildreth, and T. Lowe, *Arch. Biochem. Biophys.*, **162**, 73-82 (1974).
13. "The Photochemistry of 4-Methylverbene," P.S. Mariano and D. Watson, *J. Org. Chem.*, **39**, 2774-2778 (1974).
14. "Preparation of 3-Alkylidene-2-3-dihydrofurans," P.S. Mariano and M. Peters, *Tetrahedron Lett.*, 2670-2674 (1974).

1975

15. "The Photochemistry of Di-π-Silanes," P.S. Mariano, E. Krochmal, and D.H. O'Brien, *J. Org. Chem.*, **40**, 1137-1142 (1975).
16. "The Separation of Water-Soluble Diastereomertic Compounds on Sephadex," P.S. Mariano, G. Glover, and T.J. Wilkinson, *Separation Science*, **10**, 795-799 (1975).
17. "The Reaction of N-β-Styryl-1,2-dihydropyridine with Dimethyl Acetylene Dicarboxylate. Preparation of an N-Vinyldihydroazocine," P.S. Mariano, M. Osborn, and E. Krochmal, *Tetrahedron Lett.*, 2741-2744 (1975).
18. "The Di-π-Methane Rearrangement. Interesting Observations from the Photochemistry of 1,3-Dimethyl-3-β-Styrylcyclohexene," P.S. Mariano and D. Watson, *Tetrahedron Lett.*, 3439-3552 (1975).

1976

19. "Di-π-Methane Photochemistry. The Effect of Structural Features Which Preclude Rearrangement by Preferred Modes," P.S. Mariano, R.B. Steitle, D.H. Watson, M. Peters, and E. Bay, *J. Am. Chem. Soc.*, **98**, 5899-5906 (1976).
20. "The Separation of Diastereomeric Organic Acids on Sephades G-10. Generality of the Method," P.S. Mariano, G. Glover, and S. Cheowtirakul, *Separation Science*, **11**, 147-157 (1976).
21. "The Photochemistry of Modified Proteins. Interesting Photochemistry of Poly-p-Benzoylphenylacetimido-Bovine Serum Albumin," P.S. Mariano, G.I. Glover, and T. J. Wilkinson, *Photochemistry and Photobiology*, **23**, 147-154 (1976).
22. "The Mechanism of Energy Transfer from Poly-p-Benzoylphenylacetimido Bovine Serum Albumin to Small Molecule Triplet Energy Acceptors," P.S. Mariano, G.I. Glover, and T.J. Wilkinson, *Photochemistry and Photobiology*, **23**, 155-162 (1976).

23. "Affinity Chromatography Separations of Chemically Modified σ-Chymotrypsin," T. J. Wilkinson, P.S. Mariano, and G.I. Glover, *Separation Science*, **11**, 383-387 (1976).
24. "A Reinvestigation of Phenacyl Bromide Modification of σ-Chymotrypsin, P.S. Mariano, G.I. Glover, and J.R. Peterson, *Biochemistry*, **15**, 3754-3759 (1976).

1977

25. "The Di-π-Methane Rearrangement. The Effect of 1,4-Diene Structure and Conformation on the Reaction Efficiency and Stereochemistry," P.S. Mariano, D.G. Watson, and E. Bay, *Tetrahedron*, **33**, 11-17 (1977).
26. "Stilbene-Like Photocyclizations of 1-Phenylvinyl-2-pyridones. Preparation of 4-H-Benzo[a]-quinolizin-4-ones," P.S. Mariano, E. Krochmal, and A. Leone, *J. Org. Chem.*, **42**, 1122-1125 (1977).
27. "Azocine Chemistry. Intermediates for the Synthesis of Pyrrolizidines," P.S. Mariano, B.C. Gunn, D. Dunaway-Mariano, and M.E. Osborn, *J. Org. Chem.*, **42**, 2903-2910 (1977).
28. "Novel Photocyclization Reactions of 1-Vinyl-2-pyridones Leading to Oxazolo-[3,2a]pyridinium Salts," P.S. Mariano, A. Leone, and E. Krochmal, *Tetrahedron Lett.*, 2227-2230 (1977).
29. "7,8-Dicarbomethoxy-9-oxa-2-azabicyclo[4.2.1.]non-7-ene-2-toluene-sulfonamide," P.S. Mariano, R.C. Petersen, M.E. Osborn, and D. Dunaway-Mariano, *Crystal Structure Communications*, **6**, 471-476 (1977).
30. "The Photochemistry of N-Allyliminium Salts. A Novel Photocyclization Reaction Leading to Pyrrolidines," P.S. Mariano, J.L. Stavinoha, and R. Swanson, *J. Am. Chem. Soc.*, **99**, 6781-6782 (1977).
31. "Novel Approaches to the Synthesis of Hydroisoquinolines Using Aza-Claisen Arrangements of N-Vinylisoquinuclidenes," P.S. Mariano, D. Dunaway-Mariano, P.L. Huesmann, and R.L. Beamer, *Tetrahedron Lett.*, 4299-4302 (1977).
32. "Energy Transfer from p-Benzoylbenzyl-Bovine Serum Albumin to Small Molecule Quenchers. Maximization of the Affinity-Controlled Mechanism and the Triplet Sensitized Photochemistry of Sodium-8-Methylene-4,9-decadienoate. An Ideal Water Soluble Triplet Energy Quencher," P.S. Mariano, G.I. Glover, and R.A. Hildreth, *Photochem. Photobiol.*, **26**, 3412-3431 (1977).

1978

33. "Phenacyl α-Chymotrypsin. Evidence for a pH Dependent Irreversible Formation of a Stable Conformation," P.S. Mariano, G.I. Glover, and J.R. Petersen, *Biochem., J.*, **171**, 115-122 (1978).
34. "General Synthetic Methods for the Preparation of 1-Substituted 1-Vinyl-2-pyridones," P.S. Mariano, E. Krochmal, R.L. Beamer, P.L. Huesmann, and D. Dunaway-Mariano, *Tetrahedron*, **34**, 2609-2616 (1978).
35. "The Diels-Alder Chemistry of 1-Vinyl-2-pyridones," P.S. Mariano, P.L. Huesmann, R.L. Beamer, and D. Dunaway-Mariano, *Tetrahedron*, **24**, 2617-2626 (1978).
36. "Kinetic Analysis and Solvent Polarity Effects on the Ylid Forming Photocyclization Reaction of 1-Vinyl-2-pyridones," P.S. Mariano and A. Leone, *J. Am. Chem. Soc.*, **100**, 3947-3949 (1978).

1979

37. "Novel Photochemical Reactions of Iminium Salts. Electron-Transfer Initiated Addition Reactions of Olefins to 2-Phenyl-1-pyrrolinium Perchlorate," P.S. Mariano and J.L. Stavinoha, *J. Am. Chem. Soc.*, **100**, 7114-7116 (1978).
38. "The Excited State Chemistry of 1-Alkenyl-2-pyridones," P.S. Mariano and A.A. Leone, *J. Am. Chem. Soc.*, **101**, 3607-3617 (1979).
39. 'The Amino-Claisen Rearrangement of N-Vinylisoquinuclidenes in Novel Approaches to the Synthesis of Hydroisoquinolines," P.S. Mariano, D. Dunaway-Mariano, and P. Huesmann, *J. Org. Chem.*, **43**, 124-133 (1979).
40. "The Photochemistry of Iminium Salts. Mechanisms and Synthetic Applications," P.S. Mariano, J. Stavinoha, and T. Tiner-Harding, Papers of the Joint ACS-IPS-JCS Photochemistry Symposium Honolulu, Hawaii, April, 1979, Pet. Chem. Div., 79-93 (1979).

1980

41. "Novel Photocyclization Reactions of 1-Alkenyl-2-pyridones," P.S. Mariano, T.L. Rose, A. Leone, and L. Fisher, Chemical Methods for Solar Energy Storage, ed. R. Kutal, R. Hautala, and R.B. King, Humana Press, N.J., 1979.

42. "Substituent Control of Cyclopropylcarbinyl Diradical Ring Opening Reactions," P.S. Mariano and E. Bay, *J. Org. Chem.*, **45**, 1763-1769 (1980).
43. "Mechanistic Aspects of Gas Phase Photodecarbonylation Reactions of Bicyclo[3.1.0]-hexan-3-ones," P.S. Mariano, E. Bay, D. Watson, T.L. Rose, and C. Bracken, *J. Org. Chem.*, **45**, 1753-1762 (1980).
44. "Photochemistry of Iminium Salts in the Presence of n-Electron Donating Alcohols and Ethers," J. Stavinoha, E. Bay, A. Leone, and P.S. Mariano, *Tetrahedron Lett.*, 3455-3458 (1980).
45. "Photocycloadditions of Electron Poor Olefins to 2-Aryl-1-pyrrolinium Salts," P.S. Mariano and A. Leone-Bay, *Tetrahedron Lett.*, 4581-4584 (1980).

1981

46. "3-Heteroatom Substituted 1,4-Diene Photochemistry," A. Leone and P.S. Mariano, Reviews of Chemical Intermediates, ed. O.P. Strausz and E.M. Lown, 4, 81-119 (1981).
47. "Photocyclizations of N-Allyliminium Salts Leading to the Production of Substituted Pyrrolidines," J.L. Stavinoha, P.S. Mariano, A. Leone-Bay, R. Swanson, and C. Bracken, *J. Am. Chem. Soc.*, **103**, 3148-3160 (1981).
48. "The Electron Transfer Photochemistry of Iminium Salts. Olefin Photoadditions to 2-Phenyl-pyrrolinium Perchlorate," J.L. Stavinoha and P.S. Mariano, *J. Am. Chem. Soc.*, **103**, 3136-3148 (1981).
49. "Photochemistry of Iminium Salts. Electron Transfer Mechanisms for Singlet Quenching and Photoaddition of n-Electron Donating Alcohols and Ethers," P.S. Mariano, J.L. Stavinoha, and E. Bay, *Tetrahedron*, **37**, 3385-3395, (1981).
50. "Selectivity in β-Enaminone Anion Generation and Alkylation," Y.P. Chen, P.S. Mariano, D. O'Brien, and P.L. Huesmann, G. Little, *J. Org. Chem.*, **46**, 4643-4654, (1981).
51. "Syn-9-Cyano(6,7)benzo-2-azaspiro(4,4)non-6-ene Hydrogen Perchlorate," G. Pepe, E.F. Meyer, J.L. Stavinoha, and P.S. Mariano, *Cryst. Struct. Commun.*, **10**, 951-956 (1981).

1982

52. "1,3,3,5-Pentamethyl-2-exo-methoxy-4-phenyl-7-azabicyclo[2.2.1]-heptane Hydrogen Perchlorate," R. Swanson, J. Stavinoha, and Patrick S. Mariano, *Cryst. Struct. Commun.*, **11**, 799-804 (1982).
53. "Intramolecular Photoarylations of N-Haloarylethyl-β-enaminones," T. Tiner-Harding, and P.S. Mariano, *J. Org. Chem.*, **47**, 482-485 (1982).
54. "The Hydroazocine Route to Highly Functionalized Pyrrolizidines," L.V. Yerino, M.E. Osborne, P.S. Mariano, *Tetrahedron*, **38**, 1579-1595 (1982).
55. "The Electron Transfer Initiated Photoaddition of Allylsilanes to 1-Methyl-2-phenylpyrrolinium Perchlorate, A Novel Allylation Methodology," K. Ohga, P.S. Mariano , *J. Am. Chem. Soc.*, **104**, 617-619 (1982).
56. "Electron Transfer Initiated Photocyclizations of N-Allylpyridinium and Quinolinium Salts. Preparations of Indolizidines," U.C. Yoon, S.L. Quillen P.S. Mariano, *Tetrahedron Lett.*, 919-922 (1982).
57. "Electron Transfer Initiated Iminium Salt Photospirocyclization Methodologies. Model Studies for Harringtonine Alkaloid Synthesis," T. Tiner-Harding, J.W. Ullrich, F. T. Chiu, S.F.Chen, P.S. Mariano, *J. Org. Chem.*, **47**, 3360-3362 (1982).
58. "Exploratory and Mechanistic Aspects of the Electron Transfer Photochemistry of Olefin-N-Heteroaromatic Cation Systems," U.C. Yoon, S.L. Quillen, P.S. Mariano, R. Swanson, J.L. Stavinoha, and E. Bay, *J. Am. Chem. Soc.*, **104**, 1204-1218 (1982).

1983

59. "Electron Transfer Mechanisms in Photochemical Transformations of Iminium Salts," P.S. Mariano, *Acc. Chem. Res.*, **16**, 130-137 (1983).
60. "The Photochemistry of Iminium Salts and Related Heteroaromatic Systems," P.S. Mariano, *Tetrahedron Reports*, **39**, 3845-3879 (1983).
61. "Mechanistic and Synthetic Aspects of the Acid-Catalyzed Amino-Claisen Rearrangement of N-(β-Ketovinyl)isoquinuclidenes," Y. P. Chen, P.L. Huesmann, and P.S. Mariano, *Tetrahedron Lett.*, 1021-1024 (1983).

62. "Sequential Electron Transfer-Desilylation Pathways for C-Vinyl-Azomethine Ylid Formation in the Photochemistry of N-(1-Triethylsilyl)-allyl)iminium Salts," S.F.Chen, J.W. Ullrich, and P.S. Mariano, *J. Am. Chem. Soc.*, **105**, 6160-6162 (1983).
63. "A Novel Synthetic Approach to Reserpine Based Upon Amino-Claisen Rearrangement of Zwitterionic N-Vinylisoquinuclidenes," F.A. Kunng, J.M. Gu, S.Chao, Y. P. Chen, and P.S. Mariano, *J. Org. Chem.*, **48**, 4262-4266 (1983).
64. "Intramolecular Photoarylations of Haloarylethyl-$\alpha-$ and β-Enaminoketones. A Correction and Further Results," M.A. Brumfield, P.S. Mariano, and U.C. Yoon, *Tetrahedron Lett.*, 5567-5570 (1983).

1984

65. "Exploratory and Mechanistic Studies of the Electron Transfer Initiated Photoaddition Reactions of Allylsilane-Iminium Salt Systems," K. Ohga, U.C. Yoon, and P.S. Mariano, *J. Org., Chem.*, **49**, 213-219 (1984).
66. "Electron Transfer Initiated Photospirocyclization Reactions of β-Enaminone Derived N-Allyliminium Salts," J.W. Ullrich, F.T. Chiu, T. Tiner-Harding, and P.S. Mariano, *J. Org. Chem.*, **49**, 220-227 (1984).
67. "Model Studies Examining the Application of N-Allyliminium Salt Spirocyclization Methodologies in Synthetic Approaches to the Harringtonine Alkaloids," F.T. Chiu, J.W. Ullrich, and P.S. Mariano, *J. Org. Chem.*, **49**, 228-235 (1984).
68. "Synthetic Aspects of Electron Transfer Photochemistry," P.S. Mariano, Synthetic Organic Photochemistry, ed. W. Horspool, Plenum, 1984, 145-258.
69. "3,5-Dimethoxy-4-(2-propenyldimethylamino)-1-cyclopentene Iodide," R. Swanson, U.C. Yoon, and P.S. Mariano, *Acta Cryst.*, **C40**, 1967-1969 (1984).
70. "Electron Transfer Photochemistry of Allene-Iminium Salt Systems. Theoretical and Chemical Probes of Allene Cation Radical Structure," K. Somekawa, K. Haddaway, P.S. Mariano, and J.A. Tossell, *J. Am. Chem. Soc.*, **106**, 3060-3062 (1984).
71. "A Rauwolfia Alkaloid Synthetic Approach Employing a Zwitterionic Amino-Claisen Rearrangement," S. Chao, F.A. Kunng, J.M. Gu, H.L. Ammon, P.S. Mariano, *J. Org. Chem.*, **49**, 2708-2711 (1984).
72. "A Novel Method for Heteroatom-Substituted Free Radical Generation by Photochemical Electron Transfer Induced Desilylation of R-XCH_2-TMS Systems," M.A. Brumfield, S.L. Quillen, U.C. Yoon, P.S. Mariano, *J. Am. Chem. Soc.*, **106**, 6855-6856 (1984).
73. "A Novel Method for 2-Aza-1,3-diene Synthesis Through N-(1-Triethylsilylallyl)-amine Protodesilyation," S.F.Chen, P.S. Mariano, *Tetrahedron Letters*, 47-50 (1984).
74. "Arene Iminium Salt Photochemistry. Dramatic Effects of Sequential Electron Transfer-Desilylation Pathways on the Nature and Efficiency of Photoaddition and Photocyclization Processes," A. Lan, S.L. Quillen, R.O. Heuckeroth, P.S. Mariano, *J. Am. Chem. Soc.*, **106**, 6439-6440 (1984).

1985

75. "Diradical Cyclization Methodologies. Model Studies Probing the Applications of Photoinduced Electron Transfer Processes in Synthetic Routes to the Protoberberine and Spirobenzyl Isoquinoline Alkaloids," G.D. Ho, J.Y. Lan, P.S. Mariano, *Tetrahedron Lett.*, 5867-5870 (1985).
76. "Sequential Electron Transfer-Desilylation Methods for Diradical Photogeneration as Part of Synthetic Routes for Erythrina Alkaloid Synthesis," R. Ahmed-Schofield, P.S. Mariano, *J. Org. Chem.*, **50**, 5667-5677 (1985).
77. "Mechanistic Aspects of the Boron Trifluoride Catalyzed Intermolecular Diels-Alder Cycloadditions of an Unactivated 2-Aza-1,3-diene with Electron Donating Substituted Dienophiles," Y.S. Cheng, E. Ho, P.S. Mariano, *J. Org. Chem.*, **50**, 5678-5686 (1985).

1986

78. "Allylstannane Photoadditions to Iminium Salts. Efficiencies of Sequential Electron Transfer Destannation Versus Desilylation Pathways," R.M. Borg, P.S. Mariano, *Tetrahedron Lett.* 2821-2824 (1986).

1987

79. "The Photochemistry of Substances Containing the C=N Moiety with Emphasis on Electron Transfer Processes," P.S. Mariano in Organic Photochemistry, ed. by A. Padwa, Vol. 9, **1987**, 1-128, Marcel Dekker, New York.
80. "Novel Photochemical Diradical Cyclization Methods For Protoberberine Alkaloid Synthesis. Preparation of (±)-Xylopinine and (±)-Stylopine," G.D. Ho, P.S. Mariano, *J. Org. Chem.*, **52**, 704-706 (1987).
81. "A Photochemical Route for Erythrinane Ring Construction," R. Ahmed-Schofield, P.S. Mariano, *J. Org. Chem.*, **52**, 1478-1482 (1987).
82. "Arene-Iminium Salt Electron Transfer Photochemistry. Mechanistically Interesting Photoaddition Processes," R.M. Borg, R.O. Heuckeroth, A.J.Y. Lan, S.L. Quillen, P.S. Mariano, *J. Am. Chem. Soc.*, **109**, 2728-2737 (1987).
83. "Electron Transfer Induced Photocyclization Reactions of Arene-Iminium Salt Systems. Effects of Cation Diradical Deprotonation and Desilylation on the Nature and Efficiencies of Reaction Pathways Followed," A.J.Y. Lan, R.O. Heuckeroth, P.S. Mariano, *J. Am. Chem. Soc.*, **109**, 2738-2745 (1987).
84. "Dual Diradical and Cation-Diradical Cyclization Mechanisms for Silylalkenyl-Iminium Salt, Electron Transfer Induced Photocyclization Reactions," C.L. Tu, P.S. Mariano, *J. Am. Chem. Soc.*, **109**, 5287-5288 (1987).
85. "Electron Transfer Photochemistry of α-Silylamine-Cyclohexenone Systems. Medium Effects on Reaction Pathways Followed," U.C. Yoon, J.U. Kim, E. Hasegawa, P.S. Mariano, *J. Am. Chem. Soc.*, **109**, 4421-4423 (1987).
86. "The Chemistry of Allene Cation Radicals Probed by Use of Theoretical and Electron Transfer Photochemical Methods," K. Haddaway, K. Somekawa, P. Fleming, J.A. Tossell, P.S. Mariano, *J. Org. Chem.*, **52**, 4239-4253 (1987).

1988

87. "Conjugate Addition of Methanol to α,β-Enones. Photochemistry and Stereochemical Details," Z. Benko, B. Fraser-Reid, P.S. Mariano, A.L.J. Beckwith, *J. Org. Chem.*, **53**, 2066-2072 (1987).
88. "Electron Transfer Photochemistry of Iminium Cations, P.S. Mariano in *Single Electron Transfer Photochemistry*, ed. by M.A. Fox and M. Chanon, Part C,**1988**, 372-420, Elsevier, New York.
89. "Investigation of the Bacillus Cereus Phosphonoacetaldehyde Hydrolase. Evidence for a Schiff Base Mechanism," D.B. Olsen, T.W. Hepburn, M. Moos, P.S. Mariano, D. Dunaway-Mariano, *Biochemistry*, **27**, 2229-2234 (1988).
90. "Photocyclization Reactions of 1-Benzyl-1-pyrrolinium Salts by Diradical and Diradical Cation Pathways. Novel Photochemical Pictet-Spengler Cyclizations," I.S. Cho, P.S. Mariano, *J. Org. Chem.*, **53**, 1590-1592 (1988).
91. "Photoadditions of Ethers, Thioethers and Amines to 9,10-Dicyanoanthracene by Electron Transfer Pathways," E. Hasegawa, M. Brumfield, U.C. Yoon, P.S. Mariano, *J. Org. Chem.*, **53**, 5435-5442 (1988).
92. "Electron Transfer Induced Photoadditons of the Silylamine, Et_2NCH_2TMS, to α,β-Unsaturated Cyclohexenones. Dual Reaction Pathways Based on Ion Pair Selective Cation Radical Chemistry," E. Hasegawa, W. Xu, P.S. Mariano, U.C. Yoon, S.U. Kim, *J. Am. Chem. Soc.*, **109**, 8089-8111 (1988).
93. "Exploratory, Mechanistic and Synthetic Aspects of Silylarene-Iminium Salt SET-Photochemistry. Studies of Diradical Cyclization Processes and Applications to Protoberberine Alkaloid Synthesis", G.D. Ho, P.S. Mariano, *J. Org. Chem.*, **53**, 5113-5127 (1988).
94. "Acid Catalyzed Intramolecular 2-Aza-1,3-diene Diels-Alder Cyclization Processes," E. Ho, Y.S. Cheng, P.S. Mariano, *Tetrahedron Lett.*, 4799-4802 (1988).
95. "A Protodesilylation Route for 2-Aza-1,3-diene Synthesis," S.F. Chen, E. Ho, P.S. Mariano, *Tetrahedron* , **44**, 7013-7026 (1988) .

1989

96. "Novel Electron Transfer Photocyclization Reactions of α-Silylamine α,β-Unsaturated Ketone and Ester Systems," W. Xu, Y.T. Jeon, E. Hasegawa, U.C. Yoon, P.S. Mariano, *J. Am. Chem. Soc.*, **111**, 406-408 (1989).
97. "Electron Transfer Induced Photochemical Reaction in Imide $RXCH_2TMS$ Systems,'' U.C. Yoon, H.J. Kim, P.S. Mariano, *Hetereocycles*, 1041-1064, **29** (1989) .
98. "Stereochemical Aspects of Photo-SET Induced Diradical Cyclization Reactions as Part of Isoquinoline Alkaloid Synthetic Strategies," I.S. Cho, C.P. Lee, P.S. Mariano, *Tetrahedron Lett.*, 799-802 (1989) .

99. "Model Studies Probing the Amino-Claisen Rearrangement Approach to Yohimbane Synthesis Focusing on Stereoconytrolled Methods for Introduction of Reserpine E-Ring Functionality," E. Baxter, D. Labaree, S. Chao, P. S. Mariano, *J. Org. Chem.* 2893-2904, **54** (1989) .
100. "A Remarkable Pericyclic Mechanism for Enzyme Catalyzed P-C Bond Formation," M. S. McQueney, S-L. Lee, E. Bowman, P. S. Mariano, D. Dunaway-Mariano, *J. Am. Chem. Soc.*, **111**, 6885-6887 (1989).
101. "Application of a SET-Induced Photospirocyclization Methodology to Harringtonine Ring Construction," R. W. Kavash, P. S. Mariano, *Tetrahedron Lett.*, 4185-4188 (1989).

1990

102. "Electron Transfer Induced Photochemical Reactions of Silyl-Iminium and Benzylpyrrolinium Salts by Dual Diradical Cation and Diradical Cyclization Pathways," I. S. Cho, C. L. Tu, P. S. Mariano, *J. Am. Chem. Soc.,* **112**, 3594-3607 (1990).
103. "A Formal Total Synthesis of Deserpidine Demonstrating a Versatile Amino Claisen Rearrangement Wenkert Cyclization Strategy for the Preparation of Functionalized Yohimbanes," E. W. Baxter, D. Labaree, H. L. Ammon, P. S. Mariano, *J. Am. Chem. Soc.*, **112**, 7682-7692 (1990).
104. "A Method for Elucidating the Phosphorus Stereochemistry in Hydrolytic C-P Bond Cleavage Reactions of Phosphonates," S. L. Lee, T. W. Hepburn, P. S. Mariano, D. Dunaway-Mariano, *J. Org. Chem.*, **55**, 5435-5437 (1990).

1991

105. "Mechanistic Details for SET-Promoted Photoadditions of Amines to Conjugated Enones Arising from Studies of Aniline-Cyclohexenone Photoreactions," X-M. Zhang, P. S. Mariano, *J. Org. Chem.,* **56,** 1655-1660 (1991).
106. "Photocyclization Reactions of Phthalimide α-Silyl-n-Electron Donor Systems via Singlet Single Electron Transfer and Triplet Hydrogen and Silyl Group Abstraction Pathways," U. C. Yoon, S. J. Cho, J. H. Oh, J. S. Lee, L. T. Kang, P. S. Mariano, *J. Korean Chem. Soc.*, **12**, 241-243 (1991).
107. "Substituent Effects on Amine Cation Radical Acidities. Regiocontrol of β-Aminoethyl-cyclohexenone Photocyclizations," W. Xu, P. S. Mariano, *J. Am. Chem. Soc.*, **113**, 1431-1432 (1991).
108. "Amine-Flavin Electron Transfer Photochemistry. Potential Models for Monoamine Oxidase Catalysis and Inhibition," J. M. Kim, I. S. Cho, P. S. Mariano, *J. Org. Chem.*, **56**, 4943-4955 (1991) .
109. "Evidence for an Intramolecular, Stepwise Reaction Pathway for PEP Phosphomutase Catalyzed P-C Bond Formation," M. S. McQueney, S-L. Lee, W. H. Swartz, H. L. Ammon, P. S. Mariano, D. Dunaway-Mariano, *J. Org. Chem.* , **56**, 7121-7130 (1991).
110. "SET Promoted Photocyclization Reactions of Aminoalkylcyclohexenones. Mechanistic and Synthetic Features of Processes Involving the Generation and Reactions of Amine Cation and α-Amino Radicals," W. Xu, X-M. Zhang, P. S. Mariano, *J. Am. Chem. Soc.,* **113**, 8863-8878 (1991).
111. "Radical Cyclization Reactions of α-Silylamine α,β-Unsaturated Ketone and Ester Systems Promoted by SET-Photosensitization," Y. T. Jeon, C-P. Lee, P. S. Mariano, *J. Am. Chem. Soc.*, **113**, 8847-8863 (1991).
112. "SET-Photochemistry of Flavin-Cyclopropylamine Systems. Models for Proposed Monoamine Oxidase Inhibition Mechanisms," J-M. Kim, M. A. Bogdan, P. S. Mariano, *J. Am. Chem. Soc.,* **113**, 9251-9257 (1991).
113. "Stereochemical Characteristics of SET-Promoted Photochemical Reactions of Dihydroisoquinolinium Salts," I-S. Cho, S. S. Chang, G.D. Ho, H. L. Ammon, P. S. Mariano, *Heterocycles,* **31**, 3910-3925 (1991).

1992

114. "Recent Advances in the Synthesis of Yohimbine Alkaloids," E. W. Baxter, P. S. Mariano, *Alkaloids. Chemical and Biological Perspectives*, ed. S. W. Pelletier, **Vol. 8**, Springer-Verlag, New York, (1992).
115. "Photoaddition Reactions of Acenaphthylenedione with α-Silyl-n-Electron Donors via Triplet SET-Desilylation and Triplet Hydrogen Atom Abstraction Pathways," U. C. Yoon, Y. C. Kim, J. J. Choi, D. U. Kim, P. S. Mariano, I. S. Cho, Y. T. Jeon, *J. Org. Chem.,* **57**, 1422-1428 (1992).
116. "Mechanistic and Synthetic Aspects of Amine-Enone SET-Photochemistry," U. C. Yoon, P. S. Mariano, *Acc. Chem. Res.*, **25**, 233-240 (1992).

117. "Investigation of the Substrate Binding and Catalytic Groups of the P-C Cleaving Enzyme, Phosphonoacetaldehyde Hydrolase," D. B. Olsen, T. W. Hepburn, S-L. Lee, B. M. Martin, P. S. Mariano, D. Dunaway-Mariano, *Arch. Biochem. Biophys.*, **296**, 144-151 (1992).
118. "A Stereochemical Probe for the Mechanism of P-C Bond Cleavage Catalyzed by the B. cereus Phosphonoacetaldehyde Hydrolase," S. L. Lee, T. W. Hepburn, W. S. Swartz, H. L. Ammon, P. S. Mariano, D. Dunaway-Mariano, *J. Am. Chem. Soc.*, **114**, 7346-7354 (1992).
119. "Exploratory Studies of α-Silylamino- and α-Silylamido-Cyclohexadienone SET Photochemistry in the Development of a Functionalized Hydroisoquinoline Synthetic Methodology," Y. S. Jung, W. H. Swartz, W. Xu, P. S. Mariano, N. J. Green, A. G. Schultz, *J. Org. Chem.,* **57**, 6037-6047 (1992).
120. "Photocyclization Reactions of N-(Trimethylsilylmethoxyalkyl)phthalimides. Efficient and Regioselective Routes to Heterocycles," Y. C. Yoon, J. U. Jim, P. S. Mariano, *Bull. Korean Chem. Soc.*, **13**, 166-172 (1992).

1993

121. "Methylbenzene Cation Radical α-Fragmentation Selectivities Revealed in SET-Photoadditions of *p*-Xylene Derivatives to 1,4-Dicyanonaphthalene," N. d'Alessandro. A. Albini, P. S. Mariano, *J. Org. Chem.*, **58**, 937-942 (1993).
122. "The Operation of H-Atom and TMS-Group Transfer Processes in the Photochemistry of Silylamidoalkyl- and Silylalkyl-Ketones and -Phthalimides," Y. J. Lee, C. P. Lee, Y. T. Jeon, P. S. Mariano, U. C. Yoon, *Tetrahedron Lett.*, **34**, 5855-5858 (1993).
123. "A Novel Azomethine Ylid Forming Photoreaction of N-Trimethylsilylmethyl-phthalimides," U. C. Yoon, D. U. Kim, J. C. Kim, J. G. Lee, P. S. Mariano, Y. J. Lee, H. L. Ammon, *Tetrahedron Lett.*, **34**, 5859-5862 (1993).
124. "A New Strategy for Yohimbane Synthesis Based On A Silylamido-Cyclohexadienone Photoinduced Radical Cyclization Process," Y. S. Jung, P. S. Mariano, *Tetrahedron Lett*, **34**, 4611-4614 (1993).
125. "Preparation of Enantioenriched Tetrahydropyridines by Iminium Ion-Vinylsilane Cyclizations," P. Castro, L. E. Overman, X. M. Zhang, P. S. Mariano, *Tetrahedron Lett.*, **34**, 5243-5246 (1993).
126. "Oxidative Methods for Promoting Iminium Cation Cyclization Reactions," X. M. Zhang, P. S. Mariano, M. A. Fox, P. S. Martin, J. Merkert, *Tetrahedron Lett.*, **34**, 5239-5242 (1993).
127. "3-Methyllumiflavin Promoted Oxidative Deamination of Amines. A Model for Catalysis by Monoamine Oxidases," J. M. Kim, M. A. Bogdan, P. S. Mariano, *J. Am. Chem. Soc.*, **115**, 10591-10595 (1993).
128. "Photochemical Models for Monoamine Oxidase Catalysis and Inhibition," P. S. Mariano, J. M. Kim, M. A. Bogdan, *Recent Advances in Photoscience;* M. Yoon and P. S. Song editors, Chungnam National University, 35-43 (1993).

1994

129. "A Novel Method for Synthesis of Functionalized Piperidines," S. K. Khim, P. S. Mariano, *Tetrahedron Lett.*, **35**, 999-1002 (1994).
130. "Photoinduced Electron Transfer Chemistry of Amine and Related Electron Donors," U. C. Yoon, P. S. Mariano, R. S. Givens, B. W. Atwater, *Advances in electron Transfer Chemistry,* P. S. Mariano editor, JAI Press, Volume 4, 117-206 (1994).
131. "The Dynamics of α-CH Deprotonation and Desilylation Reactions of Tertiary Amine Cation Radicals," X-M. Zhang, S-R. Yeh, S. Hong, M. Freccero, A. Albini, D. E. Falvey, P. S. Mariano, *J. Am. Chem. Soc.*, **116**, 4211-4220 (1994).
132. "SET Photochemical Reactions Between 1,4-Naphthalenedicarbonitrile and Benzylic Donors. Medium Effects," E. Fasani, N, d'Alessandro, A. Albini, P. S. Mariano, *J. Org. Chem.*, **59**, 829-836 (1994).
133. "Exploratory Studies of the Photocyclization Reactions of N-(Trimethylsilylmethylthioalkyl)phthalimides," U. C. Yoon, S. J. Lee, K. J. Lee, S. J. Cho, C. W. Lee, P. S. Mariano, *Bull. Korean Chem. Soc.*, **15**, 154-161 (1994).
134. "Indolizidine and Quinolizidine Ring Formation in The SET-Photochemistry of a-Silylamines," S. E. Hoegy, P. S. Mariano, *Tetrahedron Lett.*, **36**, 8319-8322 (1994).
135. "A Cephalotaxine Synthesis Founded on a Mechanistically Interesting, Quasi-Biomimetic Strategy," X-D. Lin, R. W. Kavash, P. S. Mariano, *J. Am. Chem. Soc.*, **116**, 9791-9792 (1994).

1995

136. "Flavin Chemical Models for Monoamine Oxidase Inactivation by Cyclopropylamines, α-Silylamines and Hydrazines," J-M. Kim, S. E. Hoegy, P. S. Mariano, *J. Am. Chem. Soc.*, **117**, 100-105 (1995).
137. "Location of the Catalytic Site for PEP Formation within the Primary Structure of *Clostridium Symbiosum* Pyruvate Phosphate Dikinase I. Identification of an Essential Cysteine by Chemical Modification with [1-14C]Bromopyruvate and Site Directed Mutagenisis," Y. X. Xu, L. Yankie, S. Li, Y. S. Jung, P. S. Mariano, D. Dunaway-Mariano. *Biochemistry,* **95**, 2181-2187 (1995).
138. "Novel and Efficient Azomethine Ylide Forming Photoreactions of N-Silylmethylphthalimides and Related Acid and Alcohol Derivatives," U. C. Yoon, D. U. Kim, C. W. Woo, Y. S. Choi, Y. L. Lee, H. L. Ammon, P. S. Mariano, *J. Am. Chem. Soc.*, **117**, 2698-2710 (1995).
139. "Investigations of Novel Azomethine Ylid Forming Photoreactions of Silylmethylimides," U.C. Yoon, S.J. Cho, Y.J. Lee, M.J. M. Real, P.S. Mariano, *J. Org. Chem.*, **60**, 2353-2360 (1995).

1996

140. "SET-Induced Inter- and Intra-Molecular Additions to Iminium Cations" P. S. Mariano, *A Handbook of Organic Photochemistry and Photobiology*, ed. W. M. Horspool and P. S. Song, CRC Press, Boca Raton, 867-878 (1995).
141. "Stereochemical Aspects of the Oxidative Mannich Cyclization of α-Silylamino and α-Silylamido Vinylsilanes and Allylsilanes," S. K. Khim, X-D. Wu, P. S. Mariano, *Tetrahedron Lett..*, **37**, 571-574 (1996).
142. "SET-Photosensitized Reactions of α-Silylamino-Enones and α-Silylamino-Ynones Proceeding by 6-Endo α-Amino Radical Cyclization Pathways," S. K. Khim, E. Cederstrom, D. C. Ferri, P. S. Mariano, *Tetrahedron*, **52**, 3195-3222 (1996).
143. "Exploratory Studies of H-Atom Abstraction and Silyl-Transfer Photoreactions of Silylakylketones and Silylakylphthalimides," Y. J. Lee, R. Ling, P. S. Mariano, U. C. Yoon, D. U. Kim, *J. Org. Chem.,* **61**, 3304-3314 (1996).
144. "Exploratory Investigations Probing a Preparatively Versatile, Pyridinium Salt Photoelectrocyclization - Solvolytic Aziridine Ring Opening Sequence," R. Ling, M. Yoshida, P. S. Mariano, *J. Org. Chem.,* **61**, 4439-4449 (1996).
145. "Strategies for Spirocyclic Amine Synthesis Based on N-Trimethylsilylmethallyl-Iminium Salt SET Photochemistry," R. W. Kavash, P. S. Mariano, *Photosciences,* **32**, 49-60 (1996).
146. "Two Interrelated Strategies for Cephalotaxine Synthesis," X. D. Lin, R. W. Kavash, P. S. Mariano, *J. Org. Chem.,* **61**, 7335-7347 (1996).

1997

147. "Synthetic Applications of Photochemistry," P.S. Mariano, U. C. Yoon, in *Plenary Lectures III Congreso De Fotoquimica*, Ed. D. Armesto, Universidad Nacional De Education A Distancia, Madrid, 1996, pp. 112-124.
148. "Single Electron Transfer Induced Photocyclization Reactions of N-[(N-Trimethylsilyl-methyl)aminoalkyl]phthalimides," U. C. Yoon, J. W. Kim, J. Y. Ryu, S. J. Cho, S. W. Oh, P. S. Mariano, *J. Photochem. Photobiol.,* **106**, 145-154 (1997).
149. "The Dynamics of α-Anilino Acid and Related Cation Radical α-Heterolytic Fragmentation Processes," Z. Su, D. E. Falvey, U. C. Yoon, P. S. Mariano, *J. Am. Chem. Soc.*, **119**, 5261-5262 (1997).
150. "Mechanistic and Synthetic Aspects of Amine Oxidations Promoted by 3-Methyl-5-ethyllumiflavinium Perchlorate," S. E, Hoegy, P. S. Mariano, *Tetrahedron,* **53**, 5027-5047, (1997).

1998

151. "An Oxidative Mannich Cyclization Methodology for the Stereocontrolled Synthesis of Highly Functionalized Piperidines," X.M. Zhang, S.K. Khim, X. D. Wu, E.M. Cederstrom, P.S. Mariano, *J. Org. Chem.*, **63**, 841-859 (1998).
152. "Oxidative Pictet-Spengler Cyclizations," H.J. Kim, U.C. Yoon, Y.S. Jung, N.S. Park, E.M. Cederstrom, *J. Org. Chem.*, **63**, 860-863 (1998).
153. "A New Strategy for the Design of Monoamine Oxidase Inactivators. Exploratory Studies with Tertiary Allylic and Propargylic Amino Alcohols," J-M. Kim, M. Bogdan, K. A. VanHouten, D. C. Ferri, P. S. Mariano, *J. Am. Chem. Soc.,* **120**, 5864-5872 (1998).

154. "A Demonstration of the Synthetic Potential of Pyridinium Salt Photochemistry by its Application to a Stereocontrolled Synthesis of (+)-Mannostatin A", R. Ling, P.S. Mariano, *J. Org. Chem,* **63**, 6072-6076 (1998).
155. "The Dynamics of Anilinium Radical α-Heterolytic Fragmentation Processes. Electrofugal Group, Substituent and Medium Effects on Desilylation, Decarboxylation and Retro-Aldol Cleavage Pathways", Z. Su, D.E. Falvey, U.C. Yoon, S.W. Oh, P.S. Mariano *J. Am. Chem. Soc.,* **120**, 10676-10686 (1998).

1999

156. "Mechanistic Studies of the Azomethine Ylid Forming Photoreactions of N-Silylmethylphthalimides and N-Phthaloyl-Glycine," Y. Takahashi, T. Miyashi, U.C. Yoon, S. W. Oh, M. Mancheno, Z. Su, D.F. Falvey, P.S. Mariano, *J. Am. Chem. Soc.,* **121**, 3926-3932 (1999).
157 "A Solvent Effect that Influences the Preparative Utility of N-Silylalkyl-Phthalimide and N-Silylalkyl-Maleimide Photochemistry," U.C. Yoon, S.W. Oh, S.M. Lee, S.J. Cho, J. Gamlin, P.S. Mariano, *J. Org. Chem.* **64**, 4411-4418 (1999).
158. "Exploratory Studies Probing the Intermediacy of Azomethine Ylids in the Photochemistry of N-Phthaloyl Derivatives of α-Amino Acids and β-Amino Alcohols," U. C. Yoon, C. W. Lee, S. W. Oh, P. S. Mariano, *Tetrahedron*, **55**, 11997-12008 (1999).

2000

159. "A Versatile Approach to the Synthesis of Mannostatin A Analogs," S. J. Cho, R. Ling, P.S. Mariano, *J. Org. Chem.* **65**, 1574-1577 (2000).
160. "An Oxidative Prins Cyclization Methodology," C. Chen, P.S. Mariano, *J. Org. Chem.*, **65**, 3252-3254 (2000).
161. "A Potentially General Method to Control Relative Stereochemistry in Enone-Olefin 2+2-Photocycloaddition Reactions by Using Eniminium Salt Surrogates," X. Cai, V. Chang, C. Chen, H-J. Kim, P.S. Mariano, *Tetrahedron Lett.*, **41**, 9445-9449 (2000).

2001

162. "Applications of Phthalimide Photochemistry to Macrocyclic Polyether and Polyamide Synthesis," U.C. Yoon, S.W. Oh, J.H. Lee, J.H. Park, K.T. Kang, P.S. Mariano, *J. Org. Chem.*, **66**, 939-943 (2001).
163. "The Synthetic Potential of Phthalimide Photochemistry," U.C. Yoon, P.S. Mariano, *Acc. Chem. Res.* **34**, 523-533 (2001).
164. "A Potentially General Strategy to Control the Absolute Stereochemistry of Enone-Olefin 2+2-Photocycloaddition Reactions," C. Chen, V. Chang, X. Cai, E. Duesler, P.S. Mariano, *J. Am. Chem. Soc.*, **123,** 6433-6434 (2001).
165. "Concise Synthesis of the (–)–Allosamizoline Aminocyclopentitol Based on Pyridinium Salt Photochemistry," H. Lu, P.S. Mariano, Y-F. Lam, *Tetrahedron Lett.*, **42**, 4755-4757 (2001).

2002

166. "Mannich Cyclizations Promoted by Ce(IV) Oxidations of α-Aminocarboxylates and α-Stannylamines," U.C. Yoon, K.T. Kim, S.W. Oh, D.W. Cho, P.S. Mariano, *Bull. Korean Chem. Soc.*, **22**, 1267-1269 (2001).
167. "A Novel Approach to the Synthesis of Amino-Sugars. Routes to Selectively Protected 3-Amino-3-deoxyaldooentoses Based on Pyridinium Salt Photochemistry," H. Lu, Z. Su, L. Song., P.S. Mariano, *J. Org. Chem.* **67**, 3525-3528 (2002).
168. "Comparison of Photomacrocyclization Reactions of Trimethylsilyl vs. Tributylstannyl-Terminated Phthalimido- and Maleimido-Polyethers," Yoon, U.C.; Jin, Y.X.; Oh, S.W.; Cho, D.W.; Park, K.H,; Mariano, P.S., *Journal Photochemistry Photobiology Chem. A,* **150**, 77-84 (2002).
169. "Photoaddition Reaction of Silylketene Acetals with Aromatic Carbonyl Compounds. A New Procedure for β-Hydroxy Ester Synthesis, " U.C. Yoon, M.J. Kim, J.J. Moon, S.W. Oh, H.J. Kim, P.S. Mariano, *Bull. Korean Chem. Soc.*, **23**, 1218-1228 (2002).

2003

170. "The Photochemistry of Silicon Substituted Phthalimides," U.C. Yoon, P.S. Mariano, *Handbook of Organic Photochemistry and Photobiology*, W. Horspool ed., CRC Press, 2003.
171. "The Dynamics and Photochemical Consequences of Aminium Radical Reactions," U.C. Yoon, Z. Su, P.S. Mariano, *Handbook of Organic Photochemistry and Photobiology*, W. Horspool ed., CRC Press, 2003.
172. "A New Look at Pyridinium Salt Photochemistry," P.S. Mariano, *Handbook of Organic Photochemistry and Photobiology*, W. Horspool ed., CRC Press, 2003.
173. "The Influence of Aminium Radical Heterolytic Fragmentation Rates on the Nature and efficiencies of SET-Promoted Photochemical Reactions," U.C. Yoon, P.S. Mariano, *J. Photosciences*, **10**, 89-96 (2003).
174. "A Synthetic Strategy for the Preparation of Cyclic Peptide Mimetics Based on SET-Promoted Photocyclization Processes," U.C.Yoon, Y.X. Jin, S.W. Oh, C.H. Park, J.H. Park, C.F. Campana, X. Cai, E.N. Duesler, P.S. Mariano, *J. Amer. Chem. Soc.*, **125**, 10664-10671 (2003).

2004

175. "The Photochemistry of Polydonor-Substituted Phthalimides. Curtin-Hammet Type Control of Competing Reactions of Potentially Interconverting Zwitterionic Biradical Intermediates," U.C. Yoon, H.C. Kwon, T.G. Hyung, K.H. Choi, S.W. Oh, S. Yang, Z. Zhao, P.S. Mariano, *J. Amer. Chem. Soc.*, **126**, 1110-1124 (2004).
176. "β-Lactam Forming Photochemical Reactions of N-Trimethylsilylmethyl- and N-Tributylstannylmethyl Substituted α-Ketoamides," R. Wang, C. Chen, E. Duesler, P.S. Mariano, U.C. Yoon, *J. Org. Chem.,* **69**, 1215-1220 (2004).
177. "Stereoselective Synthesis of Polyhydroxylated Indolizidines Based on Pyridinium Salt Photochemistry and Ring Rearrangement Metathesis," L. Song, E.N. Duesler, P.S. Mariano, *J. Org. Chem.*, **69**, 7284-7293 (2004).

2005

178. "Mechanistic and Synthetic Aspects of SET-Promoted Photocyclization Reactions of Silicon Substituted Phthalimides," U.C. Yoon, P.S. Mariano, in *Molecular and Supramolecular Photochemistry,* ed. K. Schanze, V. Ramamurthy, Marcel Dekker, Volume 15, 2005.
179. "A Novel Photochemical Approach to the Synthesis of Naphthalene Containing Lariat-Type Crown Ethers and an Evaluation of their Metal Cation Binding and Fluorescence Sensing Properties," R. Wang, Z. Zhao, U.C. Yoon, P.S. Mariano, *Photochem. Photobiol A.,* **175**, 232-241 (2005).
180. "Pyridinium Salt Photochemistry in a Concise Route for Synthesis of the Trehazolin Aminocyclitol," X. Feng, E.N. Duesler, P.S. Mariano, *J. Org, Chem.*, **70**, 5618-5623 (2005).
181. "A Concise Sequential Photochemical-Metathesis Approach for the Synthesis of (+)-Castanospermine and Possible Uniflorine-A Stereoisomers," Z. Zhao, L. Song, E.N. Duesler, P.S. Mariano, *Tetrahedron*, **61**, 8888-8894 (2005).
182. "Photocyclization Reactions of Cyclohexa- and Cyclopenta-Fused Pyridinium Salts. Factors Governing Regioselectivity," Z. Zhao, E. Duesler, C. Wang, H. Guo, P.S. Mariano, *J. Org. Chem.*, **70**, 8508-8512 (2005).
183. "Dipole Forming Photochemical Group Transfer Reactions of Phthalimides and α-Ketoamides," Yoon, U.C.; Mariano, P.S. *Journal of Photoscience*, **12**, 155-162 (2005).

2006

184. "Kinetic Analysis of Psuedomonas Aeruginosa Arginine Deiminase Mutants and Alternate Substrates Provides Insight Into Structural Determinants of Function," X. Lu, L. Li, X. Feng, Z. Li, H. Yang, C. Wang, H. Guo, A. Galkin, O. Herzberg, P.S. Mariano, B.M. Martin, D. Dunaway-Mariano, *J. Biol. Chem*, **45**, 1162-1172 (2006).
185. "Diversity of Function in the Isocitrate Lyase Enzyme Superfamily: The Dianthus Caryophyllus Petal Death Protein Cleaves a -Keto and a-Hydroxycarboxylic Acids," Z. Lu, X. Feng, L. Song, Y. Han, A. Kim, O. Herzberg, W.R. Woodson, B.M. Martin, P.S. Mariano, D. Dunaway-Mariano, *Biochem.*, 44, 16365-16376 (2006).
186. "L-Canavanine is a Time-Controlled Mechanism Based Inhibitor of Pseudomonas Aeruginosa Arginine Deiminase," X. Lu, L. Li, X. Feng, X. Wu, J. Engen, D. Dunaway-Mariano, P.S. Mariano *J. Am. Chem. Soc.*, **127**, 16412-16413 (2006).
187. "Photoinduced Electron Transfer Processes in 1,8-Naphthalimide-Linker-Phenothiazine Dyads," Cho, D.W.; Fujitsuka, A.; Sugimoto, A. Yoon, U.C.; Mariano, P.S.; Majima, T. *J. Phys. Chem. B*, **110**, 11062-11068 (2006).

188. "Application of the Photocyclization Reaction of 1,2-Cyclopenta-Fused Pyridinium Perchlorate to Formal Total Syntheses of (-)-Cephalotaxine.' Z. Zhao, P.S. Mariano, *Tetrahedron*, **62**, 7266-7273 (2006)
189. "The Synthetic Potential of SET Photochemistry of Silicon-Substituted Polydonor-Linked `Phthalimides," U.C. Yoon, P.S. Mariano, *Bull. Korean Chem. Soc.*, **27**, 1099-1114 (2006).

2007

190. "Oxaloacetate Hydrolase: The C-C Bond Lyase of Oxalate Secreting Fungi," Y. Han, H.J. Joosten, W. Niu, Z. Zhao, P.S. Mariano, M.T. McCalman, J.A.L. vanKan, P.J. Schaap, D.Dunaway-Mariano, *J. Biol. Chem.*, **282**, 9581-9590 (2007).
191. "Characterization, Kinetics and Crystal Structures of Fructose-1,6-bisphosphate Aldolase from the Human Parasite, *Giardia lamblia*." A. Galkin, L. Kulakova, E. Melamud, L. Ling Li, C. Wu, P.S. Mariano, D. Dunaway-Mariano, T. E. Nash, O. Herzberg, *J. Biol. Chem.*, **282**, 4859-4867 (2007).
192. "A Facile Approach to the Preparation of Bis-Crown Ethers Based on SET-Promoted Photomacrocyclization Reactions," N. K. Sung, D. W. Cho, J. H. Choi, K. W. Choi, U. C. Yoon, H. Maeda, P. S. Mariano, *J. Org. Chem.*, **72**, 8831 - 8837 (2007).

2008

193. "Inactivation of Microbial Arginine Deiminase by L-Canavanine," L. Li, Z. Li, D. Chen, X. Lu, A. Feng, E. Wright, N.O. Solberg, D. Dunaway-Mariano, P. S. Mariano, A. Galkin, L. Kulakova, O. Herzberg, K.B. Green-Church, L. Zhang, *J. Am. Chem. Soc.*, **130**, 1918-1931 (2008).
194. "Observations Made in Exploring a Pyridinium Salt Photochemical Approach to the Synthesis of (+)-Lactacystin," J. Zou, M. Gong, P.S. Mariano, U.C. Yoon, *Bull. Korean Chem. Soc.*, **29**, 89-93 (2008).
195. "SET-Promoted Photocyclization Reactions of Linked Acceptor-Polydonor Systems. The Effects of Chain length and Type on the Efficiencies of Macrocyclic Ring Forming Photoreactions of Tethered α-Silylether Phthalimide Substrates," D.W. Cho, J.H. Choi, S.W. Oh, C. Quan, U.C. Yoon, R. Wang, S. Yang, P.S. Mariano, *J. Am. Chem. Soc.*, **130**, 2276-2284 (2008).
196. "Structure and Function of PA4872 from Pseudomonas Aeruginosa, a Novel Oxaloacetate Decarboxylase from the PEP Mutase / Isocitrate Lyase Superfamily," B. Narayanan, W. Niu, Y. Han, J. Zou, P. S. Mariano, D. Dunaway-Mariano, O. Herzberg, *Biochem.*, **47**, 167-182 (2008).
197. "The Electrostatic Driving Force for Covalent Catalysis in Arginine Deiminase : A Combined Experimental and Theoretical Study," Ling Li, Zhimin Li, Canhui Wang, Dingguo Xu, Patrick S. Mariano, Hua Guo and Debra Dunaway-Mariano, *Biochem.*, **47**, 4721-4732 (2008).
198. "Electroluminescent Characteristics of Novel Platinum-Porphyrin Complexes," D. U. Kim, S. H. Paik, Y. H. Tak, S. D. Kim, Y. S. Han, T. J. Kim, T. H. Ko, U. C. Yoon, P. S. Mariano, *Colloids Surfaces A: Physio. Engin. Aspects*, **313**, 444-447 (2008).
199. "The Synthetic Potential of Pyridinium Salt Photochemistry," J. Zou, P. S. Mariano, *Photochem. Photobiol. Sci.*, **7**, 393-404 (2008).
200. "Crown Ether Based Heavy Metal Ion Fluorescence Sensors," H. Maeda, D. Tierney, P.S. Mariano, M. Banerjee, D.W. Cho, U.C. Yoon, *Tetrahedron.,* **64**, 5268-5278 (2008).
201. "Photoaddition Reactions of 1,2-Diketones with Silyl Ketene Acetals. Formation of β-Hydroxy-γ-ketoesters.," D.E Cho, H.Y. Lee, S.W. Oh, J.H. Choi, P.S. Mariano, U.C.Yoon, *J. Org. Chem.,* **73**, 4539-4547 (2008).
202. "Human Symbiont Bacteroides thetaiotamicron Synthesizes 2-Keto-3-deoxy-D-glycero-Dgalacto-nononic Acid (KDN) for Host Habitation," Liangbing Wang; Debra Dunaway-Mariano; Zhibing Lu; Karen N Allen; Patrick S Mariano, *Chemistry & Biology*, **15**, 893-897 (2008).

2009

203. "Mechanisms of Catalysis and Inhibition Operative in the Arginine Deiminase from the Human Pathogen Giardia lamblia," Li Z, Kulakova L, Li L, Galkin A, Zhao Z, Nash TE, Mariano PS, Herzberg O, Dunaway-Mariano D, *Bioorg. Chem.,* **37**, 149-161 (2009).

2010

204. "Divergence of Biochemical Function in the HAD Superfamily: D-G;yceroD-mannoheptose 1,7-bisphosphate Phosphatase (GhmB)," Wang, L.; Huang, H.; Nguyen, H.; Allen, K.N.; Mariano, P.S.; Dunaway-Mariano, D, *Biochemistry* (2010), **49**, 1072-1081.
205. "Studies Aimed at Elucidating Factors Involved in the Control of Chemoselectivity in Single Electron Transfer Promoted Photoreactions of Branched-Polydonor Substituted Phthalimides," Daewon Cho, Chunsheng Quan, Hea Jung Park, Jung Hei Choi, Su Rhan Kim, Tae Gyung Hyung, Ung Chan Yoon, Sung Hong Kim, Jin Ying Xue, Patrick S. Mariano, *Tetrahedron,* **66**, 3173-3186 (2010).
206. "Organic Synthesis Based on Ruthenium Carbene Catalyzed Metathesis Reactions and Pyridinium Salt Photochemistry." Daewon Cho, Patrick S. Mariano, *J. Kor. Chem. Soc.*, **54**, 261-268 (2010)
207. "A Concise, Metathesis Based Approach to Construction of the Lepadiformine/Cylindricine Tricyclic Framework." Jiwen Zou, Daewon Cho, Patrick S. Mariano, *Tetrahedron,* **66**, 5955-5961 (2010)
208. "The Nature and Kinetic Analysis of Carbon-Carbon Bond Fragmentation Reactions of Cation Radicals Derived from SET-Oxidation of Lignin Model Compounds," Dae Won Cho, Parthasarathi Ramakrishnan, Adam S. Pimentel, Gabriel D. Maestas, Hea Jung Park, Ung Chan Yoon, Debra Dunaway-Mariano, S. Gnanakaran, Paul Langan, Patrick S. Mariano, *J. Org. Chem.,* **75**, 6549–6562 (2010).
209. "Studies of Silyl-Transfer Photochemical Reactions of *N*-[(Trimethylsilyl)alkyl]saccharins", Dae Won Cho, Sun Wha Oh, Dong Uk Kim, Hea Jung Park, Jin Ying Xue, Ung Chan Yoon, Patrick S. Mariano, *Bull. Kor. Chem. Soc.* **31**, 2453-2458 (2010)

2011

210. "Rational Design and Evaluation of First Generation Inhibitors of the Giardia *lamblia* Fructose-1,6-biphosphate Aldolase," Zhimin Li, Zhengang Liu, Daewon Cho, Jiwen Zou, Maozhen Gong, Robert M. Breece, Andrey Galkin, Ling Li, Hong Zhao, Gabriel D. Maestas, David L. Tierney, Osnat Herzberg, Debra Dunaway-Mariano, Patrick S. Mariano, J. Inorg. *Biochem.*, **105**, 509-516 (2011)
211. "Photochemical Approach to the Preparation of Lariat Crown Ethers Containing Peptide Sidearms" Dae Won Cho, Ung Chan Yoon, Patrick S. Mariano, *Bull. Kor. Chem. Soc.*, **32**, 503-509 (2011).
212. "Studies Leading to the Development of a SET-Photochemical Strategy for Syntheses of Macrocyclic Poly-Ethers, -Thioethers, and –Amides" Dae Won Cho, Ung Chan Yoom, Patrick S. Mariano, *Acc. Chem. Res.*, **44**, 204-215 (2011).
213. "Regioselectivity of Enzymatic and Photochemical Single Electron Transfer Promoted Carbon-Carbon Bond Fragmentation Reactions of Tetrameric Lignin Model Compounds" Dae Won Cho, John A. Latham, Hea Jung Park, Ung Chan Yoon, Paul Langan, Debra Dunaway-Mariano, Patrick S. Mariano, *J. Org. Chem.*, **76,** 2840–2852 (2011).
214. "Exploration of Photochemical Reactions of *N*-Trimethylsilylmethyl-Substituted Uracil, Pyridone, and Pyrrolidone Derivatives", Dae Won Cho, Chan Woo Lee, Jong Gu Park, Sun Wha Oh, Nam Kyoung Sung, Hea Jung Park, Kyung Mok Kim, Patrick S. Mariano, Ung Chan Yoon, *J. Photochem. Photobiol.*, **10**, 1169-1180 (2011).

2012

215. "A Strategy for the Preparation of Cyclic Polyarenes Based on Single Electron Transfer Promoted Photocyclization Reactions", H. J. Park, J. H. Choi, B. N. Park, U. C. Yoon, D. W. Cho and P. S. Mariano, *Res. Chem. Intermed.*, 38, 847-862 (2012).
216. "Photoaddition Reactions of Acetylpyridines with Silyl Ketene Acetals", Hea Jung Park, Ung Chan Yoon, Hyang-Yeol Lee, Dae Won Cho, Dae Won Cho, Patrick S. Mariano, *J. Org. Chem., 77*, 10304-10313 (2012).
217. "Design, Synthesis and Evaluation of Inhibitors of Pyruvate Phosphate Dikinase", Chun Wu, Debra Dunaway-Mariano, Patrick S. Mariano, *J. Org. Chem.* (2012).

College of Arts and Sciences
Faculty Vitae

Name: Charles E. Melançon III
Department: Chemistry and Chemical Biology
Date: November 29, 2012

Educational History:

PhD, 2006, The University of Texas at Austin, Biochemistry
Dissertation title: Investigation and Engineering of Macrolide Antibiotic Sugar Biosynthesis and Glycosylation Pathways of Actinomycetes
Dissertation advisor: Dr. Hung-wen (Ben) Liu

BS, 2001, University of New Orleans, Biology
BA, 2001, University of New Orleans, Chemistry

Employment History

Assistant Professor (secondary appointment), December 2011-present, Department of Biology, The University of New Mexico, 167 Castetter Hall, MSC03 2020, 1 University of New Mexico Albuquerque, NM 87131-0001

Assistant Professor, August 2010-present, Department of Chemistry and Chemical Biology, The University of New Mexico, MSC03 2060, 1 University of New Mexico, Albuquerque, New Mexico 87131-0001

Scientific Consultant, May 2010-July 2010, Ambrx Inc., 10975 North Torrey Pines Road La Jolla, CA 92037

Postdoctoral Fellow, July 2007-July 2010, Dr. Peter G. Schultz Laboratory, Department of Chemistry and the Skaggs Institute for Chemical Biology, The Scripps Research Institute, 10550 North Torrey Pines Road, La Jolla, CA 92037

Postdoctoral Fellow, January 2007-June 2007, Dr. Hung-wen (Ben) Liu Laboratory, Medicinal Chemistry Division, College of Pharmacy, The University of Texas at Austin, 2409 University Ave. Stop A1900, Austin, TX, 78712-1113

Graduate Research Assistant, June 2003-December 2006, Dr. Hung-wen (Ben) Liu Laboratory, Medicinal Chemistry Division, College of Pharmacy, The University of Texas at Austin, 2409 University Ave. Stop A1900, Austin, TX, 78712-1113

Graduate Teaching Assistant, July 2001-May 2003, Department of Chemistry and Biochemistry, The University of Texas at Austin, 105 E. 24th St. Stop A5300, Austin, TX 78712-0165

Professional Recognition, Honors, etc.

Kirschstein Postdoctoral Fellowship, a postdoctoral fellowship that provides full financial support for three years, (2007-2010), National Institutes of Health

University of Texas Continuing Fellowship, awarded to one outstanding graduate student per division per year within the Department of Chemistry and Biochemistry, provides a full one year research assistantship, (2005-2006), The University of Texas at Austin

Ravel Fellowship, a cash award for outstanding achievement in graduate research, The University of Texas at Austin (2005)

Lewis Award, a cash award for outstanding achievement in graduate research, The University of Texas at Austin (2004)

College of Natural Sciences Dean's Excellence Award, a cash award given to outstanding graduate applicants, The University of Texas at Austin (2001)

Short Narrative Description of Research, Teaching and Service Interests.

The focus of our research program is on bioactive chemicals produced by living organisms (natural products) that function as mediators of important biological and ecological processes. These compounds are also important as a source of new therapeutic agents. We currently have three main efforts: 1) discovery of novel natural products from microbes with sequenced genomes by genome mining and phylogenetics, 2) discovery of new natural products, producing organisms, and natural product-mediated ecological processes in extreme environments such as caves and oceans, and 3) creation of new molecular tools for manipulating natural product biosynthetic pathways and for detecting natural products in living cells. The long-term objectives of my research are to develop and implement innovative technologies for identifying novel natural products with therapeutic potential and for manipulating natural product biosynthetic pathways to make compound analogs with improved bioactivity.

I have initially chosen a set of projects that are intended to be innovative and synergistic. We use a multidisciplinary approach, encompassing aspects of biological, organic, and analytical chemistry, molecular biology, genetics, microbiology, and bioinformatics. We are engaged in ongoing collaborations with research groups at the University of New Mexico, including the Departments of Biology and Computer Science, Pathology and Molecular Genetics and Microbiology.

Our program integrates conceptual and practical training at the Biology/Chemistry interface for both undergraduate and graduate students. I have mentored seven undergraduate students so far, four of whom are currently working with me; three others have graduated – two have entered PhD programs in Chemistry and Biochemistry at Colorado University at Boulder, while another is currently a first-year medical student at the University of New Mexico School of Medicine. I am also mentoring three second-year Chemistry graduate students. I strive to train my students to be technically proficient, to think independently, and to communicate effectively. I motivate my students to excel by providing them with support and encouragement, leading by example, and by developing a close-knit laboratory culture.

I am also committed to excellence in classroom teaching. I have spent time developing the curriculum for CHEM 425, The Organic Chemistry of Biological Pathways, a unique upper division undergraduate course designed to furnish students with a detailed understanding of the chemical bases of biological processes. Since taking this course over in 2009, I have strived to increase the enrollment and enhance its reputation among undergraduate Chemistry, Biology, and Biochemistry majors. The course has enjoyed an average enrollment of 45 students per semester, making it among the two most popular upper-division courses in the department. Overall, student evaluation have been very high (IDEA Summary Evaluation Score = 4.3 out of a possible 5.0 in Spring 2012). I look forward to continuing to teach 425, further developing CHEM 545, the graduate version of 425, and in the future, developing a new cross-listed undergraduate/graduate course in Synthetic Biology.

I also take pride in my service to my department and university. In my first year I served on the Graduate Recruiting and Admissions Committee. I was also involved in re-designing the departmental website to highlight graduate research and in overseeing design and production of a mail-out graduate recruiting poster. Our incoming graduate class size rose significantly (from 5 to 14) after these efforts. In the 2011-2012 academic year I co-organized the departmental colloquium and served on the Building Renovations Committee. I have hosted 7 departmental seminar speakers to date. I have also served on 3 dissertation defense committees and 9 PhD candidacy examination committees thus far. I particularly enjoy committee work aimed at making our graduate program stronger and more interdisciplinary.

Scholarly Achievements:

Articles in Refereed Journals († denotes equal contribution by authors)

Articles published: 12
Citations: 528
Citations since 2008: 454
h-index: 11
i-10 index: 13
Google Scholar profile: http://scholar.google.com/citations?user=6nm0WoMAAAAJ&hl=en

Journal Impact Factors:

Nature - 36.28
Angewandte Chemie International Edition - 13.46
Journal of the American Chemical Society - 9.91
Current Opinion in Pharmacology – 6.86
ACS Chemical Biology – 6.45
Applied and Environmental Microbiology – 3.83
Biochemistry – 3.42
Bioorganic and Medicinal Chemistry Letters – 2.54

12) Guo, J.†; Melançon, C. E., III†; Lee, H. S.; Groff, D.; Schultz, P. G. Evolution of Amber Suppressor tRNAs for Efficient Bacterial Production of Proteins Containing Nonnatural Amino Acids. *Ang. Chem. Int. Ed.* 48, 9148-9151, 2009.

11) Melançon, C. E., III; Schultz, P. G. One Plasmid Selection System for the Rapid Evolution of Aminoacyl-tRNA Synthetases. *Bioorg. Med. Chem. Lett.* 19, 3845-3847, 2009.

10) Thibodeaux, C. J.; Melançon, C. E., III; Liu, H.-w. Natural Product Sugar Biosynthesis and Enzymatic Glycodiversification. *Ang. Chem. Int. Ed.* 51, 9814-9859, 2008. (review article)

9) Hong, L.; Zhao, Z.; Melançon, C. E., III; Zhang, H.; Liu, H.-w. *In Vitro* Characterization of the Enzymes Involved in TDP-D-Forosamine Biosynthesis in the Spinosyn Pathway of *Saccharopolyspora spinosa*. *J. Am. Chem. Soc.* 130, 4954-4967, 2008.

8) Zhang, H.; White, J. A.; Melançon, C. E., III; Kwon, H.-j.; Yu, W.-l.; Liu, H.-w. Elucidation of the Kijanimicin Gene Cluster: Insights into the Biosynthesis of Spirotetronate Antibiotics and Nitrosugars. *J. Am. Chem. Soc.* 129, 14670-14683, 2007.

7) Thibodeaux, C. J.; Melançon, C. E., III; Liu, H.-w. Unusual Sugar Biosynthesis and Natural Product Glycodiversification. *Nature* 446, 1008-1016, 2007. (review article)

6) Melançon, C. E., III; Liu, H.-w. Engineered Biosynthesis of Macrolide Derivatives Bearing the Non-Natural Deoxysugars 4-*epi*-D-Mycaminose and 3-*N*-Monomethylamino-3-Deoxy-D-Fucose. *J. Am. Chem. Soc.* 129, 4896-4897, 2007.
5) Melançon, C. E., III; Hong, L.; White, J. A.; Liu, Y.-n.; Liu, H.-w. Characterization of TDP-4-Keto-6-deoxy-D-glucose-3,4-ketoisomerase from the D-Mycaminose Biosynthetic Pathway of

Streptomyces fradiae: In Vitro Activity and Substrate Specificity Studies. *Biochemistry* 46, 577-590, 2007.

4) Melançon, C. E., III; Thibodeaux, C. J.; Liu, H.-w. Glyco-Stripping and Glyco-Swapping. *ACS Chem. Biol.* 1, 499-504, 2006. (commentary)

3) Melançon, C. E., III; Yu, W.-l.; Liu, H.-w. TDP-Mycaminose Biosynthetic Pathway Revised and Conversion of Desosamine Pathway to Mycaminose Pathway with One Gene. *J. Am. Chem. Soc.* 127, 12240-12241, 2005.

2) Melançon, C. E., III; Takahashi, H.; Liu, H.-w. Characterization of *tylM3*/*tylM2* and *mydC*/*mycB* Pairs Required for Efficient Glycosyltransfer in Macrolide Antibiotic Biosynthesis. *J. Am. Chem. Soc.* 126, 16726-16727, 2004.

1) Borisova, S. A.; Zhao, L.; Melançon, C. E., III; Kao, C.-l.; Liu, H.-w. Characterization of the Glycosyltransferase Activity of DesVII: Analysis of and Implications for the Biosynthesis of Macrolide Antibiotics. *J. Am. Chem. Soc.* 126, 6534-6535, 2004.

Works in Progress:

In preparation:

3) Kooser, A. S.; Yackley, B.; Van Treeck, B.; Hunt, P.; Lane, T.; Melançon, C. E. III. Global Bioinformatic Identification of Natural Product Gene Clusters in Bacteria Reveals Phylogenetic Hotspots for Secondary Metabolism and Guides Natural Product Drug Discovery (intended for submission to *Applied and Environmental Microbiology*).

2) Melançon, C. E. III. Bioinformatics-Guided Natural Product Drug Discovery. *Biochemistry* (invited review article).

1) Tegos, G.; Melançon, C. E. III. Antimicrobial Natural Products. *Curr. Opin. Pharmacol.* (invited review article).

Invited or Refereed Abstracts and/or Presentations at Professional Meetings:

4) *Invited speaker*; Title: "Bioinformatics-Guided Natural Product Drug Discovery"; Gordon Conference on Enzymes, Coenzymes, and Metabolic Pathways; Waterville Valley, NH; July 15-20, 2012

3) *Invited speaker*; Title: "Bioinformatics-Guided Natural Product Drug Discovery"; Texas Enzyme Mechanisms Conference; Austin, TX; January 6-7, 2012

2) *Invited speaker*, Title: "Application of Next-Generation Sequencing Technology to Natural Product Drug Discovery"; Federation of Analytical Chemistry and Spectroscopy Societies (FACSS) Conference, Next Generation Bioanalytics Session; Reno, NV; October 4, 2011

1) *Invited speaker*, Title: “Investigation and Engineering of Macrolide Antibiotic Sugar Biosynthesis and Glycosylation Pathways of Actinomycetes”; Texas Enzyme Mechanisms Conference, Austin, TX, January 6-7, 2006

Contributed (un-refereed) Abstracts and/or Oral Presentations at Professional Meetings:

2) *Poster presenter*, Title: “Revision of the TDP-D-Mycaminose Biosynthetic Pathway and its Application to the Glycodiversification of Macrolide Antibiotics”; Charles E. Melançon III, Haruko Takahashi, Wei-luen Yu, and Hung-wen Liu; Gordon Conference on Enzymes, Coenzymes, and Metabolic Pathways, Biddeford, ME, July 17-22, 2005

1) *Poster presenter*, Title: “Investigations of Deoxysugar Biosynthesis, Glycosylation, and Genetic Glycodiversification of Macrolide Antibiotics”; Charles E. Melançon III, Haruko Takahashi, and Hung-wen Liu; UT Austin College of Pharmacy Celebrating Research Achievements Conference, Austin, TX, April 26, 2005

Invited Research Presentations

11) *Invited speaker*; Title: “Systems and Synthetic Biology Approaches to Discovering and Bioengineering Natural Products”; University of New Mexico Health Sciences Center Department of Biochemistry and Molecular Biology Seminar; October 29, 2012

10) *Invited speaker*; Title: “Systems and Synthetic Biology Approaches to Discovering and Bioengineering Natural Products”; University of New Mexico Department of Biology Seminar, October 4, 2012

9) *Invited speaker*; Title: “Systems and Synthetic Biology Approaches to Discovering and Bioengineering Natural Products”; University of New Mexico Health Sciences Center Department of Pharmaceutical Sciences Seminar, September 10, 2012

8) *Invited speaker*; Title: “From the Liu Lab to My Lab: Macrolide Metabolic Engineering to Bioinformatics-Guided Natural Product Drug Discovery”; Ben Liu 60th Birthday Celebration and Symposium, Austin, TX, July 14, 2012

7) *Invited speaker*; Title: “Bioinformatics-Guided Natural Product Discovery, Biosynthesis, and Bioengineering”; New Mexico State University Department of Chemistry and Biochemistry Seminar, March 8, 2012

6) *Invited speaker*; Title: “Bioinformatics-Guided Natural Product Discovery, Biosynthesis, and Bioengineering”; University of New Mexico Center for Biomedical Engineering Seminar, February 22, 2012

5) *Invited speaker*; Title: “Natural Product Drug Discovery and Chemical Ecology through Microbial Genome Mining”; New Mexico Institute of Mining and Technology Department of Chemistry Seminar, October 14, 2011

4) *Invited speaker*; Title: “Natural Product Drug Discovery and Chemical Ecology through Microbial Genome Mining”; University of New Mexico Department of Chemistry and Chemical Biology Symposium, August 19, 2011

3) *Invited speaker*; Title: "From the Environment to Genomes to Drugs: Discovery, Biosynthesis, and Bioengineering of Microbial Natural Products"; University of New Mexico INCBN IGERT Seminar, February 28, 2011

2) *Invited speaker*; Title: "From the Environment to Genomes to Drugs: Discovery, Biosynthesis, and Bioengineering of Microbial Natural Products"; University of New Mexico Department of Chemistry and Chemical Biology Seminar, February 11, 2011

1) *Invited speaker*; Title: "From Soil to Genomes to Drugs: Discovery, Biosynthesis, and Bioengineering of Microbial Natural Products"; Fort Lewis College Department of Chemistry Seminar, October 29, 2010

Conferences Attended

8) Gordon Conference on Enzymes, Coenzymes, and Metabolic Pathways; Waterville Valley, NH; July 15-20, 2012

7) Texas Enzyme Mechanisms Conference; Austin, TX; January 6-7, 2012

6) Federation of Analytical Chemistry and Spectroscopy Societies (FACSS) Conference, Reno, NV; October 4, 2011

5) Enzymes Mechanisms Conference, St. Petersburg, FL, January 2-6, 2011

4) Texas Enzyme Mechanisms Conference, Austin, TX, January 6-7, 2006

3) Gordon Conference on Enzymes, Coenzymes, and Pathways, Biddeford, ME, July 17-22, 2005

2) UT Austin College of Pharmacy Celebrating Research Achievements Conference, Austin, TX, April 26, 2005

1) Enzymes Mechanisms Conference, Galveston, TX, January 3-7, 2003

Research Funding:

Project Title: Bioinformatics-Guided Natural Product Drug Discovery
Principal investigator: Charles E. Melançon III
Funding organization: UNM Research Allocations Committee (RAC)
Starting and stopping dates: 12/9/2011-9/30/2012
Amount awarded for the period listed: $8,000 (direct costs)

Pending Research Funding:

Project Title: Bioinformatics and Genomics Approach to Toxin Biothreats
Principal investigator: Edward G Moczydlowski (Sandia National Laboratory)
Co-Investigators: Amy Jo Powell, Charles E. Melançon III
Funding organization: DHS Biological Threat Characteristic Program
Status of Review: white paper submitted Jan. 23, 2013
Amount awarded: $450,000 for 1 year, extendable up to 3 additional years

Unsuccessful Applications for Research Funding:

Project Title: Targeting multidrug efflux systems of *F. tularensis* and *B. pseudomallei*
Principal investigator(s): George Tegos and Larry A. Sklar, UNM HSC Dept. of Pathology
Investigators: Terry Wu (UNM HSC); Charles E. Melançon III (UNM C&CB); Richard Houghten, Clemencia Pinilla (Torrey Pines Institute); Herbert Schweizer (Colorado State); Eleftherios Mylonakis (Harvard).
Proposed funding organization: Defense Threat Reduction Agency (DTRA)
Proposed dates: 6/1/2012-5/31/2016
Proposed amount (direct costs and indirect costs): $8,214,000; my subcontract would have been for $523,179 (direct and indirect costs) over 3 years.
Status of review: the grant was funded, but my subcontract was cut from the project

Project Title: Genome Mining-Based Discovery of Natural Product Anticancer Drugs
Principal investigator: Charles E. Melançon III
Proposed funding organization: American Cancer Society Internal Research Grant (ACS IRG)
Proposed dates: 10/1/2010-9/30/2011
Proposed amount (direct costs and indirect costs): $30,000
Status of review: not funded

Teaching

Postdoctoral Mentoring:

Dr. Yasushi Ogasawara (Research Assistant Professor); February 2012-present; Projects: "Probing the Natural Product Biosynthetic Potential of the Genus *Frankia*" and "*De novo* Genome Sequencing, Transcriptomics, and Natural Product Discovery in the Rare Azicemicin Producing Actinobacterium *Kibdelosporangium sp.* MJ126-NF4." Educational history: BS Chemistry 2000, PhD Chemistry 2005, Tokyo Institute of Technology; postdoctoral fellow, University of Texas at Austin, 2006-2012.

Masters Advisement:

Ara S. Kooser (PiBBs Fellow 2011-2013); PhD Chemistry expected December 2015; Tentative Dissertation Title: "A Combined Bioinformatic, Geomicrobiological, and Chemical Approach to Discovering Novel Natural Products from Cave Bacteria." Educational history: BA Chemistry Knox College 1997, MS Geology University of New Mexico 2012.

Shijie Huang; PhD Chemistry expected May 2016; Tentative Dissertation Title: "Development of *In Vivo* Natural Product Biosensors using Synthetic Biology Approaches." Educational history: BS Microbiology 2008, MS Microbiology 2011, South China Agricultural University.

Jingxuan He; PhD Chemistry expected May 2016; Tentative Dissertation Title: "Development of New Chemical Genetics and Biotechnology Tools for *In Vivo* Manipulation of Natural Product Pathways in *Streptomyces*." Educational history: BS Biotechnology 2011, Beijing University of Chemical Technology.

Benjamin Yackley; PhD Computer Science expected May 2013; Project Title: "Development of Python-Based Genome Mining Software and its Application to Natural Product Studies." BS Neuroscience 2006, University of California Berkeley. Benjamin is a 0.25 FTE Project Assistant (PA).

Bachelor's Honors Advisement:

Paul Hunt; May 2011; BS Biochemistry; Thesis Title: "Genome Mining of Genus *Burkholderia* for Natural Products Potentially Involved in Human Pathogenicity." Paul is currently a 1st year medical student at UNM.

Briana Van Treeck; May 2012; BS Biochemistry; Thesis Title: "Development of an Unnatural Amino Acid Incorporation System for *Streptomyces venezuelae*." Briana is currently a 1st year Biochemistry graduate student at University of Colorado Boulder.

Undergraduate Student Mentoring:

Briana Van Treeck; August 2010-August 2012; BS Biochemistry; Project Title: see above. Skills learned: Bioinformatics, Molecular Biology.

Paul Hunt; August 2010-May 2012; BS Biochemistry; Project Title: see above. Skills learned: Bioinformatics, Comparative Genomics.

Jacob Greenberg (Whaley Fellowship recipient, Summer 2011; winner of outstanding undergraduate research poster, UNM C&CB, August 2011); September 2010-September 2011; BS Biology, BA Chemistry; Project Title: "Probing the Natural Product Biosynthetic Potential of the Genus *Frankia*." Skills learned: Microbiology, Natural Product Isolation, Molecular Biology, Bioinformatics. Jake is currently a 1st year Chemistry graduate student at University of Colorado Boulder.

Joseph Villanueva (MARC Scholar; 1st place winner in Microbiology, SACNAS Conference, October 2011); June 2011-present; BS Chemistry; Project Title: "Probing the Natural Product Biosynthetic Potential of Actinomycete *Actinosynnema mirum*." Skills learned: Microbiology, Natural Product Isolation, Molecular Biology, Bioinformatics.

Laetitia Meyrueix; January 2012-present; BS Biochemistry; Project Title: "Constructing a High Resolution Phylogenetic Map of Natural Product Biosynthetic Potential in Kingdom Fungi." Skills learned: Bioinformatics, Phylogenetics.

Shane Wilder; May 2012-present; BS Biochemistry; Project Title: "Correlating Type II Polyketide Synthase Gene Sequence and Cluster Composition with Product Structure: A Systems Level View." Skills learned: Bioinformatics, Comparative Genomics.

Kaitlin Leddy (C&CB Research Award Recipient, Summer 2012); May 2012-present; BS Biology, BA Chemistry; Project Title: "Isolating and Profiling Natural Product Producing Microbes from Lechuguilla Caverns and Exploring their Chemical Ecology." Skills learned: Microbiology, Molecular Biology.

Classroom Teaching:

Lecture Courses:

2013; Spring; The Organic Chemistry of Biological Pathways; CHEM 425; 43 students
2013; Spring; The Organic Chemistry of Biological Pathways; CHEM 545; 7 students
2012; Spring; The Organic Chemistry of Biological Pathways; CHEM 425; 51 students
2012; Spring; The Organic Chemistry of Biological Pathways; CHEM 545; 8 students*
2011; Fall; The Organic Chemistry of Biological Pathways; CHEM 425; 39 students
2011; Fall; The Organic Chemistry of Biological Pathways; CHEM 545; 1 student*
2011; Spring; The Organic Chemistry of Biological Pathways; CHEM 425; 44 students
2010; Fall; The Organic Chemistry of Biological Pathways; CHEM 425; 49 students#
2010; Fall; The Organic Chemistry of Biological Pathways; CHEM 545; 1 student*,#

* CHEM 425 and 545 were taught at the same time with additional requirements for 545 students
# Team taught with Dr. Patrick Mariano, I delivered 50% of the lectures

Seminar Courses:

2013; Spring; Biochemistry Seminar; CHEM 625-004; 14 students
2012; Spring; Biochemistry Seminar; CHEM 625-004; 12 students
2011; Spring; Biochemistry Seminar; CHEM 625-004; 7 students

Research Courses:

2013; Spring; Research Readings; CHEM 650; 2 students
2013; Spring; Undergraduate Problems; CHEM 496; 3 students
2012; Fall; Research Readings; CHEM 650; 3 students
2012; Fall; Undergraduate Problems; CHEM 495; 2 students
2012; Summer; Research Readings; CHEM 650; 2 students
2012; Summer; Undergraduate Problems; CHEM 495; 1 student
2012; Spring; Undergraduate Honors Research; BCHM 498; 1 student
2012; Spring; Undergraduate Problems; CHEM 496; 1 student
2011; Fall; Undergraduate Honors Research; BCHM 497; 1 student
2011; Fall; Undergraduate Problems; CHEM 495; 1 student
2011; Summer; Undergraduate Problems; CHEM 495; 1 student
2011; Spring; Undergraduate Honors Research; BCHM 498; 1 student
2011; Spring; Undergraduate Problems; CHEM 496; 2 students
2010; Fall; Undergraduate Honors Research; BCHM 497; 1 student
2010; Fall; Undergraduate Problems; CHEM 495; 2 students

Guest Lectures:

2012; Fall; Guide to Resources in Chemistry; CHEM 499; 12 students; gave 1 lecture
2012; Spring; Special Topics in Biochemistry; CHEM 567; 11 students; gave 2 of 13 lectures
2012; Fall; General Chemistry I; CHEM 121; ~250 students; gave 1 lecture
2011; Fall; General Chemistry I; CHEM 121; ~400 students; gave 1 lecture

Service:

Administrative work in Department, College, University committees

2012-2013 Member, C&CB Building Renovations Committee
2011-2012 Replacement Member, C&CB Graduate Committee; Duties: evaluate graduate applications, provide input on graduate curriculum
2011-2012 Member, C&CB Building Renovations Committee; Duty: provide input on building renovation plans
2011-2012 Co-organizer, C&CB Departmental Colloquium; Duty: coordinate scheduling of seminar speakers.
2010-2011 Member, C&CB Graduate Admissions and Recruitment Committee; Duties: evaluate graduate applications, oversee updating of departmental website, produce graduate recruiting flyer.
2010-2011 Member, C&CB Faculty Search Committee (Liang hire)

Dissertation defense committees:

John Latham; Dunaway-Mariano Group; July 6, 2012
Danqi Chen; Dunaway-Mariano Group; November 3, 2010
Hong Zhao; Dunaway-Mariano Group; October 25, 2010

PhD Candidacy Exam committees:

Xiaobei Chen; Wang Group; May 23, 2012
Fei Li; Qin Group; April 19, 2012
Lucas Zimney; Dunaway-Mariano Group; May 3, 2011
Sarah Toews; Dunaway-Mariano Group; May 3, 2011; update October 27, 2011
Tyrel Bryan; Dunaway-Mariano Group; April 28, 2011
John Latham; Dunaway-Mariano Group; April 28, 2011
Aiguo Song; Wang Group; April 21, 2011
Weimin Xuan; Wang Group; March 24, 2011
Yanting Cao; Wang Group; November 23, 2010

Seminar host for:

Vahe Bandarian; University of Arizona Chemistry and Biochemistry; August 31, 2012
Mike Heagy; New Mexico Tech Chemistry; March 8, 2012
Pieter Dorrestein; UC San Diego Pharmacy and Pharmaceutical Sciences; February 3, 2012
Larry Sklar, UNM HSC Pathology; November 18, 2011
Alex Kornienko; New Mexico Tech Chemistry; October 28, 2011
Hun-wen (Ben) Liu; UT Austin Pharmacy; April 29, 2011
Jeremy Edwards; UNM HSC Molecular Genetics and Microbiology; January 21, 2011

Name: Robert T. Paine
Birth: December 15, 1944, Colorado Springs, CO
Major Field: Inorganic Chemistry
Education: B.S. Chemistry, University of California, Berkeley, CA, 1966 with Honors
Ph.D. Chemistry, University of Michigan, Ann Arbor, MI, 1970.

Experience:

1970 - 1972	Postdoctoral Research Associate, Northwestern University
1972 - 1974	Postdoctoral Research Associate, Los Alamos Scientific Laboratory
1974 - 1978	Assistant Professor of Chemistry, University of New Mexico
1978 - 1983	Associate Professor of Chemistry, University of New Mexico
1976 - 1982	Assistant Chairman, Chemistry Department, University of New Mexico
1983 - 2005	Professor of Chemistry, University of New Mexico
2005-present	Distinguished Professor of Chemistry, University of New Mexico
1987 - 1988	Acting Chair, Chemistry Department

Awards

1966 - 1968	National Aeronautics and Space Administration, Graduate Fellow
1982	Fellow, American Association for Advancement of Science
1995	40^{th} University of New Mexico Research Lecturer
2005	UNM Distinguished Professor
2006	Boron in the Americas Award

Professional and Honorary Societies:

American Chemical Society; Materials Research Society, American Ceramics Society; Sigma Xi, Phi Lambda Upsilon

Professional Service:

Treasurer, Central New Mexico Section of the American Chemical Society (two years)
Member, American Chemical Society, Committee on Science, 1982-1987; Vice chairman 1983-84
Associate, American Chemical Society, Publications Committee, 1982-85
Inorganic Division, ACS, Nominating and Symposium Committee, 1984
Editorial Board, *Inorganic Chemistry*, 1987-1990
Editorial Board, *Organometallics*, 1990-1993
Petroleum Research Fund - American Chemical Society Advisory Board, 1988-1991
External Reviewer, Oak Ridge National Laboratory, Chemical Techn. Div., 1986-1987, 1992;
Chemistry Division 1988
AFOSR/NRC Chemical Sciences Review Panel (1990-93, 94-96)
CIES Chemistry Review Panel (1990-93)
Canvassing Committee ACS Award in Pure Chemistry, 1992-95
Canvassing Committee, ACS Award in Organometallic Chemistry, 2000-2002
Visiting Associate, ACS Committee on Professional Training, 1991-present
Councilor, Inorganic Division, ACS, 1993-95
Associate, Committee on Divisional Activities, ACS, 1994
Panel Member, Postdoctoral Fellowship Program, NSF, 1994
Visiting Staff Member and Collaborator, Los Alamos National Laboratory, 1974-2000
NRC/NAS Postdoctoral Review Panel, 1997-2002
DOE-EMSP Program Proposal Review Panel, 2000-2001

DOE-BES Program Review Committee, 2002
DOE-Chemical Sciences, E.O. Lawrence Award Committee, 2002

Lectureships:

1997 Bayer Lecturer, University of New Hampshire
1997 E.L. King Summer Lecturer, University of Colorado
1998 E. Wiberg Lecturer, Universität München

Research Publications and Activities:

A. Publications

1. R.T. Paine and R.W. Parry, "The Synthesis of Tetrafluorodiphosphine Bis[borane(3)]," *Inorg. Chem.*, *11*, 210 (1972).
2. R.T. Paine and R.W. Parry, "The Acid-Assisted Base-Displacement Reaction: The Preparation of Halodifluorophosphine and Carbonyl Triborane(7) Complexes," *Inorg. Chem.*, *11*, 268 (1972).
3. R.T. Paine and R.W. Parry, "The Synthesis, Characterization and Stability of Halodifluorophosphine Borane(3) and Tetra-borane(8) Complexes," *Inorg. Chem.*, *11*, 1237 (1972).
4. R.T. Paine, G. Sodeck and F.E. Stafford, "Molecular Beam Mass Spectra and Pyrolyses of Fluorophosphine Triborane(7) Complexes. Formation and Mass Spectrum of Triborane(7)," *Inorg. Chem.*, *11*, 2593 (1972).
5. R.T. Paine, "Partial Hydrolysis of Rhenium and Osmium Hexafluorides. An Improved Synthesis and Characterization of $ReOF_4$," *Inorg. Chem.*, *12*, 1457 (1973).
6. R.T. Paine, K.L. Treuil and F.E. Stafford, "Vibrational Spectra of $ReOF_4$," *Spectrochim. Acta*, *29*, 1891 (1973).
7. L.B. Asprey and R.T. Paine, "One Electron Reduction Synthesis of Uranium Pentafluoride," *Chem. Comm.*, 920 (1973).
8. R.T. Paine and L.B. Asprey, "Reductive Fluoride Elimination Synthesis of Transition Metal Fluorides. The Synthesis of Molybdenum Pentafluoride and Molybdenum Tetrafluoride," *Inorg. Chem.*, *13*, 1519 (1974).
9. R.T. Paine and R.S. McDowell, "Gas Phase Composition and Structure of Metal Oxide Tetrafluorides," *Inorg. Chem.*, *13*, 2366 (1974).
10. R.S. McDowell, L.B. Asprey and R.T. Paine, "Vibrational Structure Analysis of Uranium Hexafluoride," *J. Chem. Phys.*, *61*, 3571 (1974).
11. R.T. Paine, R.R. Ryan and L.B. Asprey, "Synthesis, Characterization and Molecular Structure of Uranium Oxide Tetrafluoride," *Inorg. Chem.*, *14*, 1113 (1975).
12. R.T. Paine and L.B. Asprey, "Reductive Fluoride Elimination Syntheses. The Synthesis and Characterization of Pentafluorides and Tetrafluorides of Rhenium, Osmium and Iridium," *Inorg. Chem.*, *14*, 1111 (1975).
13. R.T. Paine and R.W. Parry, "Preparation of Bis-(Halodifluorophosphine)-Diborane(4) Complexes," *Inorg. Chem.*, *14*, 689 (1975).
14. R.T. Paine, S.,B. Roeder and E. Fukushima, "NMR of Solid Triborohydride Salts," *Chem. Phys. Lett.*, *32*, 566 (1975).

15. R.T. Paine and L.A. Quarterman, "Solution Properties of Inorganic Pentafluorides and Oxide Tetrafluorides in Anhydrous Hydrogen Fluoride," *J. Inorg. Nucl. Chem.*, H.H. Hyman, Memorial Issue, p. 85, 1976.
16. R.T. Paine, R.S. McDowell, L.B. Asprey and L.H. Jones, "Vibrational Spectroscopy of Matrix Isolated UF_6 and UF_5," *J. Chem. Phys.*, *64*, 3081 (1976).
17. R.R. Ryan, R.A. Penneman, L.B. Asprey and R.T. Paine, "Single Crystal X-Ray Study of β-UF_5; The Eight Coordination of U(V)," *Acta Cryst.*, *32B*, 3111 (1976).
18. W.B. Lewis, L.B. Asprey, R.S. McDowell, L.H. Jones and R.T. Paine, "Electronic Spectroscopy of Matrix Isolated UF_6," *J. Chem. Phys.*, *65*, 2707 (1976).
19. E. Fukushima, R.T. Paine and S.B. Roeder, "Boron-11 NMR Study of the Large Angle Anisotropic Motion of $B_3H_8^-$ in $(CH_4)_4NH_3H_8$," *J. Chem. Phys.*, *67*, 1614 (1977).
20. R.T. Paine and L.B. Asprey, "Metal Pentafluorides," *Inorg. Syn.*, *19*, 137 (1978).
21. R.T. Paine, "Borane Coordination Chemistry of Bidentate Ligands, The Preparation and Characterization of $F_2PN(CH_3)PF_2B(H_2)B(H_2)$," *J. Am. Chem. Soc.*, *99*, 3884 (1977).
22. R.T. Paine, "The Synthesis and Characterization of Methyla-mino-bis-difluorophosphine Borane(3), Bis-Borane(3) and Triborane(7) Complexes," *Inorg. Chem.*, *16*, 2996 (1977).
23. R.W. Light and R.T. Paine, "The Interaction of the Dicoordinate Phosphorus Cation 1,3-Dimethyl-1,3,2-Diazaphospholidide with Transition Metal Nucleophiles," *Am. Chem. Soc.*, *100*, 2230 (1978).
24. R.W. Light, C.F. Campana, R.T. Paine and B. Morosin, "The Crystal Structure of 2-Fluoro-1,3-Dimethyl-1,2-Diazaphospholidine Sulfide," *Acta Cryst.*, *B34*, 3671 (1978).
25. R.T. Paine and R.W. Light, "The Synthesis and Coordination Chemistry of Cyclopentadienylfluorophosphine Ligands," *Inorg. Chem.*, *18*, 368 (1979).
26. L.H. Jones, R.C. Taylor and R.T. Paine, "Potential Constants of Borane Carbonyl," *J. Chem. Phys.*, *70*, 749 (1979).
27. R.T. Paine, R.W. Light and M. Nelson, "Vibrational Spectra of Uranium(IV) Borohydride and Uranium(IV) Borodeuteride," *Spectrochim. Acta*, *35A*, 213 (1979).
28. R.T. Paine, P.R. Schonberg, R.W. Light, W.C. Danen and S.M. Freund, "Photochemistry of $U(BH_4)_4$ and $U(BD_4)_4$," *J. Inorg. Nucl. Chem.*, *41*, 1577 (1979).
29. R.W. Light and R.T. Paine, "The Formation of Diphosphine Monocations and Dications from Methylamino-bis-di-fluorophosphine," *Inorg. Chem.*, *18*, 2345 (1979).
30. P.R. Schonberg, R.T. Paine and C.F. Campana, "The Synthesis, Characterization and Molecular Structure of an Aluminum Pentamethylcyclopentadienyl Complex, $[\eta^3\text{-}(CH_3)_5C_5Al(Cl)CH_3]_2$: An Organometallic Analog of Benzvalene," *J. Amer. Chem. Soc.*, *101*, 7726 (1979).
31. R.W. Light and R.T. Paine, "The Interaction of SO_2 with Aminophosphine Ligands," *Phosphorus and Sulfur*, *8*, 255 (1980).
32. R.T. Paine and M.S. Kite, "The Photochemistry of Uranium Compounds," in "Chemistry of the Actinides," *Amer. Chem. Soc., Symp. Ser.*, *131*, 369 (1980) N. Edlestein, Ed.
33. R.W. Light, L.D. Hutchins, R.T. Paine and C.F. Campana, "Reactions of Aminophosphines with CO_2, COS, and CS_2. The Crystal and Molecular Structure of Tris-dimethylamino-phosphine Tris CS_2," *Inorg. Chem.*, *19*, 3597 (1980).

34. L.D. Hutchins, R.W. Light, R.T. Paine and C.F. Campana, "Structure and Bonding of the Dicoordinate Phosphorus Cation 1,3-Dimethyl-1,3,2-diazaphospholide with η^5-$C_5H_5Mo(CO)_3^-$," *Am. Chem. Soc.*, *102*, 4521 (1980).
35. J.S. Jessup, R.T. Paine and C.F. Campana, "The Synthesis and Characterization of Borane(3) Complexes of 1,3-Di(tert-butyl)-2,4-difluorodiazadiphosphetidine. The Crystal and Molecular Structure of the Bis Borane(3) Complex," *Phosphorus and Sulfur*, *9*, 279 (1981).
36. S.M. Bowen, E.N. Duesler and R.T. Paine, "Synthesis and Crystal and Molecular Structure of a Diethyl N,N-Diethyl-carbamoylmethylenephosphonate Thorium Nitrate Complex," *Inorg. Chem.*, *21*, 261 (1982).
37. L.D. Hutchins, R.W. Light and R.T. Paine, "Synthesis, Structure and Bonding of the Bis-Phosphenium Ion-Dicobalt Carbonyl Complex $Co_2(CO)_5$ [μ-$PN(CH_3)CH_2CH_2N(CH_3)]_2$," *Inorg. Chem.*, *21*, 266 (1982).
38. S.M. Bowen, E.N. Duesler, R.T. Paine and C.F. Campana, "The Acidity and Coordination Properties of Carbamoylmethylene-phosphonate Ligands: Synthesis and Molecular Structure of Dialkylcarbamoylmethylenephosphonate Mercury(II) Nitrate Complexes," *Inorg. Chim. Acta*, *59*, 53 (1982).
39. P.R. Schonberg, R.T. Paine and C.F. Campana, "Synthesis and Crystal and Molecular Structures of Pentamethylcyclopenta-dienyl Aluminum Halide Complexes: [η^3-$(CH_3)_5C_5Al(Cl)CH_3]_2$ and η^3-$(CH_3)_5C_5Al(Cl)(i\text{-}C_4H_9)]_2$," *Organometallics*, *1*, 799 (1982).
40. S.M. Bowen, E.N. Duesler and R.T. Paine, "Synthesis and Crystal and Molecular Structure of Diisopropyl N,N-Diethyl-carbamoylmethylenephosphonate Samarium Nitrate and Erbium Nitrate Complexes," *Inorg. Chim. Acta*, *61*, 155 (1982).
41. R.T. Paine, D.C. Moody and E.N. Duesler, "Synthesis and Structure of a Supersandwich Pentanuclear Uranium(IV) Complex," *Organometallics*, *1*, 1097 (1982).
42. L.D. Hutchins, E.N. Duesler and R.T. Paine, "Structure and Bonding in a Phosphenium Ion-Iron Complex: (η^5-$(CH_3)_5C_5)Fe(CO)_2[PN(CH_3CH_2CH_2N(CH_3)]$," *Organometallics*, *1*, 1254 (1982).
43. S.M. Bowen, E.N. Duesler and R.T. Paine, "Synthesis and Crystal and Molecular Structure of Bis(nitrato)[di-isopropyl-N,N-diethylcarbamoylmethylenephosphonate]-dioxouranium(VI)," *Inorg. Chem.*, *22*, 286 (1983).
44. J.J. Jessup, E.N. Duesler and R.T. Paine, "Synthesis and Crystal and Molecular Structure of a Palladium Phosphonate Complex, Pd[(i-$C_3H_7O)_2P(O)CH_2C(O)N(C_2H_5)_2](NO_3)_2$," *Inorg. Chim. Acta*, *73*, 261 (1983).
45. D.A. DuBois, R.W. Light, E.N. Duesler and R.T. Paine, "Synthesis and Structure of a Bimetallic Diphosphenium Ion Complex Containing a Diazadiphosphetidine Ring," *Organometallics*, *2*, 1903 (1983).
46. R.T. Paine, L.D. Hutchins, D.A. DuBois and E.N. Duesler, "Developments in the Coordination Chemistry of Dicoordinate Phosphenium Ion Ligands," *Phosphorus and Sulfur*, *18*, 263 (1983).
47. S.M. Bowen, E.N. Duesler and R.T. Paine, "Synthesis and Crystal and Molecular Structure of a Methyl N,N,Diethylcarbamoylmethylenephosphonate Dysprosium Thiocyanate Complex," *Inorg. Chim. Acta*, *84*, 221 (1984).

48. D.C. Moody and R.T. Paine, "Low Valent Actinides as Hydrogenation Catalysts," *J. Cat*, *85*, 536 (1984).
49. L.D. Hutchins, E.N. Duesler and R.T. Paine, "Synthesis and Characterization of Metallophosphenium Ion Complexes Derived from Aminohalophosphites. Crystal and Molecular Structure of $Mo(\eta^5\text{-}C_5H_5)(CO_2)[POCH_2CH_2NC(CH_3)_3]$," *Organometallics*, *3*, 399 (1984).
50. D.A. DuBois, E.N. Duesler and R.T. Paine, "Synthesis and Structural Characterization of an Eight-Membered P_4N_4 Cage Compound Analog of S_4N_4 and P_4S_4," *J. Chem. Soc. Chem. Commun.*, 488 (1984).
51. H.J. Wasserman, D.C. Moody, R.T. Paine, R.R. Ryan and K.V. Salazar, "Tetrahydroborate Complexes of Uranium with 2-(Diphenylphosphine) Pyridine," *J. Chem. Soc. Chem. Commun.*, 533 (1984).
52. D.A. DuBois, E.N. Duesler and R.T. Paine, "Synthesis and Structure of a Bimetallic Iron Carbonyl Diazadiphosphetidine Complex," *Organometallics*, *3*, 1913 (1984).
53. D.A. DuBois, E.N. Duesler and R.T. Paine, "Formation and X-Ray Crystal Structure Determination of an Unusual Phosphorus-Phosphorus Coupled Bicyclodiphosph(III)azane Complex," *Inorg. Chem.*, *24*, 3 (1985).
54. S.M. Bowen, D.J. McCabe, E.N. Duesler and R.T. Paine, "Synthesis and Crystal and Molecular Structure of *cis* Dioxodichloro-(diisopropyl-N,N-diethylcarbamoyl-methylene-phosphonate)molybdenum(VI)," *Inorg. Chem.*, *24*, 1191 (1985).
55. J.M. Ritchey, A.J. Zozulin, D.A. Wrobleski, R.R. Ryan, H.J. Wasserman, D.C. Moody and R.T. Paine, "An Organothorium-Nickel Phosphido Complex with a Short Th-Ni Distance. The Structure of $Th(C_5Me_5)_2(\mu\text{-}PPh_2)_2Ni(CO)_2$," *J. Am. Chem. Soc.*, *107*, 501 (1985).
56. L.J. Caudle, E.N. Duesler and R.T. Paine, "Formation and Crystal and Molecular Structures of Dioxouranium(VI) Complexes Containing Bidentate Carbamoylmethyl-phosphinate and Phosphine Oxide Ligands," *Inorg. Chim. Acta*, *110*, 91 (1985).
57. L.J. Caudel, E.N. Duesler and R.T. Paine, "Preparation and Structure of a Neodymium Complex Containing Bidentate Carbamoylmethylphosphine Oxide Ligands," *Inorg. Chem.*, *24*, 4441 (1985).
58. D.J. McCabe, E.N. Duesler and R.T. Paine, "Monodentate Coordination by a Tripodal Ligand System: Synthesis and Crystal and Molecular Structure of a Bis-Diisopropyl [1,2-bis(diethylcarbamoyl)ethyl] Phosphonate Erbium Nitrate Complex," *Inorg. Chem.*, *24*, 4626 (1985).
59. D.A. Wrobleski, R.R. Ryan, H.J. Wasserman, K.V. Salazar, R.T. Paine and D.C. Moody, "Synthesis and Characterization of Bis (Diphenylphosphide) Bis (Pentamethylcyclopentadienyl) Thorium (IV)," *Organometallics*, *5*, 90 (1986).
60. W.F. McNamara, E.N. Duesler, R.T. Paine, P. Kölle and H. Nöth, "Synthesis and Structure of a Metallophosphenium-borane (3) Complex Containing a Bridging BH_3 Group," *Organometallics*, *5*, 380 (1986).
61. S.M. Bowen and R.T. Paine, "Diethyl {(N,N-Diethylcarbamoyl-methyl} phosphonates," *Inorg. Syn.*, *24*, 101 (1986).
62. D.J. McCabe, S.M. Bowen and R.T. Paine, "Synthesis of Dialkyl [1,2-bis(diethylcarbamoyl)ethyl] Phosphonates," *Synthesis*, 320 (1986).

63. C.K. Narula, R.T. Paine and R. Schaeffer, "Precursors to Boron-Nitrogen Macromolecules and Ceramics," *Mat. Res. Soc. Symp. Proc.*, *73*, 383 (1986).

64. P. Kölle, H. Nöth and R.T. Paine, "Synthese und Struktur eines 1,3,2,4-Diphosphadiboretans," *Chem. Ber.*, *119*, 2681 (1986).

65. C.K. Narula, J.F. Janik, E.N. Duesler, R.T. Paine and R. Schaeffer, "Convenient Synthesis, Separation and X-Ray Structure Determination of 1(e),3(e),5(e) Trimethyl-borazane and 1(e),3(e),5(a) Trimethylcycloborazene," *Inorg. Chem.*, *25*, 3346 (1986).

66. W.F. McNamara, E.N. Duesler and R.T. Paine, "Formation and Structure of a Ferro Phosphacyclopentenone," *Organometallics*, *5*, 1747 (1986).

67. R.T. Paine, W.F. McNamara, J.F. Janik and E.N. Duesler, "Synthesis and Reactivity of Metallophosphanes," *Phosph. and Sulfur*, *30*, 241 (1987).

68. D.J. McCabe, E.N. Duesler and R.T. Paine, "Synthesis and Structure of Dialkyl-N,N Diethylcarbamoylmethylthiophosphonate Molybdenum (IV) Dichloride," *Inorg. Chem.*, *26*, 2300 (1987).

69. H. Jelinek-Fink, E.N. Duesler and R.T. Paine, "Structure of Pentacarbonyltribromo-phosphine Chromium(0), $Br_3PCr(CO)_5$," *Acta Cryst.*, *C43*, 635 (1987).

70. J.J. Hunt, E.N. Duesler and R.T. Paine, "Structural Study of $Mn_2(CO)_8[P(NMe_2)_3]_2$," *J. Organometal. Chem.*, *320*, 307 (1987).

71. D.J. McCabe, A.A. Russell, S. Karthikeyan, R.T. Paine, R.R. Ryan and B. Smith, "Synthesis and Coordination Chemistry of 2-(diethylphosphonate) and 2-(diphenylphosphine oxide) Pyridyl N-oxides. Crystal and Molecular Structures of Bis(nitrato) [2-diethylphosphonate) Pyridyl N-oxide] dioxouranium (VI) and Bis(nitrato) [2-(diphenylphosphine oxide) Pyridyl N-oxide] dioxouranium (VI)," *Inorg. Chem.*, *26*, 1230 (1987).

72. J.F. Janik, E.N. Duesler and R.T. Paine, "Structural Investigations of Alumino-Amino Carbene Complexes," *J. Organometal. Chem.*, *323*, 149 (1987).

73. G.L. Wood, C.K. Narula, E.N. Duesler, R.T. Paine and H. Nöth, "Synthesis and Structure of a Novel Phosphane Borane Cage Compound, $P_2[BNiPr]_3$," *J. Chem. Soc. Chem. Commun.*, 496 (1987).

74. L.H. Hutchins, H.U. Reisacher, E.N. Duesler and R.T. Paine, "Synthesis and Structure of Metallophosphenium Complexes Derived From Related Cyclic and Acyclic Aminohalophosphanes," *J. Organometal. Chem.*, *335*, 229 (1987).

75. C.K. Narula, R.T. Paine and R. Schaeffer, "Precursors to Non-Oxide Macromolecules and Ceramics," *ACS Symp. Ser.*, *360*, 378 (1987).

76. C.K. Narula, R. Schaeffer and R.T. Paine, "Synthesis of Boron Nitride Ceramics From Polyborazinyl Amine Precursors," *J. Am. Chem. Soc.*, *109*, 5556 (1987).

77. J.F. Janik, E.N. Duesler and R.T. Paine, "Reactions of Tris-(trimethylsilyl) Aluminum and Ammonia. Formation, Structure and Thermal Decomposition of $[(Me_3Si)_2Al(NH_2)]_2$," *Inorg. Chem.*, *26*, 4341 (1987).

78. C.K. Narula, R.T. Paine and R. Schaeffer, "Precursors to Non-Oxide Ceramics," *Polym. Preps. (Am. Chem. Soc. Div. Polym. Chem.)*, *28*, 454 (1987).

79. J.F. Janik, C.K. Narula, E.G. Gulliver and R.T. Paine, "Reaction Chemistry of Tris(trimethylsilyl)amine with Monohaloboranes," *Inorg. Chem.*, *27*, 1222 (1988).

80. W.F. McNamara, E.N. Duesler and R.T. Paine, "Formation and Molecular Structure of a Dimeric Manganese Isocyanophosphane Complex: $\{CpMn(CO)[CNP(Ph)N(SiMe_3)_2]\}_2$," *Organometallics*, *7*, 384 (1988).

81. D.J. McCabe, E.N. Duesler and R.T. Paine, "Synthesis and Coordination Chemistry of Tripodal Ligands: [Dialkyl[1,2-bis(diethylcarbamoyl)ethyl]phosphonates with Lanthanide Nitrates," *Inorg. Chim. Acta*, *147*, 265 (1988).

82. D.J. McCabe, E.N. Duesler and R.T. Paine, "Tridentate Coordination by a Tripodal Ligand System: Synthesis and Crystal and Molecular Structure of Diisopropyl [1,2-bis(diethylcarbamoyl)ethyl]phosphonate] erbium (III)," *Inorg. Chem.*, *27*, 1220 (1988).

83. S. Karthikeyan, R.T. Paine and R.R. Ryan, "Model Fluorogenic Ligand-Actinide and Lanthanide Coordination Chemistry. Formation and Crystal and Molecular Structure of $[(i\text{-}C_3H_7O)_2P(O)CH(CH_2C_6H_4NO_2)C(O)N(C_2H_5)_2]UO_2(NO_3)_2$," *Inorg. Chim. Acta*, *144*, 135 (1988).

84. W.F. McNamara, E.N. Duesler and R.T. Paine, "Synthesis and Alkylation of an Iron Phosphane Complex, Crystal and Molecular Structure Determinations for $CpFe(CO)_2\{P(C_6H_5)\{N[Si(CH_3)_3]_2\}\}$ and $CpFe(CO)_2\{P(CH_3)(C_6H_5)\{N[Si(CH_3)_3]_2\}\}$," *Organometallics*, *7*, 1313 (1988).

85. G.S. Conary, E.N. Duesler and R.T. Paine, "Coordination Chemistry of 2-Diethylphosphonate-4,6-dipiperidino-1,3,5-triazine with Uranyl Nitrate," *Inorg. Chim. Acta*, *145*, 149 (1988).

86. G.S. Conary, A.A. Russell, R.T. Paine and R.R. Ryan, "Synthesis and Coordination Chemistry of 2-(Diisopropyloxy-phosphino) pyridine N,P-dioxide. Crystal and Molecular Structure of Bis-2-(diisopropoxyphosphino)pyridine N,P-dioxide Lanthanum Nitrate," *Inorg. Chem.*, *27*, 3242 (1988).

87. P. Kölle, G. Linti, H. Nöth, G.L. Wood, C.K. Narula and R.T. Paine, "Synthesis and Structures of New 1,3,2,4-Diphosphadiboretans," *Chem. Ber.*, *121*, 871 (1988).

88. P. Kölle, H. Nöth, R.T. Paine and W. Rattay, "Synthese, Struktur and Reactionen eines 1,3,2,4 Aza λ^3 Phosphadiboretidin Derivats," *Z. Naturforsch*, *43b*, 1439 (1988).

89. J.F. Janik, E.N. Duesler and R.T. Paine, "Formation and Molecular Structure of a Novel Six Coordinate Amino Alane Complex $\{[(CH_3)_3Si]_2Al(NH_2)_2\}_3Al$," *Inorg. Chem.*, *27*, 4335 (1988).

90. R.T. Paine, J.F. Janik and C.K. Narula, "Synthesis of AlN and AlN/SiC Ceramics from Polymeric Precursors," *Mat. Res. Soc. Symp. Proc.*, *121*, 461 (1988).

91. S.L. Blaha, D.J. McCabe, R.T. Paine and K.W. Thomas, "Extraction of Lanthanides with 2-(Dihexylphosphino)pyridine N,P Dioxide," *Radiochim. Acta*, *46*, 123 (1989).

92. G.L. Wood, E.N. Duesler, R.T. Paine and H. Nöth, "Coordination Chemistry of the Cage $P_2(BN\,Pr^i_2)_3$," *Phosphorus and Sulfur*, *41*, 267 (1989).

93. J.F. Janik, E.N. Duesler, W.F. McNamara, M. Westerhausen and R.T. Paine, "Synthesis and Characterization of Phosphinosilyl Alanes from $[(CH_3)_3Si]_3Al$. Crystal and Molecular Structure Determinations of $\{[(CH_3)_3Si]_2AlP(C_6H_5)_2\}_2$, $\{[(CH_3)_3Si]_2AlP(C_6H_5)[Si(CH_3)_3]_2\}_2$, $\{[(CH_3)_3Si]_2AlP(H)(c\text{-}C_6H_{11})\}_3$ and $[\{P(CH_3)_3Si]_2N\}(C_6H_5)P]_2$," *Organometallics*, *8*, 506 (1989).

94. S. Karthikeyan, R.T. Paine and R.R. Ryan, "Synthesis and Coordination Properties of α-Phosphoryl Sulfone, α-Phosphoryl Sulfoxide and α-Phosphoryl Sulfonamide

Ligands. Crystal and Molecular Structure Determinations of $UO_2(NO_3)_2[(i\text{-}C_3H_7O)_2P(O)CH_2S(O)_2(C_6H_{11})]_2$ and $Gd(NO_3)_3[(i\text{-}C_3H_7O)_2P(O)CH_2S(O)C_6H_4CH_3]•H_2O$," *Inorg. Chem.*, *28*, 2783 (1989).

95. S.L. Blaha, L.J. Caudle, G.S. Conary, R.T. Paine and K.W. Thomas, "Synthesis and Separation Properties of a Carbamoylmethylphosphonate Immobilized on a Polystyrene Support," *Radiochim. Acta*, *48*, 59 (1989).
96. P. Kölle, H. Nöth and R.T. Paine, "Darstellung und Reactionen eines 3-Amino-1,2,3-azaphosphaboriridlins," *Chem. Ber.*, *122*, 423 (1989).
97. C.K. Narula, R. Schaeffer, R.T. Paine and A.K. Datye, "Synthesis of Boron Nitride Ceramics from 2,4,6-Triaminoborazine," *Inorg. Chem.,. 28*, 4053 (1989).
98. C.K. Narula, A.K. Datye, R. Schaeffer and R.T. Paine, "Formation of Boron Nitride Coatings on Metal Oxide Substrates," *Chem. Mater.*, *1*, 486 (1989).
99. A.K. Datye, R.T. Paine, C.K. Narula and L.F. Allard, "Novel Approach for High Resolution TEM Studies of Ceramic-Ceramic Interfaces," *Proc. Mat. Res. Soc.*, *153*, 97 (1989).
100. R.T. Paine, G.S. Conary, A.A. Russell, D.J. McCabe, E.N. Duesler, S. Karthikeyan, R. Schaeffer, R.R. Ryan and D. Cromer, "Synthesis of Polyfunctional Organophosphonate Extractants," *Solv. Extr. Ion Exch*., *7*, 767 (1989).
101. R.T. Paine, S.L. Blaha, A.A. Russell and G.S. Conary, "Polymeric Materials for Metal Ion Separations," *Solv. Extr. Ion Exch.*, *7*, 925 (1989).
102. R.T. Paine and C.K. Narula, "Synthetic Routes to Boron Nitride," *Chem. Rev.*, *90*, 73 (1990).
103. R.R. Rye, T.T. Borek, D.A. Lindquist and R.T. Paine, "Chemical Reactions During the Processing of Borazine Polymers," *J. Amer. Ceram. Soc.*, *73*, 1409 (1990).
104. D.A. Lindquist, T.T. Borek, S.J. Kramer, C.K. Narula, G. Johnston, R. Schaeffer, D.M. Smith and R.T. Paine, "Formation and Microstructure of Boron Nitride Aerogels," *Amer. Ceram. Soc.*, *73*, 757 (1990).
105. C.K. Narula, D.A. Lindquist, M.M. Fan, A.K. Datye, W.F. Hammetter, R. Schaeffer and R.T. Paine, "Models and Polyborazene Precursors for Boron Nitride Ceramics," *Chem. Mater.*, *2*, 377 (1990).
106. C.K. Narula, R. Schaeffer, A.K. Datye, T.T. Borek, B.M. Rapko and R.T. Paine, "Synthesis of Boron Nitride Ceramics from Polymeric Precursors Derived from 2-Dimethylamino-4,6-Dichloroborazenes," *Chem. Mater.*, *2*, 384 (1990).
107. D. Cromer, R.R. Ryan, S. Karthikeyan and R.T. Paine, "Structural Studies of Uranyl Complexes of Diphenyl-aminosulfonylmethyl Phosphide Oxide and Diisopropyl-tolysulfinylmethyl phosphonate," *Inorg. Chim. Acta*, *172*, 165 (1990).
108. M.T. Paffett, R.J. Simonson, P. Papin and R.T. Paine, "Borazine Absorption and Decomposition at Pt(111) and Ru(001) Surfaces," *Surf. Sci.*, *232*, 286 (1990).
109. A.K. Datye, Q. Xiaomei, T.T. Borek, R.T. Paine and L.F. Allard, "Stability of Boron Nitride Coatings on Ceramic Substrates," *Proc. Mat. Res. Soc.*, *180*, 807 (1990).
110. D.A. Lindquist, D.M. Smith, A.K. Datye, G.P. Johnston, T.T. Borek, R. Schaeffer and R.T. Paine, "Boron Nitride and Composite Aerogels from Borazine Based Polymers," *Proc. Mat. Res. Soc.*, *180*, 1029 (1990).

111. R.R. Rye, T.T. Borek, D.A. Lindquist and R.T. Paine, "Chemical Reactions During the Thermal Processing of Borazine Polymers," *Proc. Mat. Res. Soc.*, *180*, 1401 (1990).

112. G.L. Wood, C.K. Narula, E.N. Duesler, R.T. Paine and H. Nöth, "Formation of Phosphinoborane Rings. A Reinvestigation of the Reaction of $[(CH_3)_2Si]_3P$ and Borane(3)," *Chem. Ber.*, *123*, 1455 (1990).

113. G. Linti, H. Nöth, K. Polborn and R.T. Paine, "An Allene-analogous Boranylidenephosphane with B=P Double Bond: 1,1-Diethylpropyl (2,2,6,6-tetramethylpiperidino)-boranylidene phosphane-P-pentacarbonylchromium," *Angew Chem. Intl. Ed.*, *29*, 682 (1990).

114. R.R. Rye, T.T. Borek, D.A. Lindquist and R.T. Paine, "Chemical Reactions During the Thermal Processing of Borazine Polymers," *J. Am. Ceram. Soc.*, *73*, 1409 (1990).

115. X. Qiu, A.K. Datye, T.T. Borek and R.T. Paine, "Development of Crystallinity in Turbostratic Boron Nitride Derived From Polymeric Precursors," *Proc. Electron Microsc. Soc.*, 954 (1991).

116. R.R. Rye, D.R. Tallant, T.T. Borek, D.A. Lindquist and R.T. Paine, "Mechanistic Studies of the Conversion of Borazine Polymers to Boron Nitride," *Chem. of Mater*. *3* 286 (1991).

117. G.S. Conary, R.L. Meline, E.N. Duesler and R.T. Paine, "Synthesis of Bifunctional Phosphonates and Phosphine Oxides. Structural Study of Diphenyl [1-(N,N-diethylcarbamoyl)-2-(phenyl)ethyl] Phosphine Oxide with Uranyl Nitrate," *Inorg. Chim. Acta*, *189*, 59 (1991).

118. D.A. Lindquist, T.T. Kodas, D.M. Smith, Q. Xiaomei, S. Hietala and R.T. Paine, "Boron Nitride Powders Formed by Aerosol Decomposition of Polyborazinylamine Solutions," *J. Amer. Ceram. Soc.*, *74*, 3126 (1991).

119. L.F. Allard, A.K. Datye, T.A. Nolan, S.L. Mahan and R.T. Paine, "High Resolution Electron Microscopy of BN on MgO. A Model Ceramic-Ceramic Interface," *Ultramicroscopy*, *37*, 153 (1991).

120. T.T. Borek, W. Ackerman, D.W. Hua, R.T. Paine and D.M. Smith, "Highly Porous Boron Nitride for Gas Adsorption," *Langmuir*, *7*, 2844 (1991).

121. T.T. Borek, X. Qiu, L.M. Rayfuse, A.K. Datye and R.T. Paine, "Boron Nitride Coatings on Oxide Substrates: Role of Surface Modification," *J. Amer. Ceram. Soc.*, *74*, 2587 (1991).

122. D.A. Lindquist, J.F. Janik, A.K. Datye, R.T. Paine and B. Rothman, "Boron Nitride Fibers Processed from Polyborazinyl-Amine Solutions," *Chem. Mater.*, *4*, 17 (1992).

123. D. Dou, G.L. Wood, E.N. Duesler, R.T. Paine and H. Nöth, "Synthesis and Chemistry of Diborylphosphines," *Inorg. Chem.*, *31*, 1695 (1992).

124. D. Dou, G.L. Wood, E.N. Duesler, R.T. Paine and H. Nöth, "Synthesis and Structures of $P_2(BNR_2)_3$ Cages," *Inorg. Chem.*, *31*, 3756 (1992).

125. X. Qiu, A.K. Datye, R.T. Paine and L.F. Allard, "The Oxidation Stability of Boron Nitride Thin Films on MgO and TiO_2 Substrates," *Proc. Mat. Res. Soc. 250*, 275 (1992).

126. R.T. Paine, "Processing of Boron-Nitrogen Preceramic Polymers," *J. Inorg. Organomet. Polymers*, *2*, 183 (1992).

127. G.S. Conary, R.L. Meline, R. Schaeffer and R.T. Paine, "Synthesis and Coordination Chemistry of Trifunctional Phosphono-Bis-Carbonyl Alkane Ligands," *Inorg. Chim. Acta*, *201*, 165 (1992).

128. D. Dou, E.N. Duesler, R.T. Paine and H. Nöth, "Formation of a Novel P-B-N-C Ring via an Intramolecular Cyclization Process," *J. Am. Chem. Soc.*, *114*, 9691 (1992).
129. G.S. Conary, D.J. McCabe, R.L. Meline, E.N. Duesler and R.T. Paine, "Synthesis and Coordination Chemistry of Trifunctional Carbonyl-Bis Phosphonate Alkane Ligands," *Inorg. Chim. Acta*, *203*, 11 (1993).
130. D. Dou, M. Westerhausen, G.L. Wood, E.N. Duesler, R.T. Paine and H. Nöth, "Synthesis and Reaction Chemistry of Aminophosphinoboranes," *Chem. Ber.*, *126*, 379 (1993).
131. H. Nöth, S. Staude, M. Thomann and R.T. Paine, "Darstellung und Reactionen Monomerer Tetraorganylphosphanylborane," *Chem. Ber.*, *126*, 611 (1993).
132. B.M. Rapko, E.N. Duesler, P.H. Smith, R.T. Paine and R.R. Ryan, "Chelating Properties of 2-(Diphenylphosphinomethyl)pyridine N,P-Dioxide and 2,6-Bis(Diphenylphosphinomethyl)pyridine, N,P,P-Trioxide Toward f-Element Ions," *Inorg. Chem.*, *32*, 2164 (1993).
133. G.S. Conary, D.J. McCabe, L.J. Caudle, E.N. Duesler and R.T. Paine, "Synthesis and Structural Studies of Selected Multifunctional Phosphonate and Phosphonic Acid Ligands," *Inorg. Chim. Acta*, *207*, 213 (1993).
134. D. Dou, E.N. Duesler, R.T. Paine and H. Nöth, "Synthesis of Cage Compounds Containing P, B, and Si Atoms," *Inorg. Chem.*, *32*, 3056 (1993).
135. J.F. Janik and R.T. Paine, "The System $LiAlH_4/NH_4X$ as a Precursor Source for AlN," *J. Organometal. Chem.*, *449*, 39 (1993).
136. R.T. Paine, D. Dou, M. Westerhausen, E.N. Duesler, G. Linti and H. Nöth, "Synthesis and Reactivity of Borylphosphanes," *Phosph. Sulfur and Silicon*, *77*, 61 (1993).
137. B. Kaufmann, H. Nöth, R.T. Paine, K. Polborn and M. Thomann, "Carbonyl-Metal Complexes of Diphosphadiboretane $(MesBP^tBu)_2$ and Triphosphatriborinane $(MesBP^tBu)_3$," *Angew. Chem. Intl. Ed.*, *32*, 1446 (1993).
138. J.F. Janik, E.N. Duesler and R.T. Paine, "Synthesis of a Novel Azaalane Ring," *Chem. Ber.*, *126*, 2649 (1993).
139. M.E. Bartram, T.A. Michalski, J.W. Rogers and R.T. Paine, "Nucleation and Growth of AlN: Self-limiting Reactions and Regeneration of Active Sites Using Sequential Exposures of Trimethylaluminum and Ammonia on Silica at 600°K," *Chem. Mat.*, *5*, 1424 (1993).
140. G. Linti, H. Nöth and R.T. Paine, "On the Complex Formation of 1,3,2,4-Diphosphadiboretanes with Pentacarbonylchromium and the Preparation and Reactivity of Borylidenephosphane Complexes," *Chem. Ber.*, *126*, 875 (1993).
141. R.T. Paine, M. Fan, A. Hanprasopwattana and A.K. Datye, "Synthesis and Processing of Boron Nitride Polymers," *Polym. Prepr. (Am. Chem. Soc. Div. Polym. Chem.)*, *34*, 336 (1993).
142. T. Chen, E.N. Duesler, R.T. Paine and H. Nöth, "Assembly of a Spirocyclic $[(R_2NB)_2P_2]_2Si$ Cage," *Phosph. Sulfur and Silicon*, *87*, 41 (1994).
143. R.T. Paine, J.F. Janik and M. Fan, "Some Recent Developments in Precursor Routes to Ceramic Nanocomposites," *Polyhedron*, *13*, 1225 (1994).
144. D. Dou, M. Fan, T. Chen, E.N. Duesler, H. Nöth and R.T. Paine, "Synthesis and Reactivity of New Diborylphosphanes," *Inorg. Chem.*, *33*, 2151 (1994).

145. J.F. Janik, W.C. Ackerman, R.T. Paine, D.W. Hua, A. Maskara and D.M. Smith, "Boron Nitride as a Selective Gas Adsorbent," *Langmuir*, *10*, 514 (1994).

146. B. Kaufmann, N. Metzler, H. Nöth and R.T. Paine, "1,3,5-Triphenyl-2,4,6-trimesityl-1,3,5,2,4,6-triphosphatriborinane: a 6π-electron Heteroaromatic Ligand," *Chem. Ber.* *127*, 825 (1994).

147. H. Nöth, S. Staude, M. Thomann, J. Kroner and R.T. Paine, "Reactions of Monomeric Phosphanylboranes with Acyl Chlorides: 1-Oxa-3-oxonia-5-phospha-2-borata-3,5-cyclohexadienes," *Chem. Ber.*, *127*, 1923 (1994).

148. R.T. Paine and L.G. Sneddon, "Borazine-based Polymers Close in on Commercial Performance," *CHEMTECH*, July, 1994, 29.

149. R.T. Paine and L.G. Sneddon, "Recent Developments in Borazine Based Polymers," *ACS Symp. Ser.*, *572*, 358 (1994).

150. T. Chen, E. Duesler, R.T. Paine and H. Nöth, "Synthesis of Main Group Ring and Cage Compounds," *Phosph. Sulfur and Silicon*, *93*, 73 (1994).

151. H. Nöth and R.T. Paine, "Recent Advances in Phosphinoborane Chemistry," *Chem. Rev.*, *95*, 343 (1995).

152. A.A. Russell, R.L. Meline, E.N. Duesler and R.T. Paine, "Synthesis and Coordination Chemistry of 2,6-Bis(diethoxyphosphino)pyridine P,P-dioxide. Crystal and Molecular Structure of $\{[(EtO)_2P(O)]_2C_5H_3N\}UO_2(NO_3)_2$," *Inorg. Chim. Acta*, *231*, 1 (1995).

153. U. Englehardt, B.M. Rapko, E.N. Duesler, D. Frutos and R.T. Paine, "Synthesis and Molecular Structures of Complexes of Bismuth Nitrate with 2,6-Bis(Phosphinomethyl)pyridine N,P,P' Trioxide ," *Polyhedron*, *14*, 2361 (1995).

154. X. Gan, E.N. Duesler, E. Bond, P.H. Smith and R.T. Paine, "Synthesis and Coordination Properties of 6,6'Bis(Diphenylphosphinomethyl)2,2'bipyridine N,N'P,P' Tetraoxide," *Inorg. Chim. Acta*, *247*, 29 (1996).

155. B. Nieslanik, E.N. Duesler, L. Miao, S.C. Jackels and R.T. Paine, "PyO_2[18]diene N_6•4HBr•H_2O," *Acta Cryst. C*, *C52*, 205 (1996).

156. H.U. Reisacher, E.N. Duesler and R.T. Paine, "Formation of Metallophosphenium Cluster Complexes. Crystal and Molecular Structure of CpMo(CO)(u-CO)$Fe(CO)_3P(C_6H_5)\{N[Si(CH_3)]_3\}_2$,", *Chem. Ber.*, *129*, 279 (1996).

157. D. Dou, G. Linti, E.N. Duesler, R.T. Paine and H. Nöth, "Formation and Coordination Chemistry of Aminophosphanylboranes," *Inorg. Chem.*, *35*, 3626 (1996).

158. B. Kaufmann, H. Nöth and R.T. Paine, "Formation, Structure, and Reactions of a P,P'-Bi(1,3,2,4-diphosphodiboretane," *Chem. Ber.*, *129*, 557 (1996).

159. S. Grundei, H. Nöth and R.T. Paine, "Reactions of a 1,2-Diphospha-3, 4-Diboretane With Some Metal Carbonyls," *Chem. Ber.*, *129*, 1233 (1996).

160. E.M. Bond, U. Engelhardt, T.P. Deere, B.M. Rapko, R.T. Paine and J.R. Fitzpatrick, "The Solvent Extraction of Americium(III) in Nitric Acid Solutions by 2,6-Bis[(Diphenyldiphosphino)methyl]Pyridino N,P,P' Trioxide," *Solv. Extract. Ion Exch.*, *15*, 381 (1997).

161. W.F. McNamara, H.U. Reisacher, E.N. Duesler and R.T. Paine, "Reactions of Molybdenum and Tungsten Phosphenium Complexes with Sulfur and Selenium," *Organometallics*, *16*, 449 (1997).

162. T.Chen, E.N. Duesler, B. Kaufmann, R.T. Paine and H. Nöth, "Synthesis of Cage Compounds Containing Boron, Phosphorus and Tin," *Inorg. Chem*., *36*, 1070 (1997).

163. T. Chen, E.N. Duesler, R.T. Paine and H. Nöth, "Synthesis of Cage Compounds Containing Boron, Phosphorus and Germanium," *Inorg. Chem*., *36*, 802 (1997).

164. T. Chen, E.N. Duesler, R.T. Paine and H. Nöth, "Assembly of a Triple Cage Species Containing B, P and Si Atoms," *Inorg. Chem*., *36*, 1534 (1997).

165. T. Chen, E. N. Duesler, R. T. Paine and H. Nöth, "Synthesis and Assembly Mechanism for Spirocyclic Cage Compounds Containing B, P and Si atoms," *Chem. Ber*., *30*, 933 (1997).

166. H.U. Reisacher, E.N. Duesler and R.T. Paine, "Reactions of Molybdenum Phosphenium Complexes with Carbenoid Reagents," *J. Organometal. Chem*., *539*, 36 (1997).

167. J. F. Janik, E. N. Duesler and R. T. Paine, "Preparation and Characterization of Bis-(Trimethylsilyl)Aminoalanes, $[H_2AlN(SiMe_3)_2]\cdot NMe_3$ and $\{HAl[N(SiMe_3)_2]_2\}_n$. Crystal Structure Determination for Tris-(Trimethylsilyl)Alane Trimethylamine Adduct, $(Me_3Si)_3Al\cdot NMe_3$," *J. Organometal. Chem*., *539*, 19(1997).

168. T. Chen, R. T. Paine, E. N. Duesler and H. Nöth, "New BP Cage Species," *Phosphorus, Sulfur and Silicon*, *124/125*, 1 (1997).

169. H.U. Reisacher, E.N. Duesler and R.T. Paine, "Reactions of Protic Reagents with a Tungsten Phosphenium Ion Complex", *J. Organometal. Chem.*, *564*, 13 (1998).

170. E.M. Bond, U. Engelhardt, T.P. Deere, B.M. Rapko, R.T. Paine and J.R. Fitzpatrick, "The Solvent Extraction of Americium(III) from HCl Solutions by 2,6-Bis[Diphenyl-phosphino)methyl]pyridine N,P,P' Trioxide," *Solvent Extr. and Ion Exchange*, *16*, 967 (1998).

171. T. Chen, E. N. Duesler, R. T. Paine and H. Nöth, "Formation of Cage Compounds Containing Boron, Phosphorus and a Transition Metal Atom," *Inorg. Chem*., *37*, 490 (1998).

172. E. M. Bond, X. Gan, J. R. FitzPatrick and R. T. Paine, "Coordination Chemistry and Extraction Properties of Phosphonopyridine N,P Oxides," *J. Alloys and Compounds*, *271-273,* 172 (1998).

173. B. Kaufmann, H. Nöth, M. Schmidt and R. T. Paine, "Some Oxidative Addition Reactions with a Diphosphadibora[1.1.0]bicyclobutane: Formation of Cage Compounds and an Unusual Trinuclear Coordination Compound of Palladium," *Inorg. Chim. Acta,* **269**, 101 (1998).

174. D. Srivastava, M. Fan, E.N. Duesler and R.T. Paine, "Synthesis and Utilization of Silyl-borazines as Precursors to Silicon Containing Boron Nitride," *Eur. J. Inorg. Chem.*, 855 (1998).

175. D. Dou, E.N. Duesler and R.T. Paine, "Synthesis and Structural Characterization of New Polyphosphorus Ring and Cage Compounds," *Inorg. Chem*., **38**, 788 (1999).

176. T. Chen, J. Jackson, S.A. Jasper, E. N. Duesler, H. Nöth and R.T. Paine, "Coordination Chemistry of Aminoborylphosphanes," *J. Organometal. Chem*., **582**, 25 (1999).

177. M.P. Wilkerson, C.J. Burns, R.T. Paine and B.L. Scott, "Synthesis and Crystal Structure of $UO_2Cl_2(THF)_3$: A Simple Preparation of Anhydrous Uranyl Reagents," *Inorg. Chem.*, **38**, 4156 (1999).

178. R.T. Paine, W. Koestle, T.T. Borek, E.N. Duesler, G.L. Wood and M.A. Hiskey, "Synthesis, Characterization and Explosive Properties of the Nitrogen Rich Borazine $[H_3N_3B_3(N_3)_3]$," *Inorg. Chem.*, **38**, 3738 (1999).
179. T. Chen, E.N. Duesler, R.T. Paine and H. Nöth, "Synthesis and Chemistry of Boraphosphinosilanes and Germanes," *Inorg. Chem.*, **38**, 4993 (1999).
180. E.A. Pruss, G.L. Wood, W.J. Kroenke and R.T. Paine, "Aerosol Assisted Vapor Synthesis (AAVS) of Spherical Boron Nitride Powders," *Chem. Mater.*, **12**, 19 (2000).
181. M.P. Wilkerson, C.J. Burns, R.T. Paine and B.L. Scott "Synthesis and Structure of Tetrakis(2,6-dichlorophenoxide)bis(THF)Uranium(IV)" *J. Chem. Crystall.* **30**, 7 (2000).
182. M.P. Wilkerson, C.J. Burns, H.J. Dewey, J.M. Martin, D.E. Morris, R.T. Paine and B.L. Scott, "Basicity of Uranyl Oxo Ligands upon Coordination of Alkoxides" *Inorg. Chem.*, **39**, 5277 (2000).
183. X.-M. Gan, S. Parveen, W.L. Smith, E.N. Duesler and R.T. Paine, "Synthesis, Characterization and Coordination Chemistry of a New Structurally Hindered Trifunctional Ligand, 4,5-Bis(diphenylphosphino)-*sym*-octahydroacridine N,P,P′-trioxide," *Inorg. Chem.* **39**, 4591 (2000).
184. E.M. Bond, E.N. Duesler, R.T. Paine, M.P. Neu, J.H. Matonic and B.L. Scott, "Synthesis and Molecular Structure of a Plutonium (IV) Coordination Complex: $[Pu(NO_3)_2\{2,6\text{-}[(C_6H_5)_2P(O)CH_2]_2\ C_5H_3NO\}_2](NO_3)_2 \cdot 1.5H_2O\text{–}0.5MeOH$," *Inorg. Chem.* **39**, 4152 (2000).
185. E.M. Bond, E.N. Duesler, R.T. Paine and H. Nöth, "Isolation and Structure of a Europium (III) Chloride Complex of 2,6-Bis{(Diphenyl phosphino)methyl]pyridine N,P,P′ Trioxide," *Polyhedron*, **19**, 2135 (2000).
186. T. Chen, E.N. Duesler, H. Nöth and R.T. Paine, "Synthesis and Coordination Behavior of a Zirconocene Bis(Borylphosphane)," *J. Organometal. Chem.*, **614-615**, 99 (2000).
187. R.F. Hill, R. Danzer and R.T. Paine, "Synthesis of Aluminum Oxide Platelets," *J. Amer. Ceram. Soc.*, **84**, 514 (2001).
188. G.L. Wood, E.A. Pruss and R.T. Paine, "Aerosol Assisted Vapor Phase Synthesis of Gallum Nitride Powders," *Chem. Mater.*, **13**, 12 (2001).
189. Y.-C. Tan, X.-M. Gan, J.L. Stanchfield, E.N. Duesler and R.T. Paine, "Synthesis and Lanthanide Ion Coordination Chemistry of 2,6-Bis(diphenylphosphinomethyl)benzene," *Inorg. Chem.,* **40**, 2910 (2001).
190. X.Gan, E.N. Duesler and R.T. Paine, "Synthesis and Coordination Properties of New Bis(Phosphonomethyl) Pyridine N,P,P′ Trioxides," *Inorg. Chem.*, **40**, 4420 (2001).
191. R.T. Paine, Y.C. Tan and X. Gan, "Synthesis and Coordination Chemistry of 2,6-bis(Phosphinomethyl)Phenol P,P'-Dioxides," *Inorg. Chem.*, **40**, 7009 (2001).
192. R.T. Paine, E.A. Pruss, G.L. Wood, C. Schwierkowski, R.F. Hill, C. Chapelle and W.J. Kroenke "Boron Nitride Fillers for Organic Polymer Composites", ACS Symp. **804**, 27 (2001).
193. E.M. Bond, N. Donhart, E.N. Duesler, H. Nöth and R.T. Paine, "Synthesis and Coordination Properties of 1-Diphenylphosphineoxide-1-(2-Pyridyl N-Oxide) Propane," *Inorg. Chem.*, **41**, 444 (2002).

194. J.H. Matonic, M.P. Neu, R.T. Paine and B.L. Scott, "Synthesis and Crystal Structure of a Ten Coordinate Plutonium(IV) Ion Complexed by the Extractant Diphenyl phosphinomethylpyridine N,P-Dioxide $Pu(NO_3)_3\{2-[(C_6H_5)_2P(O)CH_2]C_5H_4NO]$ $[Pu(NO_3)_6]_{0.5}$," *J. Chem. Soc. Dalton Trans*., 2328 (2002).

195. M.P. Wilkerson, C.J. Burns, D.E. Morris, R.T. Paine and B.L. Scott "Steric Control of Substituted Phenoxide Ligands on Product Structures of Uranyl Aryloxide Complexes" *Inorg. Chem.* **41**, 3110 (2002).

196. K.L. Nash, C. Lavallette, M. Borkowski, R.T. Paine and X. Gan, "Features of the Thermodynamics of Two-Phase Distribution Reactions of Americium (III) and Europium (III) Nitrates into Solutions of 2,6-bis[(di-2-ethylhexylphosphino)methyl]pyridine-N,P,P-trioxide" *Inorg. Chem.* **41**, 5849 (2002).

197. J.H. Matonic, A.E. Enriquez, B.L. Scott, R.T. Paine and M.P. Neu "Eight and Nine Coordinate Plutonium (IV) Complexes of the f-Element Extractant 2,6-Bis(diphenylphosphinomethyl) Benzene P,P´Dioxide" *J. Nucl. Sci. Tech.* (Suppl. 3) 400 (2002).

198. X. Gan, R.T. Paine, E.N. Duesler and H. Nöth "Synthesis and Coordination Chemistry of Arene Soluble 4-Alkyl-2,6-bis[(diphenylphosphino)methyl] pyridine N,P,P´-trioxide Ligands" *J. Chem. Soc.* (Dalton) 153 (2003).

199. M. Fan, E.N. Duesler and R.T. Paine "Syntheses and Structure of an Amidoimidotitanium Cage Complex" *Applied Organometal. Chem.* **17**, 549 (2003).

200. X. Gan, E.N. Duesler and R.T. Paine "Synthesis of Trifunctional Ligands Containing Thiophosphoryl, Pyridine and Pyridine N-oxide Donor Groups", *J. Chem. Soc.*(Dalton), 4704 (2003).

201. J.F. Janik, M. Drygas, C. Czosnek, M. Kaminska, M. Palczewska and R.T. Paine "Carbothermally-assisted Aerosol Synthesis of Semiconducting Materials in the System GaN/Mn". *J. Phys. Chem. Solids* **65**, 639 (2004).

202. X. Gan, I. Binyamin, B.M. Rapko, J. Fox, E.N. Duesler and R.T. Paine "Layered Framework Structures Constructed from 2-(Pyridyl N-oxide) methylphosphonic Acid Ligands and Er (III). *Inorg. Chem*. **43**, 2443 (2004).

203. X. Gan, B.M. Rapko, E.N. Duesler, I. Binyamin, R.T. Paine and B.P. Hay "Synthesis and Lanthanide Coordination Chemistry of 2,6-Bis[(dicyclohexylphosphino)methyl]pyridine N,P,P-Trioxide" *Polyhedron* **24**, 469 (2005).

204. G.L. Wood, J.F. Janik, M.Z. Visi, D.M. Schubert and R.T. Paine "New Borate Precursors for Boron Nitride", *Chem. Mater.* **17**, 1855 (2005).

205. R.T. Paine, H. Nöth, T. Habereder, J.F. Janik, E.N. Duesler and D. Dreissig "Recent Developments in Boron-Phosphorus Ring and Cage Chemistry" *ACS Symp. Ser.* **917**, 152, (2005).

206. K. Knabel, T.M. Klapötke, H. Nöth, R.T. Paine and I. Schwab "A Bicyclic P-P bridged 1,3,2,4-diphosphadiboretane Cation and an Imido(phosphinidene)borane $AlBr_3$ Adduct" *Eur. J. Inorg. Chem.* 1099 (2005).

207. M. Drygas, C. Czosnek, R.T. Paine and J.F. Janik "Aerosol-assisted Vapor Phase Synthesis of Powder Composites in the Target System GaN/TiN for Potential Electronic Applications" *Mater. Res. Bull.* **40**, 1136 (2005).

208. G.L. Wood, J.F. Janik, E.A. Pruss, D. Dreissig, W.J. Kroenke, T. Habereder, H. Nöth and R.T. Paine "Aeorosol Synthesis of Spherical Morphology Boron Nitride Powders from Organoborate Precursors" *Chem. Mater.* **18**, 1434 (2006).

209. J. Janik, M. Drygas, S. Stelmakh, E. Grzanka, B. Palosz and R.T. Paine "Tuning aerosol-assisted vapor phase processing towards low oxygen GaN powders" *Phys. Status, Solidi(a)* **203**, 1301 (2006).

210. X. Gan, B.M. Rapko, J. Fox, I. Binyamin, S. Pailloux, E.M. Duesler and R.T. Paine "A Three Dimensional Framework Structure Constructed from 2-(Pyridyl N-oxide) Ethylphosphonic Acid and Nd(III)" *Inorg. Chem.* **45**, 3741 (2006).

211. K. Knabel, H. Nöth, and R.T. Paine"Behavior of 1,3-Di(tert-butyl)-2,4-bis(tetramethylpiperidino)-1,3,2,4-diphosphodiboretane towards Boron Halides and Adduct Formation of a Bicyclo [1.1.0] diphosphodiboretane with Tris(pentafluorophenyl)borane" *Z. Naturforsch* Sect. B **61**, 265 (2006).

212. M. Drygas, C. Czosnek, R.T. Paine and J.F. Janik "Two-Stage Aerosol Synthesis of Titanium Nitride TiN and Titanium Oxynitride TiO_xN_y Nanopowders of Spherical Particle Morphology" *Chem. Mater.* **18**, 3122 (2006).

213. I. Binyamin, S. Pailloux, E.N. Duesler, B.M. Rapko and R.T. Paine "Synthesis and Lanthanide Coordination Properties of New 2,6-Bis(N-t-Butylacetamido) Pyridine and 2,6-Bis(N-t-Butylacetamido) Pyridine N-oxide Ligands" *Inorg. Chem.* **45**, 5886 (2006).

214. X. Gan, I. Binyamin, S. Pailloux, E.N. Duesler and R.T. Paine "Formation of a Layered Framework Structure Based Upon 4-Methyl-2,6-Bis(methylphosphonic acid)Phenol" *J. Chem. Soc. Dalton* 3912 (2006).

215. J. Gosk, M. Drygas, J.F. Janik, M. Palczewska, R.T. Paine and A. Twardowski "Magnetic and Optical properties of (GaMn)N nanocrystalline powders obtained by the aerosol-assisted vapor phase synthesis and anerobic imide route methods" *J. Phys. D. Applied Phys.* **39**, 3717 (2006).

216. X. Gan, I. Binyamin, B.M. Rapko, J. Fox, E.N. Duesler and R.T. Paine "Formation of a 1-D Chain Structure from Nd(III) and 2,6-bis(methylphosphonic acid)pyridine N-oxide" *Polyhedron* **25**, 3387 (2006).

217. G.L. Wood and R.T. Paine "Aerosol Synthesis of Hollow Spherical Morphology Boron Nitride Particles" *Chem. Mater.* **18**, 4716 (2006).

218. M. Fan, R.T. Paine, E.N. Duesler and H. Nöth "Synthesis and Molecular Structure of Tris[(trimethylsilyl)silyl](diisopropylamino)(diphenylphosphino) borane" *Z. Anorg. Allgem. Chem* **632**, 2443 (2006).

219. I. Binyamin, S. Pailloux, B.P. Hay, E.N. Duesler, B.M. Rapko and R.T. Paine "Synthesis of Propionamide Pyridine and Pyridine N-oxide Ligands" *J. Heterocyclic Chem.* **44**, 99 (2007).

220. M. Fan, E.N. Duesler, J.F. Janik and R.T. Paine "Transamination Reactivity of $Ti(NMe_2)_4$ and $Zr(NMe_2)_4$ with 1,3,4,5,6-Pentamethyl-2-amino Borazine and Aryl Amines. Model Chemistry for the Formation of Metalloborazine Preceramic Polymers and MN/BN (M = Ti, Zr) Ceramic Composites" *J. Inorg. Organomet. Polym. Mater.* **17**, 423 (2007).

221. H. Nöth, B. Gemünd and R.T. Paine "N(2,4,6-trimethylborazinyl) substituted Phosphanes, Arsanes and Stibanes" *Eur. J. Inorg. Chem.* 4282 (2007).

222. R. Jetzfehlner, H. Nöth and R.T. Paine "Phosphino[tris(trimethylsilyl)methyl] Boranes and 2,4-Bis[tris(trimethylsilyl)methyl]1,3,2,4-diphosphadiboretanes" *Z. Anorg. Allgem. Chem* **633**, 548 (2007).

223. T. Habereder, H. Nöth and R.T. Paine "Synthesis and Reactivity of New Bis(tetramethylpiperidino)(phosphino)alanes" *Eur. J. Inorg. Chem.* 4298 (2007).

224. S. Pailloux, I. Binyamin, S. Kim, L.M. Deck, B.M. Rapko, B.P. Hay, E.N. Duesler, L. Zakharov, A.L. Rheingold and R.T. Paine "Oxidation Reactivity Channels for 2-(Pyridin-2-yl)-N,N-diphenyl acetamide *J. Org. Chem.* **72**, 9195 (2007).

225. R. Jetzfehlner, H. Nöth and R.T. Paine "Dimeric Phosphinoboranes $[R'(Hal)B\text{-}PHR]_2$ and some of their Reactions" *Z. Anorg. Allgem, Chem.* **633**, 917 (2007).

226. M. Drygas, Z. Olejniczak, E. Grzanka, M.M. Bucko, R.T. Paine and J.F. Janik "Probing the Structural Diversity and Thermal Stability of Various Nanocrystalline Powders of Gallium Nitride, GaN" *Chem. Mater*. **20**, 6816 (2008).

227. S. Pailloux, C.E. Shirima, A.D. Ray, E.N. Duesler, R.T. Paine, J.R. Klaehn, M.E. McIlwain and B.P. Hay "Synthesis and Coordination Chemistry of Trifluoromethyl Decorated Derivatives of 2,6-Bis[(diphenylphosphinoyl)methyl]pyridine N-Oxide Ligands with Lanthanide Ions" *Inorg. Chem*. **48**, 3104(2009).

228. S. Pailloux, C.E. Shirima, E.N. Duesler, R.T. Paine, J.R. Klaehn, M.E. McIlwain and B.P. Hay "Synthesis and Lanthanide Coordination Chemistry of Trifluoromethyl Derivatives 0f Phosphinoylmethyl-pyridine N-oxides" *J. Chem. Soc. Dalton Trans*. 7486 (2009).

229. S. Pailloux, E.N. Duesler, R.T. Paine, J.R. Klaehn and M.E. McIlwain "Direct synthesis of trifluoromethyl-decorated diphenyl phosphites. Unusual non-bonded structural features in bis[(2-trifluoromethyl)phenyl phosphite: $[2\text{-}(CF_3)C_6H_4]_2P(O)H$" *Main Group Chem.* **8**, 207 (2009).

230. S. Pailloux, I. Binyamin, L.M. Deck, B.P. Hay, L.N. Zakharov, W.S. Kassel, A.L. Rheingold and R.T. Paine "Unexpected Chelation Interaction for 2-Hydroxy-2-(1-oxy-pyridin-2-yl)-N,N-diphenyl acetamide" *Polyhedron* **28**, 3979 (2009).

231. M. Fan, E.N. Duesler, H. Nöth, and R.T. Paine "Reactions of Organyl and Silyl Alanes with 1,3,4,5,6-Pentamethyl-2-amino Borazine" *Inorg. Chem.* **49**, 2983 (2010).

232. S. Pailloux, C.E. Shirima, K.A. Smith, E.N. Duesler, R.T. Paine, N.J. Williams and R.D. Hancock "Synthesis and Reactivity of (Benzoxazol-2-ylmethyl)phosphonic Acid" *Inorg. Chem.* **49**, 9369 (2010).

233. K.L. Swancutt, S.P. Mezyk, L.R. Martin, R.D. Tillotson, S. Pailloux, M. Chakravarty and R.T. Paine "Kinetics and Efficiencies of Radiolytic Degradation in Lanthanide/Actinide Separation Ligands – NOPOPO" *ACS Symp. Ser.* **1046**, 231 (2010).

234. M. Fan, E.N. Duesler and R.T. Paine "Reactions of Tris(Trimethylsilyl) Aluminum with Aniline and 2,6-Diisopropylaniline" *Main Group Chem*. **10**, 37 (2011).

235. J.M. Camus, S. Pailloux, C.E. Shirima and R.T. Paine "Synthesis of 2,5-bis(phosphinoylmethyl)- and 2,5-bis(thiophophinoylmethyl)-thiophenes" *Main Group Chem.* **10,** 25 (2011).

236. S. Pailloux, C.E. Shirima, E.N. Duesler, K.A. Smith and R.T. Paine "Synthesis and lanthanide coordination chemistry of 2[(phosphinoyl)methyl]-4,5-dihydrooxazole and 2-[(phosphinoyl)methyl)benzoxazole ligands" *Polyhedron* , **30**, 2746 (2011).

237. T. Chen, E.N. Duesler, H. Nöth, and R.T. Paine "Synthesis and reactivity of a zirconocene bis-(aminoborylphosphane)" *Main Group Chem*. **10**,279 (2011).

238. M. Chakravarty, S. Pailloux, E.N. Duesler, K.A. Smith, R.T. Paine, N.J. Williams and R.D. Hancock "Synthesis and metal coordination chemistry of (phenyl)(pyridine-2-ylmethyl)phosphinodithioic acid, [2-C_5H_4N]CH_2P(S)(SH)(Ph)" *Polyhedron*, **33**, 327 (2012).

239. J. Sulakova, R.T. Paine, M. Chakravarty and K.L. Nash "Extraction of Lanthanide and Actinide Nitrate and Thiocyanate Salts by 2,6-Bis[(bis 2-n-octyl)phosphino)methyl]pyridine N,P,P'-trioxide in Toluene" *Sep. Sci. Tech*., **47**, 1, 2012.

240. D. Rosario-Amorin, E.N. Duesler, R.T. Paine, B.P. Hay, S. Reilley, B.L. Scott and A. J. Gaunt "Synthesis and Coordination Chemistry of Phosphino Oxide Decorated Dibenzofuran Platforms" *Inorg. Chem.,* **51**, 6667 (2012).

241. D. Rosario-Amorin, S. Ouizem, D.A. Dickie, Y. Wen, R.T. Paine, J. Gao, J. K.Grey, A. de Bettencourt-Dias, B.P. Hay and L.H. Delmau "Synthesis, Coordination Chemistry and Liquid-Liquid Extraction Performance of CMPO-decorated Pyridine and Pyridine N-oxide Platforms" *Inorg. Chem.* accepted

242. D. Rosario-Amorin, D.A. Dickie, Y. Wen and R.T. Paine "A New Hybrid CMPO/NOPOPO Ligand: Synthesis and Selected Lanthanide Coordination Chemistry" *Phosp. Sulfur, Silicon and Rel. Elem*. accepted.

243. S. Ouizem, D.A. Dickie, M.J. Katz and R.T. Paine "Unexpected Transformation of a Schiff-base Pyridine N-oxide in the Presence of $Pr(NO_3)_3 \cdot 6H_2O$" *Phosp. Sulfur, Silicon and Rel. Elem*. accepted.

244. S. Pailloux, D. Rosario-Amorin, M. Chakravarty, J. M. Camus, K.A. Smith, E.N. Duesler, D.A. Dickie, R.T. Paine, K. K. Klausmeyer, B. P. Hay, and L. H. Delmau " Synthesis and Properties of New (Phosphinoylmethyl) Pyridine N-Oxides" *Zeitschrift für Anorganische und Allgemeine Chemie*, submitted.

245. S. Ouizem, S. Pailloux, A.D Ray, K.A. Smith, E.N. Duesler and R.T. Paine "Synthesis and Coordination Chemistry of a Dissymmetric Phosphinoylmethyl Pyridine N-Oxide Ligand" *Inorg. Chem*., manuscript in preparation.

B. Chemtracts Commentaries

1. R.T. Paine, "GaN Thin Films" on "Growth of GaN Layers from the Single Source Precursor $(Et_2GaNH_2)_3$" in *Chem. Mater.* **1998**, *10*, 2251. *Chemtracts*, submitted.
2. R.T. Paine, "Sterically Hindered Phosphines" on "PH Functionalized Phosphines with 1,1´-Biphenyl-2,2´-bis(methylene) and 1,1´-Binaphthyl-2,2´-bis(methylene) Backbones," *Inorg. Chem.* **1998**, *37*, 6408. *Chemtracts*, submitted.

C. Patents

Issued

1. R.T. Paine, R. Schaeffer, C.K. Narula, U.S. Patent No. 4,971,779, November 20, 1990. "Process for the Pyrolytic Conversion of a Polymeric Precursor Composition to Boron Nitride."
2. R.T. Paine, C .K. Narula, R. Schaeffer, U.S. Patent No. 5,082,693, January 21, 1992. "Precursor for Boron Nitride Ceramic Coating."

3. R.T. Paine, C.K. Narula, R. Schaeffer, U.S. Patent No. 5,188,757, February 23, 1993. "Precursor Composition for Conversion to Boron Nitride."
4. R.T. Paine, C.K. Narula, R. Schaeffer, D.A. Lindquist and T.T. Borek, U.S. Patent No. 5,204,295, April 20, 1993. "Precursors for Boron Nitride Coatings."
5. R.T. Paine, W.J. Kroenke, E.A. Pruss U.S. Patent No. 6,348,179 BI February 19, 2002 "Spherical Boron Nitride Process, System and Product of Manufacture".
6. R. T. Paine, W. J. Kroenke, E. A. Pruss U.S. Patent 6,824,753, November 30, 2004 "Organoboron Route and Process for Preparation of Boron Nitride".
7. R. T. Paine, G. L. Wood, J. F. Janik, W. J. Kroenke U.S. Patent 7,060,237 "Non-Aqueous Borate Route to Boron Nitride" June 13, 2006.
8. R. T. Paine and G. L. Wood, U.S. Patent 7,192,644 "Non-Aqueous Borate Routes to Boron Nitride" March 20, 2007.

D. Book Chapters

1. R.T. Paine, "Formation of Nonoxide Ceramics from Inorganometallic Precursors," *Inorganometallic Chemistry*, T.P. Fehlner, Ed., Plenum Publ. Co. (1992): p. 359-385.
2. R.T. Paine, "Boron-Nitrogen Compounds" in *Encyclopedia of Inorganic Chemistry*, R.B. King, Ed., J. Wiley, (1994).
3. R.T. Paine, "Design and Synthesis of F-Element Selective Ligands," in *F-Element Separations*, K.L. Nash and G.R. Choppin, Eds., Plenum Press: New York, (1995): p. 173.

E. Book Reviews

1. "Techniques and Applications of Plasma Chemistry," by J.R. Hollahan and A.T. Bell, J. Wiley and Sons, NY, 1974, appeared in *J. Am. Chem. Soc*., 98, 1646 (1976).
2. "Structural Inorganic Chemistry," by A.F. Wells, Oxford University Press, 1984, appeared in *J. Am. Chem. Soc*.
3. "Advanced Inorganic Chemistry," by G. Wilkinson and F. A. Cotton, 5th Ed. *J. Am. Chem. Soc*.

F. Present Research Areas

1. Coordination Properties of Low Coordinate Main Group Ligands.
2. Design of Advanced Chemical Extractant Systems.
3. Synthesis and Processing of Main Group Ceramic Precursors.
4. Systematic Construction of Main Group Ring, Cage, and Cluster Compounds.

G. Present Research Support

1. Department of Energy, 8/1/12-7/30/14, $260,000, "Preorganized and Immobilized Ligands for Metal Ion Separations".

H. Past Research Support

1. Petroleum Research Fund -- Type G, American Chemical Society, three years support, 1976-79, $9,000 (award was returned at agency's request when SURP grant was received by R.T. Paine), "Low Temperature Cocondensation Chemistry" (see below).
2. Sandia University Research Program (SURP), two years support, 1974-76, $36,259, "Low Temperature Reactive Condensation Chemistry."

3. National Science Foundation-Departmental Instrumentation Grant -- Department Grant, organized by R.T. Paine, 1976, $35,000.
4. Los Alamos Scientific Laboratory, 1976-present, $30,000, Equipment Loan for Cocondensation Chemistry.
5. Los Alamos Scientific Laboratory, one year, 1976, $5,720, "Luminescence Spectra of Uranium Hexafluoride and Borohydride," joint with W.F. Coleman of Chemistry Dept., UNM.
6. Research Corporation, 1977, $6,000, "The Synthesis and Photospectroscopy of Actinide Compounds."
7. Kirtland Weapons Laboratory, 5/77-12/77, $1,500, "The Synthesis of Xenon Fluorides."
8. Los Alamos Scientific Laboratory, 1/78-12/78, $10,023, "Synthesis, Spectroscopy and Photochemistry of $U(BH_4)_4$."
9. Department of Energy-Sandia Laboratories, 9/77-9/79, $59,811, "Chemistry Related to the Carlsbad Waste Isolation Pilot Plant."
10. Department of Energy, 8/79-6/82, $140,718, "The Development of Surface Immobilized Ligands."
11. Sandia Laboratory, 7/81-6/82, $16,000, "Mechanisms for Semiconductor Etching."
12. American Chemical Society-Petroleum Research Fund, 8/81-8/84, $45,000. "Chemistry, Structures, and Bonding Patterns in Metallophosphenium Ion Complexes."
13. Department of Energy, 7/82-6/84, $201,000, "Development of Surface Immobilized Ligands for Actinide Separations."
14. Sandia Laboratory, 7/82-6/85, $51,000, "Mechanisms for Semiconductor Etching."
15. Sandia Laboratory, 1/85-12/87, $140,000, "Synthesis of B-N Compounds Suitable for Ceramic Precursors," joint with R.O. Schaeffer.
16. Sandia Laboratory, 7/84-6/85, $17,000, "Mechanisms for Semiconductor Etching."
17. Los Alamos National Laboratory, 10/85-9/87, $80,000, "Synthesis of Actinide Extractants."
18. North Atlantic Treaty Organization, 1/84-1/87, $4,500 travel grant. Joint with Professor H. Nöth.
19. American Chemical Society Petroleum Research Fund, 9/84-8/87, $52,500, "Organometallic Chemistry of Low Coordinate Phosphorus Ligands."
20. Department of Energy, 6/85-5/88, $228,000, "Development of Surface Immobilized Ligands for Actinide Separations."
21. National Science Foundation, 7/85-6/88, $171,000, "Synthesis and Chemistry Organometallic and Metal Cluster Complexes Containing Low Coordinate Main Group Ligands."
22. Sandia National Laboratory, 4/88-3/89, $45,000, "Synthesis of B-N Compounds Suitable for Ceramic Precursors," joint with R.O. Schaeffer.
23. Los Alamos National Laboratory, 10/88-9/89, $40,000, "Studies of Actinide Extraction Complexes."
24. Los Alamos National Laboratory, 10/89-9/90, $40,000, "Studies of Actinide Extraction Complexes."
25. Department of Energy, 6/88-5/91, $270,000, "Development of Surface Immobilized Ligands for Actinide Separations."

26. Center for Microengineered Ceramics, National Science Foundation, 7/89-6/90, $80,000, "Ceramic Materials from Polymeric Precursors and Formation of Ceramic Aerogels from Polymeric Precursors."
27. Center for Microengineered Ceramics, National Science Foundation, 7/90-8/91 - $50,000, Ceramic Materials from Polymeric Precursors.
28. Sandia National Laboratory, 4/90-3/91, $45,000, "Synthesis of Al-N Compounds Suitable for Ceramic Precursors."
29. Los Alamos National Laboratory, 10/91-9/92, $50,000, "Studies of Actinide Extraction Complexes."
30. Department of Energy, 6/91-5/94, $295,000, "Synthesis of Surface Immobilized Ligands for f-element Separations."
31. Department of Energy, 4/95-3/96, $20,000 "Upgrade of NMR Spectrometer Data System."
32. National Science Foundation, 6/95-5/98, $300,000 "Synthesis and Structure of Main Group Element Cage Assemblies."
33. NSF/CMEC, 9/97-8/98, $50,000, "Development of BN-Organic Polymer Hybrids for Thermal Management."
34. American Chemical Society, Petroleum Research Fund, 6/95-5/98, $50,000, "Construction of Main Group Element Cage Compounds."
35. Department of Energy, 10/96-9/99, $499,998, "f-Element Chelation in Highly Basic Media."
36. Department of Energy, 6/97-5/00, $328,000, "Preorganized and Immobilized Ligands for Metal Ion Separations."
37. NSF/CMEM, 4/99-3/00, $90,000, "Inorganic/Organic Polymer Composites for Thermal Management."
38. NSF/CMEM, 4/00-3/01, $110,000, "Inorganic/Organic Polymer Composites."
39. NSF/CMEM, 4/01-3/02, $100,000, "Ceramic Filled Polymer Composites."
40. INEEL 1/2-9/02, $35,000 "Development of Metal Selective Chelating Agents".
41. PGRF 1/2-12/02, $50,000 "Development of New Imidophosphoranes".
42. Department of Energy, 6/00-5/03, $415,000, "Preorganized and Immobilized Ligands for Metal Separations."
43. National Science Foundation, 10/99-9/03, $250,000, "Synthesis and Processing of Spherical Morphology Boron Nitride."
44. INEEL 12/02 – 9/03, $38,000 "Development of Nanocomposite Chelators".
45. Department of Energy, 8/1/03 – 7/30/06, $405,000, "Preorganized and Immobilized Ligands for Metal Separations."
46. National Science Foundation, 6/00-5/05, $310,000, "Ring and Cage Assemblies for Main Group Elements."
47. PGRF 1/05 – 12/05, $40,000 "Development of New Imidophosphoranes".
48. Department of Energy, 8/1/06-7/30/09, $405,000, "Preorganized and Immobilized Ligands for Metal Ion Separations".
49. Department of Energy, 3/13/06-3/12/09, $295,600, "Designs and Development of Selective Extractants for An/Ln Separations".

50. Department of Energy, 8/1/09-7/30/12, $435,000, “Preorganized and Immobilized Ligands for Metal Ion Separations”.
51. Department of Energy, 10/1/07-9/30/11, $300,000, “Advanced Aqueous Separation Systems for Actinide Partitioning”, sub-contract on multi-investigator grant administered by Washington State University.

I. Invited Seminars

1. “New Developments in Multidentate Coordination Chemistry of Fluorophosphine Ligands,” Texas Tech University, 1977.
2. “Structures and Motions in Inorganic Solids: Multinuclear NMR Studies,” Symposium on Recent Applications of Isotopes, Rocky Mountain Regional Meeting, Amer. Chem. Soc., June 17, 1976.
3. “Vibrational Spectroscopy of Metal Fluorides and Oxide Fluorides,” Symposium on Infra-red Spectroscopy as a Probe of Structure and Bonding in Transition Metal Compounds, 1976, Pacific Conference on Chemistry and Spectroscopy, Phoenix, November 7, 1976.
4. “Multifunctionality of Phosphorus Ligands,” University of Utah, December 4, 1978.
5. “Multifunctionality of Phosphorus Ligands,” Utah State University, December 5, 1978.
6. “Reactivity Patterns for Dicoordinate Phosphorus,” Univ. of Texas, Austin, March 1, 1979.
7. “Reactivity Patterns for Dicoordinate Phosphorus,” Texas Christian Univ., March 2, 1979.
8. “Multifunctional Coordination Properties of Phosphine Ligands,” University of Texas, El Paso, September 28, 1979.
9. “Photochemistry of Uranium Compounds,” Symposium on Lanthanide and Actinide Chemistry, American Chemical Society National Meeting, September 13, 1979.
10. “Formation and Properties of Metallophosphenium Ion Compounds,” University of Colorado, November 12, 1979.
11. “Formation and Properties of Metallophosphenium Ion Compounds,” Colorado State University, November 13, 1979.
12. “Formation and Properties of Metallophosphenium Ion Compounds,” University of Wyoming, November 14, 1979.
13. “Multifunctional Coordination Properties of Phosphine Ligands,” U.S. Air Force Academy, November 16, 1979.
14. “Phosphorus Ligands: From Nuclear Waste Extractions to Carbene Analogs,” Argonne National Laboratory, August 5, 1980.
15. “Formation of Metallophosphenium Ion Complexes,” Northern Arizona Univ., March 24, 1981.
16. “Structural Systematics in Metallophosphenium Ion Chemistry,” Texas Tech University, November 11, 1981.
17. “Phosphorus Ligands - Their Application to Nuclear Waste Problems,” Northern Arizona University, January 28, 1982.
18. “Coordination Properties of Phosphenium Ions,” Oklahoma State Univ., December 7, 1982.
19. “Coordination Properties of Phosphenium Ions,” Central State Univ., December 8, 1982.
20. “Coordination Properties of Phosphenium Ions,” Univ. of Oklahoma, December 9, 1982.

21. “Multifunctional Coordination Chemistry of Phosphorus Ligands,” Fort Lewis College, January 27, 1983.
22. “Phosphenium Ions - Analogues of NO, SO_2 and Carbenes,” Colorado College, February 9, 1983.
23. “Phosphenium Ions - Analogues of NO, SO_2 and Carbenes,” University of Colorado, Colorado Springs, February 10, 1983.
24. “Phosphenium Ions - Analogues of NO, SO_2 and Carbenes,” Adams State College, February 28, 1983.
25. Phosphenium Ions as Reactive Intermediates,” Inorganic Gordon Research Conference, Wolfsboro, NH, August, 1983.
26. “Coordination Properties of Low Coordinate Phosphorus Fragments,” Universität of Munich, September, 1983.
27. “Coordination Properties of Low Coordinate Phosphorus Fragments,” Universität Kaiserslautern, September, 1983.
28. “Coordination Properties of Low Coordinate Phosphorus Fragments,” Universität Bonn, September, 1983.
29. “Coordination Properties of Low Coordinate Phosphorus Fragments,” Universität Braunschweig, September, 1983.
30. “New Aspects in Low Coordinate Phosphorus Chemistry,” Univ. of Colorado, May 29, 1984.
31. “Phosphonate Extractants,” University of Utah/DOE Workshop, August 27, 1984.
32. “Phosphorus in Low Coordinate Environments,” Univ. of Nevada - Reno, October 10, 1984.
33. “Reaction Chemistry of Metallophosphenium Reagents,” Texas Tech Univ., April 24, 1985.
34. “Reactivity of Metallophosphenium Complexes,” Universität München, August 1, 1985.
35. “Reactivity of Metallophosphenium Complexes,” Technische Universität München, Garching, August 2, 1985.
36. “Reactivity of Metallophosphenium Complexes,” Universität Bielefeld, August 6, 1985.
37. “Chemistry of Low Coordinate Phosphorus Fragments,” New Mexico State University, January, 1986.
38. “Development of Molecular Routes to Solid State Materials,” Los Alamos National Laboratory, May 11, 1987.
39. “Reactivity of Transition Metal-Main Group Centers,” February, 1988.
40. “Molecular Routes to Ceramic Materials,” University of Pennsylvania, November 7, 1988.
41. “Molecular Routes to Ceramic Materials,” DuPont de Nemours Co., Experimental Station, November 8, 1988.
42. “Molecular Routes to Ceramic Materials,” Michigan State University, November 10, 1988.
43. ”Polymeric Precursors to New Ceramics,” Kansas State University, January 17, 1989.
44. ”Polymeric Precursors to New Ceramics,” Washington University, January 19, 1989.
45. “Molecular Precursors to Ceramic Materials,” Duke University, March 31, 1989.
46. “Molecular Routes to Solid State Materials,” Ford Motor Co. Research Department, Dearborn, MI, May 10, 1989.

47. “Molecular Routes to Solid State Materials,” (a) Universität München, May 19, 1989; (b) Technische Universität München, May 23, 1989; (c) Universität Stuttgart, May 22, 1989; (d) Universität Göttingen, May 25, 1989
48. “Molecular Precursors to Ceramic Materials,” Univ. of Texas, Austin, October 25, 1989.
49. “Development of Polymers for Ceramic Materials,” Univ. of Minnesota, February 22, 1990.
50. “Development of Polymers for Ceramic Materials,” Univ. of Nebraska, February 23, 1990.
51. “Molecular Precursors and Novel Processing of Boron Nitride,” Southern Methodist University, September 27, 1990.
52. “Chemical Processing of Non Oxide Ceramic Precursors,” Florida Advanced Materials Chemistry Conference, Palm Coast, February 6, 1991.
53. “Polymeric Precursors for Boron Nitride,” Joint Japan-U.S. Conference on Inorganic and Organometallic Polymers, Nagoya, Japan, March 25, 1991.
54. “Synthesis and Processing of Preceramic Polymers,” JPT Organization, Tokyo, Japan, March 28, 1991.
55. “Development of Polymers for Ceramic Materials,” Dalhousie University, April 5, 1991.
56. “Ligand Design for Actinide Separations,” Batelle Pacific NW Laboratories, July 23, 1991.
57. “Formation and Processing of Preceramic Polymers,” Univ. of Utah, October 22, 1991.
58. “Inorganic Polymers: An Entryway to Solid State Materials,” Univ. of Tennessee, November 14, 1991.
59. “Ligand Designs for Improved Separations,” Oak Ridge National Lab, November 15, 1991.
60. “Synthesis and Processing of Preceramic Polymers,” GIDL-H, Japan, March 9, 1992; Tohoku University, March 12, Shin-Etsu Chemical Co., March 13, Kyoto University, March 16, and Tonen Corp., March 17.
61. “Development of Ceramic Precursors,” University of Idaho, April 17, 1992.
62. “Ceramic Precursors for Boron Nitride,” W.R. Grace Co., May 7, 1992.
63. “Development of Ceramic Precursors,” Rhone Poulenc Co., Lyon, June 1, 1992.
64. “Synthesis of Polyborazinyl Amines and Applications in Polymer Processing,” University of Lyon, June 2, 1992.
65. “Synthesis of New Phosphinoboranes,” University of Munich, July 13, 1992.
66. “Development of Organic Extractants for f-element Separations,” Los Alamos National Laboratory, August 17, 1992.
67. “Development of Polymeric Precursors for Ceramics,” Univ. of Texas, Arlington, October 15, 1992.
68. “Synthesis and Processing of Inorganic Polymers,” Fort Lewis College, October 23, 1992.
69. “Synthesis of Preceramic Inorganic Polymers,” University of Michigan, November 9, 1992.
70. “Synthesis and Processing of Preceramic Polymers,” Univ. of Illinois, November 10, 1992.
71. “Synthesis and Processing of Preceramic Polymers,” Indiana Univ., November 12, 1992.
72. “Synthesis of f-element Chelators,” Battelle Pacific Northwest Lab., August 11, 1993.
73. “Inorganic Polymers as Precursors to Ceramics,” NM State Univ., September 16, 1993.

74. “Design and Synthesis of Actinide Chelators,” First DOE Separations Science Workshop, Seattle, October 14, 1993.
75. “Inorganic Polymer Precursors to Boron Nitride,” Advanced Ceramics, Inc., Cleveland, November 1, 1993.
76. “Inorganic Polymer Precursors to Boron Nitride,” Dow Chemical Company, Midland, November 3, 1993.
77. “Inorganic Polymers in Materials,” Western Michigan University, November 4, 1993.
78. “Inorganic Polymer Precursors to BN,” Notre Dame University, November 5, 1993.
79. “Polymeric Precursors to Non Oxide Ceramics,” NM State Univ., November 6, 1993.
80. “Development of Precursors for BN,” University of Texas at El Paso, January 28, 1994.
81. “BN in Thermal Management Applications,” French/USA Materials Workshop, San Diego, March 28, 1995.
82. “Processing Advances with Boron Nitride,” Advanced Ceramics Corp., Cleveland, October 3, 1995.
83. “Main Group Rings and Cages as Precursors to Solid State Materials,” University of Colorado - Colorado Springs, February 7, 1996.
84. “Boron-Phosphorus Cage Chemistry,” Indiana University, October 19, 1996.
85. “Expressions through Synthesis,” 1997 Bayer Lecture, University of New Hampshire, March 25, 1997.
86. “Development of New Materials via Molecules,” Texas A & M University, April 23, 1997.
87. “Synthesis and Processing of BN for Thermal Applications,” Texas Instruments, May 21, 1997.
88. “B-P Chemistry: Still Gold in Them Thar Hills,” R.W. Parry Symposium, University of Michigan, June 20, 1997.
89. E. L. King Summer Lecture Series in Inorganic Chemistry, University of Colorado, June 9-11, 1997: (a) From Molecules to Materials; (b) Pathways to Inorganic Composites; (c) Development of B-P Cage Assemblies; (d) Synthesis of New Borylphosphanes; (e) Ligand Design for Selective Metal Complexation.
90. “Synthesis of B-P Cage Molecules,” University of Karlsruke, September 24, 1997.
91. “Synthesis of B-P Cage Molecules,” University of Munich, September 28, 1997.
92. “Synthesis of B-P Cage Molecules,” Technical University – Munich, September 29, 1997.
93. “Processing of Preceramic Polymers,” Texas Instruments, October 7, 1997.
94. “Expressions through Synthesis – from Molecules to Polymers to the Solid State,” Kansas State University, December 1, 1997.
95. “Synthesis of Boron-Phosphorus Cage Systems,” University of Pennsylvania, February 24, 1998.
96. “Development of Preceramic Systems for Nonoxide Materials,” Pennsylvania State University, March 5, 1998.
97. “From Molecules to Polymers to the Solid State: An Update on the Formation of Boron Nitride,” Wiberg Lecture, Universität München, June 4, 1998.
98. “Ceramic Precursors for BN Composites,” Universität München, June 5, 1998.
99. “Polymeric Precursors for BN and Its Composites,” Kansas State University, June 11, 1998.

100. “Ligand Design for Antinide Separations,” Argonne National Laboratory, Feb. 8, 1999.
101. “From Molecules to Polymers to the Solid State,” North Dakota State University, Oct. 28, 1999.
102. “From Molecules to Polymers to the Solid State,” University of North Dakota, Oct. 29, 1999.
103. “Development of New Borylphosphanes,” Ohio State University, Jan. 20, 2000.
104. “Ligand Design for Actinide Separations,” Idaho National Energy and Environmental Laboratory, March 15, 2001.
105. “Selective Extractants for Actinide Ions” DOE-BES Program Review, Aug. 2, 2001.
106. “Frontiers in Chemistry” UNM Showcase, KUNM, Aug. 22, 2001.
107. “Aerosol Synthesis of Boron Nitride” Advanced Ceramics Corp., Cleveland, OH, Nov. 8, 2001.
108. “Design of Molecular Fishhooks”, Washington State University, Dec. 3, 2001.
109. “Recent Advances in Actinide Chelate Design”, PGRF, Aug. 15, 2002.
110. “Recent Developments in BN Chemistry”, GE/ACC, Cleveland, OH, Nov. 7, 2003.
111. “Design of Ligands for Selective Actinide Chelation”, University of Arizona, Dec. 7, 2003.
112. “Aerosol Synthesis of Ceramic Nitrides”, University of Mining and Metallurgy, Krakow Poland, Oct. 13, 2004.
113. “Aerosol Synthesis of Nitrides”, University of Calgary, Aug. 5, 2005.
114. “Boron Nitride as a Hydrogen Storage Medium”, HyTEP Conference, Santa Fe, NM, Sept. 19, 2005.
115. “Ligand Design for Actinide Recognition”, University of California, Lawrence Berkeley Laboratory, May 9, 2007.

J. Contributed and Invited Papers at Professional Meetings (1974-Present)

1.* “Structure and Motion of $B_3H_8^-$ Anions in Solids. A Borane and Proton NMR Study,” coauthors, E. Fukushima and S.B. Roeder, 178th ACS National Meeting, April 10, 1975.

2. “Matrix Photospectroscopy of Metal Hexafluorides,” coauthors R.S. McDowell and L.B Asprey, 179th ACS National Meeting, August 29, 1975.

3. “Synthesis and Characterization of Coordination Compounds of Bidentate Phosphine Ligands,” Rocky Mountain Regional ACS Meeting, June 19, 1976.

4. “Synthesis and Characterization of New Metalloborane Compounds,” coauthor R.W. Light, 172nd ACS National Meeting, August 30, 1976.

5. “Synthesis and Characterization of New Uranium Compounds,” coauthors R.W. Light and P.R. Schonberg, 172nd ACS National Meeting, September 1, 1976.

6. “The Synthesis and Spectroscopic Properties of $U(BH_4)_4$,” coauthors R.W. Light, P.R. Schonberg, M. Nelson, ACS, Rocky Mountain Regional Meeting, June, 1978.

7. “The Interaction of Transition Metal Nucleophiles and Aminophosphine Bases,” coauthor R.W. Light, ACS, Rocky Mountain Regional Meeting, June, 1978.

8. “The Interaction of Aminohalophosphines and Transition Metal Nucleophiles,” coauthor R.W. Light, ACS, Southwest Regional Meeting, December, 1978.

9. “Mobilization of Radionuclides in Geologic Media,” ACS Southwest Regional Meeting, December, 1978.

10. “Mobility of Radionuclides in Geomedia,” coauthors F.C. See and S.G. Barnhart, 178th ACS National Meeting, September, 1979.

11. “Synthesis and Characterization of New Diazadiphosphe-tidine Complexes,” coauthors J.J. Jessup, D. Byers, C.F. Campana, ACS Southwest Regional Meeting, December, 1979.

12. “Synthesis and Characterization of Cp-Al Compounds,” coauthor P.R. Schonberg, ACS Southwest Regional Meeting, December, 1979.

13.* “Synthesis and Structural Properties of Phosphenium Ion Complexes,” Biennial Inorganic Symposium, June, 1980.

14.* “Substrate Binding of Bidentate Extractants,” Actinide Workshop IV, May, 1980.

15. “Pentamethylcyclopentadienyl Complexes of Metalloid Elements,” coauthor P.R. Schonberg, ACS, Rocky Mountain Regional Meeting, June, 1980.

16. “Synthesis and Coordination Properties of Dihexyl, N,N-diethyl-carbamoylmethylene Phosphonates,” coauthor S.M. Bowen, ACS Rocky Mountain Regional Meeting, June, 1980.

17. “Structure and Bonding in Metallophosphenium Ion Complexes,” ACS Rocky Mountain Regional Meeting, coauthor L.D. Hutchins, June, 1980.

18. “Synthesis and Properties of CMP-metal Complexes,” ACS 2nd Chemical Congress of the North American Continents, S.M. Bowen, August, 1980.

19. “Pentamethylcyclopentadiene Complexes of the Metalloid Elements,” ACS 2nd Chemical Congress of the North American Continent, coauthor, P.R. Schonberg, August, 1980.

20. “Structure and Bonding in Phosphenium Ion-Metal Complexes,” ACS 2nd Chemical Congress of the North American Continent, coauthors L.D. Hutchins and E.N. Duesler, August, 1980.

21. “Synthesis and Coordination Properties of Carbamoylmethylene Phosphonate Ligands,” coauthors S.M. Bowen, E.N. Duesler, International Conference on Phosphorus Chemistry, June, 1981.

22. “Synthesis and Coordination Properties of Carbamoylmethylene Phosphonate Ligands,” Actinide Workshop V, June, 1981.

23. “Synthesis and Structure of a Metallophosphinite Uranium (IV) Complex,” coauthors D.C. Moody and E.N. Duesler 183rd National ACS Meeting, March, 1982.

24.* “Coordination Chemistry of Phosphenium Ions: Parallels with Small Molecule Ligands,” 1st National Science Foundation Workshop on Non-metal Chemistry, June, 1982.

25. “Synthesis and Structural Properties of a Metallophosphenium Ion Complex $CH_3NCH_2CH_2N(CH_3)PFeCp^*(CO)_2$,” coauthors L.D. Hutchins and E.N. Duesler, 184th ACS National Meeting, September, 1982.

26. “Coordination Properties of Carbamoylmethylene Phosphonates,” coauthors S.M. Bowen, L.J. Caudle, 184th ACS National Meeting, September, 1982.

27. "Phosphenium Ions: Coordination Parallels with Other Small Molecule Ligands," R.T. Paine, L.D. Hutchins and E.N. Duesler, 185th ACS National Meeting, March, 1983.
28. "Metallophosphenium Ion Complexes Containing Diphosphetidines," D.A. DuBois, R.W. Light, E.N. Duesler and R.T. Paine, 186th ACS National Meeting, August, 1983.
29. "Metallophosphenium Ion Complexes Containing Diazadiphosphetidines and Reductive Coupling of Diazadiphosphetidines," D.A. DuBois, E.N. Duesler and R.T. Paine, 187th ACS National Meeting, April, 1984.
30. "Synthesis and Crystal and Molecular Structure of A [diisopropyl(N,N-diethylcarba-moyl)methylenephos-phonate]molybdenum Chloride Complex," S.M. Bowen, E.N. Duesler and R.T. Paine, 7th Rocky Mountain Regional ACS Meeting, June, 1984.
31. "Metallophosphenium Ion Complexes Containing An Acyclic Silylaminophosphane Fragment," W.F. McNamara, E.N. Duesler and R.T. Paine, 7th Rocky Mountain Regional ACS Meeting, June, 1984.
32. "Metallophosphenium Ion Complexes Containing Diazadiphosphetidine Fragments," D.A. DuBois, E.N. Duesler and R.T. Paine, 7th Rocky Mountain Regional Meeting, June, 1984.
33. "Synthesis of Phosphenium Ion Complexes From $PhNCH_2CH_2N(Ph)PCl$," G.L. Wood and R.T. Paine, 7th Rocky Mountain Regional Meeting, June, 1984.
34. "Synthesis, Characterization and Coordination Chemistry of New CMP Ligands," D.J. McCabe and R.T. Paine, 7th Rocky Mountain Regional Meeting, June 1984.
35. "Matrix Isolation Studies of Plasma Species Trapped on Silicon Wafers," F.C. See and R.T. Paine, 7th Rocky Mountain Regional Meeting, June, 1984.
36.* "Advances in Low Coordinate Phosphorus Chemistry," R.T. Paine, ACS/PAS Pacific Conference, October, 1984.
37. "Coordination Chemistry of Cyclodiphosph(III)azanes," D.A. DuBois, E.N. Duesler and R.T. Paine, 40th Southwest Regional ACS Meeting, December, 1984.
38.* "Coordination and Extraction Chemistry of Phosphonate Ligands," R.T. Paine and D.J. McCabe, 189th ACS National Meeting, April, 1985.
39. "Main Group Ring and Cage Compounds: Some New Avenues," R.T. Paine, 40th Northwest Regional ACS Meeting, June, 1985.
40. "Coordination Chemistry of Trifunctional Phosphonate Ligands," R.T. Paine and D.J. McCabe, 40th Northwest Regional ACS Meeting, June, 1985.
41. "Chemistry of Metallophosphane Fragments," W.F. McNamara, E.N. Duesler, J.V. Ortiz and R.T. Paine, 190th National ACS Meeting, September 9, 1985.
42.* "Inorganic Macromolecules Containing BN Units," C.K. Narula, R.T. Paine and R.O. Schaeffer, 190th National ACS Meeting, September 9, 1985.
43.* "Macromolecular Precursors to BN Materials," R.T. Paine, R.O. Schaeffer and C.K. Narula, Materials Research Society Spring Meeting, April, 1986.
44.* "Synthesis and Reactivity of Metallophosphanes," R.T. Paine, W.F. McNamara, J. Janik, International Conference on Phosphorus Chemistry, Bonn, West Germany, September 2, 1986.

45.* "Synthesis and Coordination Properties of Multifunctional Carbamoylmethylphosphonates," R.T. Paine, D.J. McCabe, S.L. Blaha and E.N. Duesler, International Conference on Phosphorus Chemistry, Bonn, West Germany, September 5, 1986.

46.* "Synthesis and Reactivity of Metallophosphanes," R.T. Paine, W.F. McNamara and E.N. Duesler, 192nd ACS National Meeting, September, 1986.

47. "Formation, Characterization and Chemistry of Silylphosphane Boranes," G.L. Wood, C.K. Narula, E.N. Duesler and R.T. Paine, 192nd ACS National Meeting, September, 1986.

48. "Chemical Studies of Novel Phosphonate Extractants," L.J. Caudle, K.W. Thomas, G.S. Conary, S.L. Blaha and R.T. Paine, 192nd ACS National Meeting, September, 1986.

49. "Nonoxide Ceramics: Precursors to B-N Materials," C.K. Narula, R.T. Paine and R.O. Schaeffer, 192nd ACS National Meeting, September, 1986.

50. "Synthesis of Boron Nitride from Polyborazinyl Amines," C.K. Narula, R.T. Paine and R.O. Schaeffer, 193rd ACS National Meeting, April, 1987.

51. "Reactions of an Organotungsten Phosphenium Complex," H.U. Reisacher and R.T. Paine, 193rd ACS National Meeting, April, 1987.

52.* "Precursors to Non-Oxide Macromolecules and Ceramics," C.K. Narula, J.F. Janik, R.T. Paine and R.O. Schaeffer, 193rd ACS National Meeting, April, 1987.

53.* "Synthesis of AlN and AlN/SiC from Polymeric Molecular Precursors," Materials Research Society Meeting, Reno, April 7, 1988.

54. "Precursors to Boron Containing Solid State Materials," Boron-USA Meeting, Dallas, April 10, 1988.

55.* Routes to Aluminum Nitride and Aluminum Phosphide," ONR Workshop on Group 3-5 Chemistry and Semiconductors, Grand Island, NY, June 3, 1988.

56.* "Synthesis and Structural Properties of Borophosphane and Aluminophosphane Complexes," 3rd Chemical Congress of North America, Toronto, June 6, 1988.

57. "Synthesis of AlN and AlN/SiC from Polymeric Molecular Precursors," Materials Research Society Meeting, Reno, April 7, 1988.

58.* "Formation of BN Ceramics from Molecular Precursors," 196th American Chemical Society Meeting, Los Angeles, September 28, 1988.

59. "Nitride Ceramic Coatings from Molecular Precursors," 4th International Conference on Ultrastructure Processing, Tucson, February 21, 1989.

60.* "Synthesis of Polyfunctional Organophosphonate Extractants," R.T. Paine, G.S. Conary, A.A. Russell, D.J. McCabe, E.N. Duesler, S. Karthikeyan, R.R. Ryan and D.J. Cromer, 197th American Chem. Society Meeting, Dallas, April 12, 1989.

61. "Polymeric Materials for Metal Ion Separations," R.T. Paine, S.L. Blaha, A.A. Russell and G.S. Conary, 197th American Chemical Society Meeting, Dallas, April 10, 1989.

62. "Molecular Precursors to Boron Nitride," International Ceramic Science and Technology Congress, November 1, 1989.

63. "Chemical Paths to Ceramics," R.R. Rye, T.T. Borek, D.A. Lindquist and R.T. Paine, Amer. Ceram. Soc./Mat. Res. Soc. Meeting, Albuquerque, October 6, 1989.

64. “Trimethyl Aluminum and Ammonia on Silica: Nucleation of an AlN Precursor on a Surface,” M.E. Bartram, J.W. Rogers, T.A. Michalske and R.T. Paine, Amer. Ceram. Soc./Mat. Res. Soc. Meeting, Albuquerque, October 6, 1989.

65. “Linear Borazene Polymer Precursors for Boron Nitride Coatings,” T.T. Borek, C.K. Narula, A.K. Datye, R.O. Schaeffer and R.T. Paine, Amer. Ceram. Soc./Mat. Res. Soc. Meeting, Albuquerque, October 6, 1989.

66. “Boron Nitride Aerogels and Composite Aerogels from Borazene Based Polymers,” D.A. Lindquist, D.M. Smith, S.J. Kramer, G.L. Johnston, T.T. Borek, R.O. Schaeffer and R.T. Paine, Amer. Ceram. Soc./Mat. Res. Soc. Meeting, Albuquerque, October 6, 1989.

67. “Functionalized Zirconium Phosphonates as Novel Chromatographic Materials,” A.A. Russell and R.T. Paine, Amer. Ceram. Soc./Mat. Res. Soc. Meeting, Albuquerque, October 6, 1989.

68. “Stability of Boron Nitride Coatings on Ceramic Substrates,” A.K. Datye, T.T. Borek and R.T. Paine, Mat. Res. Soc. Fall Meeting, November 24, 1989.

69. “Investigations of New Multidentate Actinide Complexants,” G.D. Jarvinen, B.F. Smith, P.H. Smith, R.R. Ryan, W.H. Smith, R.T. Paine and D.E. Ensor, Actinide Workshop, Idaho Falls, May 15, 1989.

70. “Synthesis and Coordination Properties of New Bifunctional and Trifunctional Extractants with Actinides and Lanthanides,” G.D. Jarvinen, B.F. Smith, M.M. Jones, P.H. Smith, R.R. Ryan, R.T. Paine and A.A. Russell, Amer. Chem. Soc. Pacific Basin Meeting, December 20, 1989.

71. “Synthesis and Structures of New Borophosphines,” D. Dou, M. Westerhausen, E.N. Duesler and R.T. Paine, 45th Northwest/10th Rocky Mountain American Chemical Society Regional Meeting, Salt Lake City, June 13, 1990.

72. “University-Federal Laboratory Transitions,” R.T. Paine, 45th Northwest/10th Rocky Mountain American Chemical Society Regional Meeting, Salt Lake City, June 14, 1990.

73.* “Main Group Building Blocks to Solid State Materials,” Symposium on Inorganometallic Chemistry, 200th American Chemical Society National Meeting, Washington, D.C., September 29, 1990.

74. “Boron Nitride and Composite Aerogels, Aerosol Powders and Fibers Processed From Polymeric Precursors,” D.A. Lindquist, D.M. Smith, A.K. Datye, T.T. Kodas and R.T. Paine, Materials Research Society Meeting, Boston, November 29, 1990.

75. “Oxidation of Boron Nitride Ceramics,” T.T. Borek, D.M. Smith, R.T. Paine, Materials Research Society Meeting, Boston, November 29, 1990.

76. “Synthesis of Novel Organic Compounds for the Extraction of F-Block Elements,” B. Rapko, E.N. Duesler and R.T. Paine, 201st American Chemical Society Meeting, Atlanta, April 16, 1991.

77. “Polymer Development for Ceramics,” R.T. Paine, 202nd American Chemical Society National Meeting, New York, August 30, 1991.

78. “Preceramic Polymer Derived BN Aerosols,” National Amer. Assoc. Aerosol Research, Traverse City, October 20, 1991.

79.* “Synthesis of Ligands for Actinide Separations,” R.T. Paine, Symposium on Advanced Separations, 203rd American Chemical Society National Meeting, San Francisco, March 7, 1992.

80. “Reactions of P=N Double Bond,” G. Paramanathan and R.T. Paine, Rocky Mountain Regional ACS Meeting, Albuquerque, June 11, 1992.

81. “Synthesis and Structures of Borylphosphanes,” D. Dou, H. Nöth and R.T. Paine, International Conference on Phosphorus Chemistry, Toulouse, France, July 8, 1992.

82.* “Synthesis and Processing of Borazinylamine Polymers,” International Ceramic Science and Technology Congress, San Francisco, November 3, 1992.

83.* “Phosphonpyridine N,P-oxides as Chelators for Selected Metal Ions,” R.T. Paine, B. Rapko, X. Gan, J. Fox, P.H. Smith and R.T. Ryan, 205th American Chemical Society Meeting, Denver, March 31, 1993.

84.* “Synthesis and Processing of BN Preceramic Polymers,” R.T. Paine, M. Fan, A. Hanprasopwattana and A.K. Datye, 205th American Chemical Society Meeting, Denver, March 31, 1993.

85. “Processing of Microporous BN,” R.T. Paine, M. Fan, D.M. Smith, Porous Expo-93, Albuquerque, May 4, 1993.

86. “Synthesis and Processing of Boron Nitride,” R.T. Paine, Inorganic Gordon Conference, Wolfsburo, July 29, 1993 (poster).

87. “Synthesis of New Boron Phosphorus Cages,” T. Chen, R.T. Paine, E.N. Duesler, B. Kaufmann, H. Nöth, 206th American Chemical Society Meeting, Chicago, August 22, 1993.

88. “Phosphonopyridine N,P-oxides and Their Coordination Chemistry,” R.T. Paine, J. Fox, E. Bond, P.H. Smith, Actinides-93, Santa Fe, September 21, 1993.

89.* “Synthesis of New Boron-Phosphorus Rings and Cages,” R.T. Paine, Southwest Regional American Chemical Society Meeting, Austin, October 27, 1993.

90.* “Design of Ligands for F-Element Separations,” R.T. Paine, 207th American Chemical Society Meeting, San Diego, March 16, 1994.

91.* “Development of Polymeric Precursors for BN Processing,” R.T. Paine, Joint U.S.-Japan Conference on Inorganic and Organometallic Polymers, Asilomar, May 18, 1994.

92.* “Group 13-15 Chemistry -- From Molecules to Rings, Cages and Polymers,” R.T. Paine, Inorganic Gordon Research Conference, Brewster Academy, August 5, 1994.

93.* “Synthesis of Boron-Phosphorus Cage Systems,” R.T. Paine, IRIS-VI, Banff, August 9, 1994.

94.* “Development of Ion Exchange Chelators for Actinide Separations,” R.T. Paine, American Chemical Society, Anaheim, April 2, 1995.

95.* “Utilization of Preceramic Polymers for Formation and Processing of BN,” R.T. Paine, American Chemical Society, Anaheim, April 5, 1995.

96.* “Development of New Separations Agents,” R.T. Paine, DOE/BES Separations Conference, Santa Fe, June 7, 1995.

97. “Synthesis of New Borylphosphanes,” R.T. Paine, Inorganic Gordon Conference, Wolfesboro, July, 24, 1995.

98. “Phosphonopyridine N-oxides as Separations Agents,” R.T. Paine, Inorganic Gordon

Conference, Wolfesboro, July 24, 1995.

99. "The Solvent Extraction of Am(III) by 2,6-bis(diphenylphosphino) methylpyridine N,P,P' Freoxide," E. Bond, J. Fitzpatrick, U. Englehardt, P. Deere, B. Rapko, R.T. Paine, 213th American Chemical Society Meeting, San Francisco, April 15, 1997.

100. "Synthesis and Structure of Uranyl Compounds Containing Sterically Demanding Alkoxide Ligands," M.P. Wilkerson, C.J. Burns, R.T. Paine and B.L. Scott, 213th American Chemical Society Meeting, San Francisco, April 17, 1997.

101. "New BP Cage Species," R. T. Paine, T. Chen, E. N. Duesler and H. Nöth, IRIS-97 Conference, Loughborough, England, August 11, 1997.

102. "Coordination and Extraction Chemistry of Phosphonopyridine N,P Oxides," E. Bond, J.R. FitzPatrick and R. T. Paine, An-97 Conference, Baden-Baden, Germany, September 23, 1997.

103.* "Ceramic Precursors for boron Nitride Composites," High Temperature Materials Workshop, Boulder, CO, May 25-28, 1998.

104. "f-Element Chelation in Highly Basic Media," DOE-EMSP Workshop, Chicago, July 27-30, 1998.

105. "Structural Preferences of Uranyl Compounds Containing Sterically Demanding Alkoxide Ligands," M.P. Wilkerson, C.J. Burns, R.T. Paine, 216th American Chemical Society Meeting, August 28, 1998.

106. "Systematic Syntheses of New Main Group Element Rings," T. Chen, E.N. Duesler, R.T. Paine and H. Nöth, 215th American Chemical Society Meeting, April 2, 1998.

107. "Solid State Structures and Solution Speciation of Uranyl Compounds Containing Sterically Demanding Ligands," M.P. Wilkerson, C.J. Burns, H.J. Dewey, D.E. Morris, R.T. Paine and B.L. Scott, 217th American Chemical Society Meeting, March 21, 1999.

108. "F-Element Solvent Extraction Properties of Phosphono pyridyl N,P-Oxides," E.M. Bond, X. Gan and R.T. Paine, American Chemical Society, 55th Southwest Regional Meeting, October 21, 1999.

109.* "Formation and Processing of Ceramic Nitride Spherical Particles," R.T. Paine, E.A. Pruss, G.L. Wood, K. Butter-Warrensford, R.F. Hill and W.J. Kroenke, American Chemical Society, 55th Southwest Regional Meeting, October 21, 1999.

110. "Phosphonopyridine N-Oxides as f-Element Chelators," R.T. Paine, X.M. Gan, S. Parveen and E.M. Bond, American Chemical Society, March 26, 2000.

111. "Development of Ceramic Fillers for Polymer Composites," R.T. Paine, E.A. Pruss, W. Kroenke, R.F. Hill, G.L. Wood, C. Sierkowski, L.J. Wood, C. Chappelle and D. Dreissig, American Chemical Society, March 26, 2000.

112. "Boron Nitride Fillers for Organic Composites," R.T. Paine, Inorganic Gordon Conference, July 25, 2000.

113.* "Synthesis of Ceramic Fillers for Composites," R.T. Paine, International Conference on Composite Interfaces (ICCI-VIII), October 12, 2000.

114. Aerosol Synthesis of BN," R.T. Paine, Boron-USA Conference, June 8, 2000.

115. "Preorganized and Immobilized Ligands for Actinide Separations," DOE – Heavy Element Conference, Argonne National Laboratories, R.T. Paine, November 20, 2000.

116. "Synthesis of New Phosphino pyridine ligands for f-Element Chelation" S. Parveen, E. Duesler and R. T. Paine, American Chemical Society Meeting, Aug. 2001.

117. "Is There Anything New in Acid-Base Chemistry" T. Habereder, R. T. Paine, H. Nöth and D. Dreissig, Boron Americas Conf., Jan. 3, 2002.

118. "Simple and Complex: The Reactions of $PhBCl_2$ with $P(SiMe_3)_3$" T. Habereder, J. F. Janik, R. T. Paine and H. Nöth, Boron Americas Conf. Jan. 3, 2002.

119. "Recent Advances in the Aerosol Synthesis of Boron Nitride" G. L. Wood, J. F. Janik, R. T. Paine and D. Dreissig, Boron Americas Conf. Jan. 3, 2002.

120. "Aerosol Synthesis of Inorganometallic Nitrides" R. T. Paine, G. L. Wood, J. F. Janik, American Chemical Society Meeting, Aug. 2002.

121.* "Routes to Main Group Nitrides: Crossing the Valley of Death" R. T. Paine Southwest Regional American Chemical Society Meeting, Nov. 4, 2002.

122. "Carbothermally-assisted Aerosol Synthesis of Semiconducting Materials in the System GaN/Mn" J.F. Janik, M. Drygas, C. Czosnek, M. Kaminska, M. Palczewska and R.T. Paine, 12th International Symposium on Intercalation Compounds – ISIC 12, June 1-5, 2003, Pozna, Poland.

123. "Magnetic and Optical Properties of GaMnN Nanocrystals Obtained by Vapor-Assisted Aerosol Synthesis" J. Gosk, M. Zajac, M. Palczewska, M. Kaminska, A. Twardowski, M. Drygas, J.F. Janik and R.T. Paine, XXXII International School on Physics of Semiconducting Compounds – Jaszowiec 2003, May 31 – June 6, 2003, Jaszowiec, Poland.

124.* "Utilization of Borates as Solid State Materials Precursors" R.T. Paine, 227th Amer. Chem. Soc. Mtg., Anaheim, Mar. 28, 2004.

125.* "Adventures in Main Group Compound Reactivity" R.T. Paine, 227th Amer. Chem. Soc. Mtg., Anaheim, Mar. 30. 2004.

126. "Synthesis of Boron Nitride from Guanidinium Nonaborate" G.L. Wood, J.F. Janik, R.T. Paine, D.M. Schubert and M.Z. Visi, Amer. Chem. Soc. Mtg., Anaheim, Mar. 31, 2004.

127. "Borates as Solid State Materials Precursors" G.L. Wood, J.F. Janik, R.T. Paine, D.M. Schubert and M.Z. Visi, Boron in the Americas IX, May 19, 2004.

128. "Magnetic and Optical Properties of GaMnN Nanocrystals Obtained by Imide Route Method" J. Gosk, M. Drygas, M. Palczewska, M. Kaminska, A. Twardowski, J.F. Janik and R.T. Paine, XXXIII International School on Physics of Semiconducting Compounds – Jaszowiec 2004, May 28 – June 4, 2004, Jaszowiec, Poland.

129. "Magnetic and Optical Properties of GaMnN Nanocrystals Obtained by Vapor-Assisted Aerosol Synthesis and Imide Route Method" J. Gosk, M. Drygas, M. Palczewska, M. Kaminska, A. Twardowski, J.F. Janik and R.T. Paine, The 3rd International Conference on Physics and Applications of Spin-Related Phenomena in Semiconductors, July 21-23, 2004, Santa Barbara.

130. "Aerosol-Assisted Vapor Phase Synthesis of Powder Composites in the Target System GaN/TiN for Potential Electronic Applications" M. Drygas, C. Czosnek, R.T. Paine and J.F. Janik, Nano and Giga Challenges in Microelectronics – Krakow 2004, September 13-17, 2004, Krakow, Poland.

131. “Tuning Aerosol – Assisted Vapor Phase Processing Toward Bulk Low Oxygen GaN Powders”, M. Drygas, S. Stelmakh, E. Grzanka, B. Palosy, R. T. Paine and J. F. Janik, Trends in Nanotechnology Conf. Oviedo, Spain 8/29-9/2, 2005.

133.* “Synthesis of Ceramic Materials” R. T. Paine, Boron in the Americas Meeting, San Juan Puerto Rico, Aug. 5, 2006.

134.* “Aerosol Methods for BN Synthesis” R. T. Paine, 231st American Chemical Society Meeting, Chicago, April 25, 2007.

135.* “Preorganized and Immobilized Ligands for Metal Ion Separations”, R. T. Paine, DOE Program Review, Annapolis MD, April 25, 2007.

136.* “Memories of R. W. Parry”, R. T. Paine, Inorganic Gordon Conference, Newport, R. I., July 19, 2007.

Student Research Direction

A. Postdoctoral Associates

1. C. Narula, 1985-1988
2. S. Karthikeyan, 1985-1988
3. U. Reisacher, 1986-1987
4. M. Westerhausen, 1987-1988
5. B. Rapko, 1989-1992
6. D. Srivastava, 1989-1990
7. J. Janik, 1990-1992
8. Xinmin Gan, 1990-1992, 1997-2001
9. Lan Miao, 1993-1994
10. Paul Fazen, 1995
11. Steven Jasper, 1995
12. Tuqiang Chen, 1997
13. Gene Pruss, 1997-1999
14. Evelyn Bond, 1998-1999
15. Wolfgang Koestler, 1998-1999
16. Tassilo Habereder, 2000-2001
17. Qing-min Cheng, 2000-2001
18. Iris Binyamin 2002-2004
19. Sung-Jun Kim 2002-2003
20. Jean-Michel Camus 2002-2004
21. Yongjun Tang, 2006
22. Sylvie Pailloux, 2005 – 2010
23. Manab Chakravarty 2009-2010
24. Sabrina Ouizem, 2010-2012
25. Daniel Rosario-Amorin, 2010-2012

B. Ph.D. Students (Graduation Date)

1. Ronald W. Light (1979)
2. Peter R. Schonberg (1981)
3. Larry D. Hutchins (1982)
4. Scott M. Bowen (1983)
5. Linda J. Caudle (1984)
6. Donn DuBois (1985)
7. Daniel J. McCabe (1987)
8. Sharon Blaha (1987)
9. Frere MacNamara (1987)
10. Gary L. Wood (1987)
11. Jerzy Janik (1987)
12. Greg Conary (1988)
13. Arthur Russell (1990)
14. David Lindquist (1990)
15. Danan Dou (1992)
16. Maomin Fan (1994)
17. Tuquiang Chen (1995)
18. Aree Hanprasopwattana (1998)
19. Evelyn Bond (1998)
20. Marianne Wilkerson (2000)
21. Dirk Dreissig (2001)
22. Sahrah Parveen (2003)
23. Cornel Edicome (2009)

C. M.S. Students

1. Ronald W. Light (1976)
2. Peter R. Schonberg (1978)
3. Marcia Kite (1980)

9. Daniel J. McCabe (1984)
10. Gary L. Wood (1984)
11. Sharon Blaha (1984)

4. Larry D. Hutchins (1981)
5. Scott M. Bowen (1981)
6. Linda J. Caudle (1981)
7. Betty J. Nusser (1981)
8. Frank C. See (1981)
12. Ted Borek (1990)
13. Guru Paramanathan (1991)
14. Bryan Meyers (1998)
15. Yufeng Wen (1998)
16. Kathleen Banjac (1999)
17. Kara Butler (2000)

D. Undergraduates

1. Ronald Voorhees
2. Joe A. Mims
3. Yolanda D. Jones
4. Joel K. Swadesh
5. James S. Horwitz
6. Bruce Cottrell
7. Mark Nelson
8. Karl S. Ricker
9. Donald E. Maier
10. John T. Shay
11. Kenneth M. Maier
12. Jenny Hunt
13. David L. Byers
14. Judith Stanton
15. Eric Gulliver
16. Ron Meline
17. Steven Kramer
18. Leann Rayfuss
19. Deanella Frutos
20. Brenda Nieslanik
21. Paul Deere
22. Kyle Findly
23. Jeff Jackson
24. Jesse Stanchfield
25. Tiffany Tinsley
26. Nathan Kersten
27. Colin Swierkowski
28. Nathan Donart
29. Sam Coulter
30. Elizabeth Bright

E. Sabbatical Leave Visitors

1. G. Lynn Wood, Valdosta State University
2. J. Janik, University of Mining and Technology, Krakow, Poland
3. Wayne Smith, Colby College

Professional Service

A. Departmental Committees

1. Assistant Department Chairman (six years)
2. Undergraduate Recruitment and Freshman Committee (six years)
3. Seminar Committee (four years)
4. Library Committee (two years)
5. Salary Committee (three years)
6. Graduate Curriculum and Studies Committee (four years)
7. Undergraduate Career Advisement Committee (Chrm., two years)
8. Building and Space Committee (three years, Chrm., one year)
9. New Equipment Planning Committee (Chrm., six years)
10. Executive Committee (eight years)
11. Graduate Selection Committee (seven years)
12. Graduate Selection Committee, Chair (seven years)

B. University Committees

1. Member, Research Policy Committee (1976-1978)

2. A-21 Advisement Committee (1980-1981)
3. SURP-BRSG Review Committee (1979-1982)
4. Arts and Sciences Tenure and Promotion Advisory Subcommittee (Natural Sciences and Mathematics) (1984-1985) Chairman 1985

C. Temporary Committees

1. Committee on Studies: Chairman for twenty-three Ph.D. candidates, committee member for numerous others.

Curriculum Vitae – Yang Qin

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Department of Chemistry & Chemical Biology
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Education Background

09/1996-07/2000	Department of chemistry, Peking University, P. R. China. Degree achieved: B.Sc. in Chemistry. Advisor: Prof. Xinru Jia.
07/2000-06/2001	Department of chemistry, Beijing University, P. R. China. Research assistant. Advisor: Prof. Xinru Jia.
08/2001-10/2006	Department of Chemistry, Rutgers University-Newark, Newark, NJ. Degree achieved: Ph.D. in Chemistry. Advisor: Prof. Frieder Jäkle. Thesis: "Synthesis, Characterization and Complexation of Well-Defined Organoboron Polymers with Different Architectures."
10/2006-08/2009	Department of Chemistry, University of Minnesota, Minneapolis, MN. Postdoctoral research fellow. Advisor: Prof. Marc A. Hillmyer.
08/2009-08/2010	Center for Functional Nanomaterials, Brookhaven National Laboratory, NY. Research Associate. Advisor: Prof. Robert B. Grubbs.
08/2010-present	Assistant Professor, Department of Chemistry & Chemical Biology, University of New Mexico

Publications

1. "Self-Assembly of a Polythiophene Block-Copolymer and a Fullerene Derivative via Complementary Hydrogen Bonding." *In preparation*.
2. "Photo-Cross-Linkable Azide-Functionalized Polythiophene for Thermally Stable Bulk Heterojunction Solar Cells." Nam, C.-Y.; Qin, Y.; Park, Y. S.; Hlaing, H.; Lu, X.; Ocko, B. M.; Black, C. T.; Grubbs, R. B. *Macromolecules*, 2012, *45*, 2338-2347.
3. "Self-Assembly of Borane End-Functionalized Polystyrene Through Tris(1-pyrazolyl)borate (Tp) Iron(II) Linkages." Qin, Y.; Shipman, P. O.; Jäkle, F. *Macromol. Rapid Commun.* 2012, *33,* 562-567.
4. "High Open-Circuit Voltage Photovoltaic Cells with a Low Bandgap Copolymer of Isothianaphthene, Thiophene and Benzothiadiazole Units." Kim, J. Y.; Qin, Y.; Stevens, D. M.; Kalihari, V.; Hillmyer, M. A.; Frisbie, C. D. *J. Phys. Chem. C* 2009, *113*, 21928-21936.
5. "Synthesis and pH-dependent Micellization of the Amphiphilic Block Copolymer Poly(styreneboronic acid)-block-Polystyrene in Water." Cui, C.; Bonder, E. M.; Qin, Y.; Jäkle, F. *J. Polym. Sci. A: Polym. Chem*. 2010, *48*, 2438-2445.
6. "Poly(3-hexyl-2,5-thienylene vinylene) by ADMET Polymerization of a Di-propenyl Monomer" Qin, Y.; Hillmyer, M. A. *Macromolecules* 2009, *42*, 6429-6432.
7. "Low Band Gap Poly(thienylene vinylene)/Fullerene Bulk Heterojunction Photovoltaic Cells." Kim, J. Y.; Qin, Y.; Stevens, D. M.; Kalihari, V.; Hillmyer, M. A.; Frisbie, C. D. *J. Phys. Chem. C* 2009, *113*, 10790-10797.
8. "Enhancement of the Morphology and Open Circuit Voltage in Bilayer Polymer/Fullerene Solar Cells." Stevens, D. M.; Qin, Y.; Hillmyer, M. A.; Frisbie, C. D. *J. Phys. Chem. C* 2009, *113*, 11408-11415.

9. “Novel Distannylated Isothianaphthene as a Versatile Building Block for Low Band-Gap Polymers.” Qin, Y.; Kim, J. Y.; Frisbie, C. D.; Hillmyer, M. A. *Macromolecules*, 2008, *41*, 5563-5570.
10. “Tris(1-pyrazolyl)borate (Scorpionate) Functionalized Polymers as Scaffolds for Metallopolymers.” Qin, Y.; Cui, C.; Jäkle, F. *Macromolecules,* 2008, *41*, 2972-2974.
11. “Synthesis of Organoboron Quinolate Polymers with Tunable Luminescence Properties.” Qin, Y.; Kiburu, I.; Shah, S.; Jäkle, F. *Macromolecules* 2007, *40*, 1413-1420.
12. “Formation of Lewis Acid-Lewis Base Complexes with Well-Defined Organoboron Polymers.” Qin, Y.; Jäkle, F. *J. Inorg. Organomet. Polym. Mater.* 2007, *17*, 149-157.
13. “Silylated Initiators for the Efficient Preparation of Borane End-Functionalized Polymers.” Qin, Y.; Jäkle, F. *Macromolecules* 2006, *39*, 9041-9048.
14. “Luminescence Tuning of Organoboron Quinolates through Substituent Variation at the 5-Position of the Quinolate Moiety.” Qin, Y.; Kiburu, I.; Shah, S.; Jäkle, F. *Org. Lett.* 2006*, 8,* 5227-5230.
15. “Boron-Bridged Poly(ferrocenylene)s as Promising Materials for Nanoscale Molecular Wires.” Heilmann, J.; Qin, Y.; Jäkle, F.; Lerner, H.; Wagner, M. *Inorg. Chim. Acta* 2006, *359,* 4802-4806.
16. “A Synthetic Route to Borylene-Bridged Poly(ferrocenylene)s.” Heilmann, J.; Scheibitz, M.; Qin, Y.; Sundararaman, A.; Jäkle, F. Kretz, T.; Bolte, M.; Lerner, H.; Holthausen, M.; and Wagner, M. *Angew. Chem. Inter. Ed.* 2006*, 45,* 920-925.
17. “Preparation of Organoboron Block Copolymers via ATRP of Silicon and Boron Functionalized Monomers.” Qin, Y.; Sukul, V.; Pagakos, D.; Cui, C; Jäkle, F. *Macromolecules* 2005*, 38,* 8987-8990.
18. “A New Route to Organoboron Polymers via Highly Selective Polymer Modification Reactions.” Qin, Y.; Cheng, G.; Achara, O.; Parab, K.; Jäkle, F. *Macromolecules* 2004*, 37,* 7123-7131.
19. “Luminescent Organoboron Quinolate Polymers.” Qin, Y.; Pagba, C.; Piotrowiak, P.; Jäkle, F. *J. Am. Chem. Soc.* 2004, *126,* 7015-7018.
20. “Lewis Acidic Organoboron Polymers.” Qin, Y.; Cheng, G.; Parab, K.; Sundararaman, A.; Jäkle, F. *Macromol. Symp.* 2003, *196,* 337-345.
21. “Well-Defined Boron-Containing Polymeric Lewis Acids.” Qin, Y.; Cheng, G.; Sundararaman, A.; Jäkle, F. *J. Am. Chem. Soc.* 2002*, 124,* 12672-12673.
22. “Fabrication of Covalently Attached Ultrathin Films Based on Dendrimers via H-Bonding Attraction and Subsequent UV Irradiation.” Zhong, H.; Wang, J.; Jia, X.; Li, Y.; Qin, Y.; Chen, J.; Zhao, X.; Cao, W.; Li, M.; Wei, Y. *Macromol. Rapid Commun.* 2001*, 22,* 583-586.
23. “Conjugation of Poly(amidoamine) Dendrimers (PAMAM) and Cytochrome C.” Chen, L.; Zhong, H.; Jia, X.; Qin, Y.; Liao, Q.; Li, M.; Wei, Y. *Acta Polymerica Sinica* 2001*, 4,* 553-556.

Patents

1. “Azide Functionalized Poly(3-hexylthiophene) and Method of Forming Same” Qin, Y.; Grubbs, R. B.; Park, Y. S. US 2012/0028191 A1; Feb 02, 2012.

Conference Proceedings

1. Cui, C.; Qin, Y.; Jäkle, F. *Polymer Preprints* 2008, *49*, 889-890.

2. Jäkle, F.; Cui, C.; Qin, Y. *Polymer Preprints* 2008, *49*, 297-298.
3. Parab, K.; Qin, Y.; Jäkle, F. *PMSE Preprints* 2008*, 98,* 189-190.
4. Parab, K.; Venkatasubbaiah, K.; Qin, Y.; Jäkle, F. *Polymer Preprints* 2007*, 48,* 699-700.
5. Jäkle, F.; Qin, Y.; Parab, K.; Cui, C. *Polymer Preprints* 2007*, 48,* 654-655.
6. Jäkle, F.; Cui, C.; Qin, Y.; Banipal, J. S. *PMSE Preprints* 2007*, 96,* 39-40.
7. Qin, Y.; Jäkle, F. *Polymer Preprints* 2006*, 47,* 54-55.
8. Cui, C.; Banipal, J. S.; Qin, Y.; Jäkle, F. *PMSE Preprints* 2006*, 95,* 699-700.
9. Jäkle, F.; Qin, Y.; Kiburu, I. *PMSE Preprints* 2006*, 95,* 26-27.
10. Jäkle, F.; Sundararaman, A.; Qin, Y.; Parab, K. *PMSE Preprints* 2005*, 93,* 786-787.
11. Parab, K.; Qin, Y.; Haleem, S.; Jäkle, F. *PMSE Preprints* 2005*, 93,* 422-423.
12. Qin, Y.; Shah, S.; Kiburu, I.; Jäkle, F. *Polymer Preprints* 2005*,* 46*,* 1026-1027.
13. Qin, Y.; Sukul, V.; Pagakos, D.; Cui, C; Jäkle, F. *Polymer Preprints* 2005*, 46,* 351-352.
14. Qin, Y.; Priya S., Pagba, C.; Piotrowiak, P.; Jäkle, F. *PMSE Preprints* 2004*, 91,* 447-448.
15. Qin, Y.; Parab, K.; Cheng, G.; Achara, O.; Jäkle, F. *Polymer Preprints* 2003*, 44,* 513-514.

Invited Presentations

1. "Conjugated Polymers for Organic Photovoltaics." *Fort Lewis College*, Oct. 14th, 2011.
2. "Supramolecular Block Copolymers for Organic Photovoltaics." *The 7th Sino-US Chemistry Professors Conference*, Guiyang, China, June 28th-30th, 2011.
3. "Nano–Structured Organic Photovoltaics." Department of Chemistry, *New Mexico Institute of Mining and Technology* (*New Mexico Tech*), Feb. 11th, 2011.
4. "Solution-Processable Organic Electronics." Integrating Nanotechnology with Cell Biology and Neuroscience (INCBN-IGERT), Center for High Technology Materials, *University of New Mexico*, Nov. 1st, 2010.
5. "Functional Polymers for Organic Electronics." Department of Physics & Astronomy, *University of New Mexico*, Oct. 11th, 2010.
6. "Functional Polymers for Organic Electronics." Department of Chemical & Nuclear Engineering, *University of New Mexico*, Sept. 21st, 2010.

Conference Presentations

Oral Presentations

1. "Novel distannylated isothianaphthene as a versatile building block for low band-gap polymers." Qin, Y.; Hillmyer, M. A. *Industrial Partnership for Research in Interfacial and Materials Engineering Annual Meeting, May 27th-29st,* 2008.
2. "Synthesis and characterization of organoboron quinolate polymers with tunable luminescence properties." Qin, Y.; Kiburu, I.; Venkatasubbaiah, K.; Shah, S.; Jäkle, F. *Boron in the Americas X, San Juan, Puerto Rico, Aug 2nd-7th,* 2006.
3. "Use of silylated initiators for the efficient preparation of borane end-functionalized polymers via ATRP." Qin, Y.; Jäkle, F. *38th Middle Atlantic Regional Meeting, Hershey, PA, June 4th-7th,* 2006.
4. "Synthesis and characterization of organoboron quinolate polymers with tunable luminescence properties." Qin, Y.; Shah, S.; Kiburu, I.; Jäkle, F. *6th National Graduate Research Polymer Conference, University of Massachusetts, Amherst, June 15th-17th,* 2005.

5. “Synthesis and characterization of organoboron quinolate polymers with tunable luminescence properties.” Qin, Y.; Shah, S.; Kiburu, I.; Jäkle, F. *230th ACS National Meeting, Washington, DC, US, Aug. 28-Sep. 1,* 2005.
6. “Luminescent organoboron quinolate polymers”, Qin, Y.; Pagba, C.; Piotrowiak, P.; Jäkle, F. *37th Middle Atlantic Regional Meeting of the American Chemical Society, New Brunswick, NJ, May 22-25,* 2005.

Poster Presentations

1. “UV Crosslinkable Polythiophene for Nano-imprinting and Photolithography toward Ordered Bulk Heterojunction in Organic Photovoltaics.” Qin, Y.; Hlaing, H.; Ocko, B.; Black, C. and Grubbs, R. B. *Gordon Research Conference: Polymers, South Hadley, MA, July 25th-30th, 2010.*
2. “Low Bandgap Poly(3-hexyl-2,5-thienylene vinylene) by ADMET Polymerization of a Dipropenyl Monomer for Photovoltaic Devices.” Qin, Y.; Hillmyer, M. A. *Gordon Research Conference: Polymers, South Hadley, MA, June 21st-29th, 2009.*
3. “Novel distannylated isothianaphthene: a versatile building block for low bandgap conjugated polymers.” Qin, Y.; Kim, J. Y.; Frisbie, C. D.; Hillmyer, M. A. *Organic Microelectronics and Optoelectronics Workshop IV, Materials Research Society, San Francisco, CA, July 7th-10th,* 2008.
4. “Synthesis of conjugated polymers and block copolymers possessing low band-gaps as potential components in bulk hetero-junction solar cells.” Qin, Y., Hillmyer, M. A. *Industrial Partnership for Research in Interfacial and Materials Engineering Annual Meeting, May 29th-31st,* 2007.
5. “Well-defined organoboron homo-, block- and telechelic polymers.” Qin, Y.; Parab, K.; Jäkle, F. *Boron in the Americas X, San Juan, Puerto Rico, Aug 2nd-7th,* 2006.
6. “Well-defined organoboron homo- and block co-polymers.” Qin, Y.; Jäkle, F. *231st ACS National Meeting, Atlant, GA, March 26th-30th,* 2006.
7. “Preparation of organoboron block copolymers via ATRP of silicon and boron functionalized monomers.” Qin, Y.; Sukul, V.; Pagakos, D.; Cui, C; Jäkle, F. *230th ACS National Meeting, Washington, DC, Aug. 28-Sept, 1,* 2005.
8. “Synthesis and characterization of novel luminescent organoboron quinolate polymers.” Qin, Y.; Priya S., Pagba, C.; Piotrowiak, P.; Jaekle, F. *228th ACS National Meeting, Philadelphia, PA, Aug. 22-26,* 2004.
9. “New Well-Defined Triarylborane Polymers: Synthesis, Characterization and formation of Lewis Acid-Lewis Base Complexes.” Qin, Y.; Parab, K.; Cheng, G.; Achara, O.; Jaekle, F. *226th ACS National Meeting, New York, September 7-11,* 2003.
10. “Synthesis and Properties of polymers containing highly Lewis acidic groups.” Qin, Y.; Cheng, G.; Sundararaman, A.; Jaekle, F. *224th ACS National Meeting, Boston, MA, August 18-22,* 2002.

Fundings & Awards

1. “DOE Early Career Award 2012” – to be submitted.
2. “NSF CAREER Award 2012” – Pending.
3. “RAC award (2010-2011) ” – University of New Mexico (11-L-04).
4. “Start-up fund (2010-2014)” – University of New Mexico.
5. “Dean’s Award for Outstanding Doctoral Dissertation” – the Graduate School, Rutgers – Newark, May 18th, 2007.

6. “Outstanding Poster Presentation at BORAM X” – Boron in the Americas X, San Juan, Puerto Rico, August 2nd-6th, 2006.
7. “Graduate Student Excellence Award” – Graduate Student Government Association, Rutgers University, May 19th, 2006.
8. “Excellence in Graduate Polymer Science Award” – Division of Polymer Chemistry, 231st ACS National Meeting, Atlanta, GA, March 26th-30th, 2006.

Students Advising

Current Students

Fei Li (Graduate Student 2010-)
Fei Chang (Graduate Student 2011-)
Keda Hu (Graduate Student 2011-)
Guoshun Yang (Graduate Student 2011-)
Jianzhong Yang (Graduate Student 2011-)
Robert Sparks (Undergraduate Student 2010-)

Former Students

Alexander Starkey (Undergraduate Student, 01/2012-05/2012)
Robert Haver (STEM Student, Mount View College, 05/31/2011-08/05/2011)

Services

1. Departmental seminar coordinator (Fall 2011 to present).
2. Graduate study committee (02/2012 to present).
3. Graduate Study committee (01/2011 to 10/2011).
4. Faculty recruiting committee (Spring 2011 for hiring Dr. Fu-Sen Liang).

Curriculum Vitae

Alisha D. Ray Chemistry and Chemical Biology 2012

Educational History:

M.S., July 2005, University of New Mexico, Albuquerque, NM, Chemistry, "An Analysis of Phosphate's Effect on Iron Incorporation and Release from Ferritin," advisor: Richard K. Watt

B.S. and B.A., May 2001, University of New Mexico, Albuquerque, NM, Anthropology and Chemistry, "It's Not All in Your Head: Determining Biological Affinity Based on Post-cranial Discriminate Function Analysis," advisor: Osbjorn Pearson

Employment History

Lecturer II, January 2006-present, University of New Mexico, Albuquerque, NM

Part-time Instructor, August 2005-December 2005, University of New Mexico, Albuquerque, NM

Laboratory Assistant, July 2001-May 2002, Maxwell Museum of Anthropology Laboratory of Human Osteology, Albuquerque, NM

Employment History – concurrent temporary or visiting appointments, consultantships

Research Assistant, 5/2009 – 8/2009 and 5/2008 – 8/2008, C&CB, University of New Mexico, Albuquerque, NM

Professional Recognition, Honors, etc. (Teaching, research, service)

Outstanding Lecturer of the Year Award, in recognition of excellent teaching and contributions towards UNM's teaching mission, 2009-2010, OSET

Clark-Person-Graham Teaching Assistant Award, in recognition of outstanding teaching, 2005, C&CB

Clark-Person-Graham Teaching Assistant Award, in recognition of outstanding teaching, 2004, C&CB

Outstanding Senior Award, in recognition of accomplishments in the University Honors Program, 2001, University Honors Program

Short Narrative Description of Teaching, Research and Service Interests.

Teaching interests:

1. Increase awareness on the role of science and technology in society. I am interested in ***developing and teaching a new chemistry course designed to introduce non-science majors to the basic chemistry required to understand a variety of scientific topics in the news and affecting our community, such as global warming, acid rain, nuclear power, plastics, drugs, and genetic engineering.*** In this course, students would develop the critical thinking skills to assess the risks and benefits of technology-based issues. By the end of the course, students would be able to critically evaluate scientific claims as presented in the popular press.
2. Captivating, motivating, engaging and challenging students. In CHEM 111L (Elements of Chemistry), I use clickers to engage students in lecture and set up a rigorous learning "routine." ***I use the routine to subtly influence the study habits of my students***. ***I also have the students work in small groups on in-class activities to help students practice the skills they need for their exam.*** When students get to work in groups they have the opportunity to improve chemistry knowledge base by asking and answering each others' questions and articulate their own questions. In addition, by working together in groups the students start to create a sense of community within the class and build their self-esteem by having them contribute to their team and the class. In addition to using clickers, and in-class activities, my CHEM 111L ***students use a web-based artificially intelligent learning and assessment system called A.Le.K.S. (Assessment and Learning in Knowledge Spaces), which provides customized supplemental instruction for the course***. This tool is able to help "catch up" students that need remedial math help, so long as they are willing to put in the time. The more advanced students are recognized and allowed to work at an accelerated pace to keep them from becoming bored. ***Since spring 2012, I've have peer-learning facilitators (PLFs) in each of my CHEM 111L classes to offer students assistance and immediate feedback.*** Because of the large amount of course material covered in my course, students can often become overwhelmed. In order to prevent burnout and loss of interest, I use relevant examples of course materials to help reinforce fundamental principles. Relating concepts taught in class to issues students find important in their own lives provides additional motivation for students to master the course materials. ***In order to provide context for mastering core principles, I started using informal weekly surveys to find out who my students are, what they hope to learn, why they are taking chemistry, and what they are struggling with in the course.*** This information allows me to identify ties between the course material and their interests that I can subsequently raise during my lectures. In addition I can tailor my lectures to the topics they struggled to learn in their reading assignments and answer some of the frequently asked questions.

Service interests:

- Help the department increase the amount of survey data on current majors and chemistry graduates
- Assist in reinstituting department graduation ceremony each May
- Volunteer at local schools to promote science and math education

TEACHING ACHIEVEMENTS

Classroom Teaching:

2012; Spring*; Elements of Chemistry; 111L; 115 students

2011; Fall; Elements of Chemistry; 111L; 122 students
2011; Fall; Integrated Organic and Biochemistry; 212; 75 students

2011; Spring; Elements of Chemistry; 111L; 114 students
2011; Spring; Integrated Organic and Biochemistry; 91 students

2010; Fall; Elements of Chemistry; 111L; 124 students
2010; Fall; Integrated Organic and Biochemistry; 212; 56 students

2010; Spring; Elements of Chemistry; 111L; 123 students
2010; Spring; Integrated Organic and Biochemistry; 58 students

2009; Fall; Elements of Chemistry; 111L; 117 students
2009; Fall; Integrated Organic and Biochemistry; 212; 46 students

2009; Spring; Elements of Chemistry; 111L; 95 students
2009; Spring; Integrated Organic and Biochemistry; 62 students

2008; Fall; Elements of Chemistry; 111L; 121 students
2008; Fall; Integrated Organic and Biochemistry; 212; 47 students

2008; Spring; Elements of Chemistry; 111L; 115 students
2008; Spring; Integrated Organic and Biochemistry; 63 students

2007; Fall; Elements of Chemistry; 111L; 122 students
2007; Fall; Integrated Organic and Biochemistry; 212; 80 students

2007; Spring; Elements of Chemistry; 111L; 122 students
2007; Spring; Integrated Organic and Biochemistry; 77 students

2006; Fall; Elements of Chemistry; 111L; 122 students
2006; Fall; Integrated Organic and Biochemistry; 212; 60 students

2006; Summer; General Chemistry; 121; 50 students

* part-time status during the spring 2012 semester

Curriculum Development or Teaching Administrative Positions:

- Implemented a new online learning system, A.Le.K.S. (Assessment and Learning in Knowledge Spaces), for CHEM 111L; spring 2010
- Incorporated informal writing assignments in CHEM 212; fall 2009
- Began using video demonstrations in CHEM 111L; fall 2009
- Developed two video tutorials for unit conversions; 2008
- Developed and tested several group learning exercises and surveys; spring and fall 2008
- Incorporated “capstone” project in CHEM 212 that involved writing a paper and giving a formal presentation; spring and fall 2008
- Instituted group discussion in recitations and eliminated the use of teaching assistants as instructors in recitation ; 2008-2009 AY
- Carried out an assessment of two learning outcomes for Chem 111; each year since 2008
- Incorporated several POGIL-style exercises into CHEM 212; fall 2008

Service:

C&CB Undergraduate Committee; 2011-2012 AY

Teaching Enhancement Committee; fall 2011-present

- TAG subcommittee; fall 2011
- chaired LATOYA selection committee; spring 2012

Volunteer at Mole Day celebration held at the National Nuclear Science and History Museum; fall 2011

C&CB Undergraduate Committee; 2010-2011 AY

Gave talk at OSET's Success in the classroom conference; 2/17/2010; "Using Clickers to Engage Students in the Classroom"

Gave talk at ALeKS conference in Austin, TX discussing the use of ALeKS in introductory chemistry; 2012

C&CB Undergraduate Committee; 2009-2010 AY

Spring Storm; 2009; community service project volunteer

Invited guest speaker at CAPS tutor training; 8/2008

Recruitment of graduate students at the Joint 63rd Northwest/21st Rocky Mountain (NORM/RMRM) ACS meeting; summer 2008

- attended POGIL workshop

Attended the New Mexico Higher Education Assessment and Retention Conference; spring 2008

Assessment Committee Chair 01/2008-12/2008

- Developed program goals and student learning outcomes (SLOs) for B.A./B.S. and M.S./PhD. programs
- Prioritized the (SLOs) and submitted pilot assessment plans for the programs.
- Submitted a General Education Core Annual Progress on Assessment Report

Scholarly Achievements (not all lecturers participate in scholarship in their disciplines, but for those who do, please list as described below:
Articles in Refereed Journals:

Sylvie Pailloux, Cornel Edicome Shirima, **Alisha D. Ray**, Eileen N. Duesler, Robert T. Paine, John R. Klaehn, Michael E. McIlwain and Benjamin P. Hay; *Synthesis and Coordination Properties of Trifluoromethyl Decorated Derivatives of 2,6-Bis[(diphenylphosphinoyl)methyl]pyridine N-Oxide Ligands with Lanthanide Ions*; Inorg. Chem.*; 48 (7); pp 3104–3113; 2009.*

Pailloux, Sylvie; Shirima, Cornel Edicome; **Ray, Alisha D**.; Duesler, Eileen N.; Smith, Karen Ann; Paine, Robert T.; Klaehn, John R.; McIlwain, Michael E.; Hay, Benjamin P.; *Synthesis and lanthanide coordination chemistry of trifluoromethyl derivatives of phosphinoylmethyl pyridine N-oxides;* Dalton Transactions; 36; 7486-7493; 2009.

Polanams, Jup.; **Ray, Alisha D**.; Watt, Richard K; *Nanophase Iron Phosphate, Iron Arsenate, Iron Vanadate, and Iron Molybdate Minerals Synthesized within the Protein Cage of Ferritin*; Inorg. Chem.; 44(9); 3203-3209; 2005.

Cutler, Chris; Bravo, Anthony; **Ray, Alisha D.**; Watt, Richard K; *Iron Loading into ferritin can be stimulated or inhibited by the presence of cations and anions: a specific role for phosphate*; J.Inorg. Biochem.; 99, 2270-2275; 2005.

Contributed (un-refereed) Abstracts and/or Oral Presentations at Professional Meetings:

The role of phosphate in iron uptake and release; Ray, Alisha D.; Watt, Richard K.; Joint Regional Meeting of the Northwest and Rocky Mountain Sections of the American Chemical Society; Logan, UT; June 6-9 2004.

Curriculum Vitae

Wei Wang

Contact Information

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Fax: 505-277-2609
Email: wwang@unm.edu
Research Group Webpage: http://www.unm.edu/~wwang/

Education

Ph.D., Organic Chemistry, February 2000
Dissertation Title: Design, synthesis and evaluation of coumarin-based prodrugs and fluorescence sensors
Advisor: Binghe Wang
Department of Chemistry, North Carolina State University, Raleigh, NC, USA

M.S., Organic Chemistry, June 1993
Thesis Title: Synthesis and QSAR studies of (+) edulinine and its analogs
Advisors: Kunjian Gu and Ruyun Ji
Department of Medicinal Chemistry, Shanghai Institute of Materia Medica, Chinese Academy of Sciences, Shanghai, China

B.S., Chemistry, July 1988
Nanjing Normal University, Nanjing, China

Awards and Honors

• Guest Editor, *Science China: Chemistry*, **2011**, *53(1)*: Special Issue on "The Frontiers of Chemical Biology and Synthesis"

• President, The Chinese-American Chemistry & Chemical Biology Professors Association, June 2010 to May 2012

• Director, The Chinese-American Chemistry & Chemical Biology Professors Association, June 2008 to May 2010

• Board Member, *Current Organic Synthesis,* September 2009 to present

• *Tetrahedron Letters* Most Cited Paper 2006-2009 Award

• The Chinese-American Chemistry & Chemical Biology Professors Association (CAPA) Distinguished Junior Faculty Award 2008

• *Tetrahedron Letters* Most Cited Paper 2004-2007 Award

• Honorary Board Member, *Organic Chemistry Insights,* August 2007 to present

• Board Member, *Letters in Organic Chemistry,* August 2007 to present

• The Bruce W. Erickson Young Investigator Award, the American Peptide Society (APS) and the APS Travel Grant Award, the 17th American peptide Symposium/2nd International Peptide Symposium, June 9-15, 2001, San Diego, CA, USA

• The Outstanding Research Award, the First Annual North Carolina State University International Research Exposition, North Carolina State University, April 16, 1999, USA

• Glaxo Graduate Fellowship, Department of Chemistry, North Carolina State University, 1998-1999, USA

• Honors Student and the University Scholarship, Nanjing Normal University, 1984-1987, China

Professional Experience

Department of Chemistry and Chemical Biology, University of New Mexico (UNM), Albuquerque, NM
Associate Professor (tenured), July 2008 to present
Assistant Professor, August 2003 to June 2008

Principal Investigator, December 2001 to August 2003
Genomics Institute of the Novartis Research Foundation, San Diego, CA

Postdoctoral Fellow (with Professor Victor J. Hruby), February 2000 to December 2001
Department of Chemistry, University of Arizona, Tucson, AZ

Teaching and Research Assistant, August 1996 to February 2000
Department of Chemistry, North Carolina State University, Raleigh, NC

Research Associate, October 1994 to July 1996
Department of Medicinal and Pharmaceutical Chemistry, College of Pharmacy, University of Oklahoma Health Sciences Center, Oklahoma City, OK

Research Associate, July 1993 to September 1994
Shanghai Combined Chemistry Institute, East China University of Science & Technology, Shanghai, China.

Research Assistant, September 1990 to June 1993
Shanghai Institute of Material Medica, Chinese Academy of Sciences, China.

High School Chemistry Teacher, August 1988 to August 1990
Sizhao High School, Dongtai City, Jiangsu Province, China

Research Interest:

Organic Chemistry

• Development of new synthetic methodology, particularly in the area of organocatalysis with an emphasis on atom-economical, environmentally friendly synthesis and catalysis in the preparation of biologically interesting molecules

Medicinal Chemistry and Chemical Biology

• *Drug discovery*: Design, synthesis, and evaluation of small molecules as therapeutic agents with focus on anti-cancer, neurodegenerative diseases and anti-bacterial.

• *Molecular imaging*: Development of fluorescent and multi-modular probes for the detection of reactive oxygen species, thiols, seleno-proteins, arsenic, Zn(II), sugars, tumor cells and toxic heavy metals and other chemicals.

• *Pharmaceutical chemistry*: Development of novel intelligent drug delivery systems for improving the properties and drug efficacy of medicinal agents.

Teaching Interest:

• Develop undergraduate general and organic chemistry curricula and graduate advanced organic chemistry courses including organic reaction mechanisms, structures, reactions and synthesis, advanced spectroscopy for determination of structures of organic molecules.
• Develop specific topics at the graduate level such as medicinal and bioorganic chemistry, modern biotechnologies and chemical biology. Ideally they would be cross-listed such that both undergraduate and graduate students could take the courses, with graduate students being assigned additional work. This would introduce both groups to important and state-of-the art topics that are not currently covered. The students' scientific education would be broadened and enhanced by the opportunity to develop and teach these courses in green and bio-related chemistry. If students were interested, they would have, if appropriate, the opportunity to apply this knowledge more practically by requesting a rotation in my laboratory.

Service Interest:

• Interested in actively participating in all level (University, College and Department) services such as faculty recruiting, instrument, safety, graduate and undergraduate study committee, student recruiting, new program development such educational projects for both undergraduate and graduate.
• Interested in actively participating, attending and organizing local and national professional organization activities, conferences and services.

Profession Affiliations

American Chemical Society
American Peptide Society
Phi Lambda Upsilon National Honorary Chemical Society and Vice President of Beta Lambda Chapter (1999-2000)
New York Academy of Sciences
Sigma Xi

Research Support

Ongoing Research Support

• NSF (CHE-1057569), "Oxidative Enamine Catalysis in Organic Synthesis," PI, 08/01/2011-07/31/2014, $455,000 total cost.
• NSF (CHE-0946690), "Acquisition of a Low-Field NMR Spectrometer for Research and Teaching," co-PI (PI, Marty Kirk), 01/14/2011-01/13/2014, $218,700.00 total cost.
• NSF (CHE-0840523), "Upgrade of a 300 MHz NMR Spectrometer for Research and Teaching," co-PI (PI, Marty Kirk), 07/30/2009-07/29/2013, $499,700 total cost.
• The National Institutes of Health (NIH, 1RC1MH088480-01), "Phosphodiesterase-2 and Mood Disorders: Target Validation and Drug Discovery," co-PI (PI, James M. O'Donnell, West Virginia University), 09/30/2009-10/31/2011, $149,630 total cost.
• NIH "NIH Roadmap Center Program" MLSCN U54, as an investigator (PI: Larry A. Sklar), 7/1/2008-6/30/2014, my portion: $180,000 direct cost.
• University of New Mexico, the Research Allocation Committee Small Grant-in-Aid for Research (#11-32) "Functionalized Organometallic Nanostructures as Recyclable and Reusable Catalysts for Water Medium Organic Reactions," PI, 03/01/2011-9/30/2011 $3,900, direct cost.

Pending Research Support
• NIH, "Organocatalyzed Reactions in Organic Synthesis," 07/01/2012-06/30/2017, PI, $1,624,908, total cost.
• NIH, "Chemical Approaches to Target Validation for Drug Resistant Pathogens," 03/01/2012-02/28/2017, as Co-PI, (PI: George Tegos, Cancer Center, University of New Mexico), my portion: $635,000 total cost.
• NIH, "Targeting Transposase Domains for Cancer Therapy," 03/01/2012-02/28/2017, as Co-PI, (PI: Robert Hromas, School of Medicine, University of Florida), my portion: $566,250 total cost.
• NSF, "Novel Fluorescence Probes for Simultaneous Detection of Multiple Toxic Heavy Metals," 07/01/2013-06/30/2016, PI, $656,644 total cost

Past Research Support
• University of New Mexico-NIH COBRE seeded fund, Development of Novel Sensitive and Selective Fluorescence Spin Probes Used for Detection of ROS in Brain 1/1/2004-7/31/2004 (PI, $15,000 direct cost).
• University of New Mexico, the Research Allocation Committee Small Grant-in-Aid for Research (#05-01) "Green" Organocatalysts for Asymmetric Michael Addition Reactions," PI, 10/1/2004-9/30/2005, $4,000, direct cost.
• University of New Mexico, the Research Allocation Committee Large Grant-in-Aid for Research (#05-L-01), "Fluorescence Spin Probes for Detection of ROS Associated Brain Injuries," PI, 1/12/2005-9/30/2005, $6,980, direct cost.
• NIH INBRE, "ICAM-1 Mimics as LFA-1 Inhibitors" PI, 10/01/2005 to 6/30/2008 $397,500, total cost.
• NIH "NIH Roadmap Center Program" MLSCN U54, as an investigator (PI: Larry A. Sklar), 7/1/2005-6/30/2008, $3,000,000, direct cost, my portion: $100,000 direct cost.
• University of New Mexico, the Research Allocation Committee Large Grant-in-Aid for Research (#06-L-08), "Recyclable and Reusable (S) Pyrrolidine Sulfonamide Organocatalyst for Asymmetric Synthesis", PI, 1/1/2006-9/30/2006, $8,000, direct cost.
• University of New Mexico Cross-Campus Collaborations in the Life Sciences, "Development of Competitive LFA-1 Antagonists for Regulating Integrin Functions," PI, 1/1/2006-12/13/06, $23,300, direct cost.

• ACS-PRF, "Recyclable and Reusable (*S*) Pyrrolidine Sulfonamide Organocatalyst for Asymmetric Synthesis," PI, 09/01/2006-08/31/2008, $35,000 direct cost.
• The Sandia National Laboratories-University Research Program (SURP), "Quantum Dots for Melanoma Tumor Imaging," PI, 10/01/2006-09/30/2008, $80,000 total cost.
• The University of New Mexico, the Research Allocation Committee Large Grant-in-Aid for Research, "Quantum Dots for Specific Melanoma Tumor Imaging," PI, 01/01/2007-09/30/2007, $8,000, total cost.
• NSF, "Bifunctional molecule mediated catalysis," PI, 05/01/2007-04/30/2010, $429,900 total cost.
• The University of New Mexico GAP Fund, "Three-Step Preparation of Anticonvulsant Lyrica and Analgesic Baclofen Using Environmentally Friendly Organocatalytic Asymmetric Processes," PI, 12/01/2008-11/30/2009 $25,000 direct cost.
• Chinese Government Award for Outstanding Self-Financed Students Abroad 2006, $5,000, for Jian Wang.
• Chinese Government Award for Outstanding Self-Financed Students Abroad 2008, $5,000, for Liansuo Zu.
• The China Scholarship Council for Chengguang Yu, September 1, 2008 to August 31, 2010, $24,000.

Publications

After joining UNM (independent research work, 8/2003-present, 113 total, *as corresponding author):

1) Xie, H.-X.; Song, A.-G.; Zhang, X.-S.; Chen, X.-B.; Li, H.; Sheng, C.-Q.;* **Wang, W.*** "Quinine-thiourea Catalyzed Enantioselective Hydrophosphonylation of Trifluoromethyl 2(1*H*)-Quinazolinones" *Chem. Commun.,* **2013,** *49*, 928-930.
2) Xie, H.-X.; Song, A.-G.; Song, X.-X.; Zhang, X.-S.; **Wang, W.*** "Organocatalytic Enantioselective Strecker Reaction of Cyclic Trifluoromethyl-ketoimines" *Tetrahedron Lett.,* **2013**, in press.
3) Xia, D.-Q.; Cheng, T.-Y.; Xiao, W.; Liu, K.-T.; Wang, Z.-L.; Liu, G.-H.* Li, H.-X. **Wang, W.*** "Imidazolium-Based Organic-Inorganic Hybrid Silica as A Functional Platform Dramatically Boosts Chiral Organometallics Performance in Asymmetric Catalysis" *ChemCatChem,* **2013**, in press.
4) Xuan, W.; Pan, R.; Cao, Y.; Liu, K.-J.; Wang, W.* "A Fluorescent Probe Capable of Detection of H_2S at a Submicromolar Range and in Cellular Imaging" *Chem. Commun.,* **2012**, *48*, 10669-10671**.**
5) Zhang, X.-S.; Song, X.-X.; Li, H.; Zhang, S.-L.; Chen, X.-B.; Yu, X.-H.; **Wang, W.*** "An Organocatalytic Cascade Approach toward Polysubstituted Quinolines and Chiral 1,4-Dihydroquinolines–Unanticipated Effect of *N*-Protecting Groups" *Angew. Chem. Int. Ed.,* **2012**, *51*, 7282-7286.
6) Song, X.-X.; Zhang, X.-S.; Zhang, S.-L.; Li, H.;* **Wang, W.*** "Direct Transformation of Simple Enals to 3,4-Disubstituted Benzaldehydes under Mild Reaction Conditions via an Organocatalytic Regio- and Chemo-selective Dimerization Cascade" *Chem. Eur. J.,* **2012**, *18*, 9770-9774.
7) Xuan, W.; Chen, C.; Cao, Y.; He, W.; Jiang, W.; Liu, K.-J.;* Wang, W.* "Rational Design of a Ratiometric Fluorescent Probe with a Large Emission Shift for the Facile Detection of Hg^{2+}" *Chem. Commun.,* **2012**, *48*, 7292-7294.
8) Wang, H.; Yang, W.; Liu, H.; **Wang, W.;*** Li, H.* "$FeCl_3$ Promoted Highly Regioselective [3+2] Cycloaddition of Dimethyl 2-Vinyl and Aryl Cyclopropane-1,1-dicarboxylates with Aryl Isothiocyanates" *Org. Biomol. Chem.,* **2012**, *10,* 5032-5035.

9) Xuan, W.-M. Sheng, C.-Q.;* Cao, Y.-T.; He, W.-H.; **Wang, W.*** "Emerging Fluorescent Probes for the Detection of Hydrogen Sulfide in Biological Systems" *Angew. Chem. Int. Ed.,* **2012**, *51,* 2282-2284 (Highlights).
10) Liu, L.; Wu, D.; Li, X.; Wang, S.; Li, H.; Li,* J.; **Wang, W.*** "Organocatalytic Enantioselective Conjugate Addition of Ketones to Isatylidine Malononitriles" *Chem. Commun.,* **2012***, 48*, 1692-1694.
11) Zhu, J.; Yu,* S.; Lu, W.-C..; Deng, J.; Li, J.; **Wang, W.*** "Direct Oxidative Conversion of 3-Aryl Propionaldehydes to 3-Aryl Acroleins Promoted by SOMO Catalysis" *Tetrahedron Lett.*, **2012**, *53*, 1207-1209.
12) Deng, J.; Wang, F.; Yan, W.-Z.; Zhu, J.; Jiang, H.-L.; **Wang, W.;*** Li, J.* "Synthesis of 3-Substituted 1,5-Aldehyde Esters via an Organocatalytic Highly Enantioselective Conjugate Addition of New Carbonylmethyl 2-Pyridinylsulfone to Enals" *Chem. Commun.*, **2012**, *48*, 148-150. Invited for "the joint ChemComm–Organic & Biomolecular Chemistry 'Organocatalysis' web themed issue."
13) Xie, H.-X.; Zhang, S.-L.; Li, H.; Zhao, S.-H.; Xu, Z.-A.; Song, X.-X.; Yu, X.-H.;* **Wang, W.*** "Total Synthesis of Polyene Natural Product Dihydroxerulin by Mild Organocatalyzed Dehydrogenation of Alcohols" *Chem. Eur. J.* **2012**, *18*, 2230-2234.
14) Zou, Z.-Q.; Deng, Z.-J.; Yu, X.-H.;* Zhang, M.-M.; Zhao, S.-H.; Lou, T.; Yin, X. Xu, H.; **Wang, W.*** "A New Facile Approach to *N*-Alkylpyrroles from Direct Redox Reaction of 4-Hydroxy-L-proline with Aldehydes" *Science China – Chemistry,* **2012,** *55*, 43-49 (invited paper).
15) Liu, L.; Wu, D.; Zheng, S.; Li, T.; Li, X.; Wang, S.; Li, J.; Li, H.;* **Wang, W.*** "Synthesis of Highly Functionalized Chiral 3, 3'-Disubstituted Oxindoles via an Organocatalytic Enantioselective Michael Addition of Nitroalkanes to Indolylidene-cyanoacetates" *Org. Lett.,* **2012**, *14*, 134-137.
16) Zhang, F.; Yang, X.-S.; Zhu, F.-X.; Huang, J.-L.; He, W.-H.; **Wang, W.*;** Li, H.-X.* "Highly Active and Reusable Organometallic Catalysts Covalently Bonded to an Ordered Mesoporous Polymer" *Chem. Sci.,* **2012**, *3*, 476-484.
17) Song, X.-X.; Song, A.-G.; Zhang, F.; Li, H.-X.;* **Wang, W.*** "Direct Stereoselective α-Arylation of Unmodified Enals Using an Organocatalytic Cross-coupling-like Reaction" *Nature Commun.,* **2011**, *2*, 524, doi:10.1038/ncomms1541. **This work has been highlighted in *Synfacts*.**
18) Xie, H.-X.; Zhang, Y.-N.; Zhang, S.-L.; Chen, X.-B.; **Wang, W.*** "Bifunctional Cinchona Alkaloid-thiourea Catalyzed Highly Efficient, Enantioselective Aza-Henry of Cyclic Trifluoromethyl-Ketimines and Application in Synthesis of Anti-HIV Drug DPC 083" *Angew. Chem. Int. Ed.*, **2011**, *50,* 11773-11776. **This work has been highlighted in *Synfacts*.**
19) Zhang, S.-L.; Xie, H.-X.; Song, A.-G.; Wu, D.-Y.; Zhu, J.; Zhao, S.-H.; Li, J.;*, Yu, X.-H.;* **Wang, W.*** "Efficient Preparation of *trans*-α, β-Unsaturated Aldehydes from Saturated Aldehydes by Oxidative Enamine Catalysis" *Science China – Chemistry,* **2011,** *54*, 1932-1936 (invited for special issue of International Year of Chemistry).
20) Zhang, S.-L.; Xie, H.-X.; Zhu, J.; Li, H.; Zhang, X.-S.; Li, J.;* **Wang, W.*** "Organocatalytic Enantioselective β-Functionalization of Aldehydes via Oxidation of Enamines and Their Application in Cascade Reactions" *Nature Commun.,* **2011**, *2,* 211, DOI: 10.1038/ncomms1214. **This work has been highlighted in *C&EN News* (March 7, 2011 issue on page 9) as "News of the Week" and *Synfacts*.**
21) Zhu, F.-X., **Wang, W.;*** Li, H.-X.* "Water-Medium and Solvent Free Organic Reactions over a Bifunctional Catalyst with Au Nanoparticles Covalently Bonded to HS/SO_3H Functionalized PMO" *J. Am. Chem. Soc.* **2011**, *133*, 11632-11640.
22) Liu, L.; Zhang, S.-L.; Xue, F.; Lou, G.-S.; Zhang, H.-Y.; Ma, S.-C.; Duan, W.-H.; **Wang, W.*** "Catalytic Enantioselective Henry Reactions of Isatins. Application in Concise Synthesis of (*S*)-(-

)-Spirobrassinin", *Chem. Eur. J.* **2011,** *17*, 7791-7795. **This work has been highlighted in *Synfacts***.

23) Chigaev, A.; Smagley, Y.; Zhang,Y.; Waller, A.; Haynes, M. K.; Amit, O.; **Wang, W.**; Larson, R. S.; Sklar, L. A. "Real-Time Analysis of the Inside-Out Regulation of Lymphocyte Function-Associated Antigen-1 Reveled Similarities and Differences with Very Late Antigen-4" *J. Bio. Chem.* **2011**, *286*, 20375-20386. This work has been featured online on the site "Global Medical Discovery" (http://globalmedicaldiscovery.com).

24) Liu, G.-X.; Zhang, S.-L.; Zhang, T.-Z.; **Wang, W.*** "Organocatalytic Enantioselective Friedel-Crafts Reactions of 1-Naphthols with Aldimines" *Org. Lett.,* **2011**, *13*, 828-831.

25) Wang, J.; Zhang, M.-M.; Xu, Z.-A.; Li, H.; Yu, X.-H.; **Wang, W.*** "Chiral Pyrrolidine Sulfonamide Catalyzed Enantioselective Michael Addition of Cyclic Ketones to Maleimides" *Synlett*, **2011**, 473-476, invited for cluster topic: "Proline and Proline-Based Organocatalyst."

26) Yu, C.-G.; Zhang, S.-L.; Li, H.; **Wang. W.*** "Cu(II) Catalyzed Oxidation-[3+2] Cycloaddition-Aromatization Cascade: Efficient Synthesis of Pyrrolo [2, 1-*a*] Isoquinolines" *Chem. Commun.,* **2011**, *47*, 2036-1038.

27) Yu, C.-G.; Zhang, Y.-N.; Song, A.-G.; Ji, Y.-F.;* **Wang, W.*** "Interplay of Direct Stereo-control and Dynamic Kinetic Resolution in a Bifunctional Amine Thiourea Catalyzed Highly Enantioselective Cascade Michael-Michael Reaction" *Chem. Eur. J.,* **2011,** *17*, 770-774.

28) Liu, C-L.; Zhang, X.-S.; Wang, R.;* **Wang, W.*** ""One-pot" Access to 4*H*-Chromenes with Formation of a Chiral Quaternary Stereogenic Center by a Highly Enantioselective Iminium-allenamine Involved Oxa-Michael-Aldol Cascade" *Org. Lett.,* **2010**, *12*, 4948-4951.

29) Gao, Z.; Zhang, T.; Wu, M.; Xiong, Q.; Sun, H.; Zhang, Y.; Zu, L.; **Wang, W.;*** Li, M.* "Isoform-specific Prolongation of KCNQ (Kv7) Potassium Channels Opening Mediated by New Molecular Determinants for Drug-Channel Interactions" *J. Bio. Chem.* **2010**, *285*, 28322-28332.

30) Zhang, X.-S.; Zhang, S.-L.; **Wang, W.*** "Iminium Allenamine Cascade Catalysis: "One-pot" Access to Chiral 4H-Chromenes by a Highly Enantioselective Michael-Michael Sequence" *Angew. Chem. Int. Ed.,* **2010,** *49*, 1481-1484. **This work has been highlighted in *Synfacts***.

31) Xue, F.; Liu, L.; Zhang, S.; Duan, W.-H.; Wang, W. "A Simple Primary Amine-Thiourea Catalyzed Highly Enantioselective Conjugate Addition of α, α-Disubstituted Aldehydes to Maleimides" *Chem. Eur. J.,* **2010**, *16*, 7979-7982. **This work has been highlighted in *Synfacts***.

32) Zhang, N.; Agbor, L. N.; Scott, J. A.; Zalobowski, T.; Elased, K. M.; Trujillo, A.; Duke, M. S.; Wolf, V.; Walsh, M. T.; Born, J. L.; Felton, L. A.; Wang, J.; **Wang, W.;** Kanagy, N. L.; Walker, M. K. "An Activated Renin-angiotensin System Maintains Normotension in Aryl Hydrocarbon Receptor Heterozygous Mice but not Null Mice" *Biochem. Pharmacol.*, **2010**, 80, 197-204.

33) Zhang, Y.-N.; Yu, C.-G.; Ji, Y.-F.;* **Wang, W.*** "Diastereo- and Enantioselective Organocatalytic Direct Conjugate Addition of γ-Butenolide to Chalcones" *Chem. Asian. J.,* **2010,** *5*, 1303-1306.

34) Jiang, W.; Cao, Y.-T.; Liu, Y.; **Wang, W.*** "Rational Design of a Highly Selective and Sensitive Fluorescent PET Probe for Discrimination of Thiophenols and Aliphatic Thiols" *Chem. Commun.,* **2010**, *46*, 1944-1966.

35) Huang, J.-L.; Zhu, F.-X.; He, W.-H.; Zhang, F.; **Wang, W.*** Li, H.-X.* "Periodic Mesoporous Organometalsilicas with Unary or Binary Organometals Inside the Channel Walls as Active and Reusable Catalysts in Aqueous Organic Reactions" *J. Am. Chem. Soc.,* **2010**, *132*, 1492-1493.

36) Yu, C.-G.; Zhang, Y.-N.; Zhang, S.-L.; He, J.;* **Wang, W.*** "Highly Enantioselective Michael-cyclization Cascade Promoted by Synergistic Asymmetric Aminocatalysis and Lewis Acid Catalysis" *Tetrahedron Lett.,* **2010**, *51*, 1742-1744.

37) Deng, J.; Zhang, S.-L.; Ding, P.; Jiang, H.-L.; **Wang, W.*** and Li, J.* "Facile Creation of Privileged 3-Indolyl-3-hydroxy-2-oxindoles by an Organocatalytic Enantioselective Friedel-Crafts Reaction of Indoles with Isatins" *Adv. Synth. Catal.,* **2010**, *352*, 833-838.

38) Zhang, S.-L.; Li, J.;* Zhao, S.-H.; **Wang, W.*** "1,3-Benzodithiole-1,1,3,3-tetraoxide (BDT) as a Versatile Methylation Reagent in Catalytic Enantioselective Michael Addition Reaction with Enals" *Tetrahedron Lett.,* **2010**, *51*, 1766-1769.
39) Liu, J.; Zhu, J.; Jiang, H.-L.; **Wang, W.;*** Li, J.* "Pd-Catalyzed Cascade Heck-Saegusa: Direct Synthesis of Enals from Aryl Iodides and Allyl Alcohol" *Chem. Commun.,* **2010,** *46*, 415-417.
40) Zhang, H.-Y.; Zhang, S.-L.; Liu, L.; Lou, G.-S.; Duan, W.-H.; **Wang, W.*** "Synthesis of Chiral 3-Substituted Phthalides by a Sequential Organocatalytic Enantioselective Aldol-lactonization Reaction. Three-step Synthesis of (*S*)-(-)-3-Butylphthalide" *J. Org. Chem.,* **2010,** *75*, 368-374.
41) Li, H.; Ji, Y.-F.; Li, J.; Zhang, S.-L.; Yu, C.-G.; **Wang, W.*** "Organocatalytic Enantioselective Michael Addition Reactions of Fluoromalonates with α, β-Unsaturated Aldehydes" *Science China – Chemistry,* **2010,** *53*, 135-139.
42) Zu, L.-S.; Zhang, S.-L.; Xie, H.-X.; **Wang, W.*** "Catalytic Asymmetric oxa-Michael-Michael Cascade for Facile Construction of Chiral Chromans via an Aminal Intermediate" *Org. Lett.,* **2009,** *11*, 1627-1630. **This work has been highlighted in *Org. Chem. Highlights.***
43) Masood, A.; Huang, Y.; Hajjhussein, H.; Xiao, L.; Li, H.; Wang, W.; Hamza, A.; Zhan, C.-G.; O'Donnell, J. M. **"**Anxiolytic Effects of Phosphodiesterase-2 Inhibitors Associated with Increased cGMP Signaling" *J. Pharmacol. Exp. Ther.* **2009**, *331*, 690-699.
44) Njus, B. H.; Chigaev, A.; Waller, A.; Wlodek, D.; Ostopovici-Halip, L.; Ursu, O.; **Wang, W.**; Oprea, T. I.; Bologa, C. G.; Sklar, L. A. "Conformational mAb as a Tool for Integrin Ligand Discovery" *ASSAY Drug Dev. Tech.,* **2009**, *7*, 507-515.
45) Mei, K.; Jin, M.; Zhang, S.-L.; Li, P.; Liu, W.-J.; Chen. X.-B.; Xue, F.; Duan, W.-H.; **Wang, W.*** "Simple Cyclohexanediamine-Derived Primary Amine Thiourea Catalyzed Highly Enantioselective Conjugate Addition of Nitroalkanes to Enones" *Org. Lett.,* **2009,** *11*, 2864-2867.
46) Liu, J.; Zhu, J.; Jiang, H.-L.; **Wang, W.;*** Li, J.* "Direct Oxidation of β-Aryl Substituted Aldehydes to α, β-Unsaturated Aldehydes Promoted by a *o*-Anisidine-Pd(OAc)$_2$ Co-catalyst" *Chem. Asian. J.,* **2009,** *4*, 1712-1716.
47) Xue, F.; Zhang, S.-L.; Liu, L.; Duan, W.-H.; **Wang, W.** "Organocatalytic Enantioselective Cross-Aldol Reactions of Aldehydes with Isatins: Formation of Two Contiguous Quaternary Centered 3-Substituted 3-hydroxyindol-2-ones" *Chem. Asian. J.,* **2009,** *4*, 1664-1667.
48) Zhang, S.-L.; Zhang, Y.-N. Ji, Y.-F. Li, H.; **Wang, W.*** "Catalytic Enantioselective Conjugate Addition of Fluorobis(phenylsulfonyl)methane to Enals: Synthesis of Chiral Monofluoromethyl Compounds" *Chem. Commun.,* **2009,** 4886-4888.
49) Jiang, W.; **Wang, W.*** "A Selective and Sensitive "Turn-on" Fluorescent Chemodosimeter for Hg^{2+} in Aqueous Media via Hg^{2+} Promoted Facile Desulfurization-lactonization Reaction" *Chem. Commun.,* **2009,** 3913-3915.
50) Luo, G.; Zhang, S.-L.; Duan, W.-H.;* **Wang, W.*** "Enantioselective Organocatalytic Synthesis of Highly Functionalized Tetrahydrothiophenes by a Michael-aldol Cascade Reaction" *Tetrahedron Lett.*, **2009**, *50*, 2946-2948.
51) Zhu, J.; Liu, J.; Ma, R.; Xie, H. Li, J.;* Jiang, H.-L.; **Wang, W.*** "A Direct Amine-Pd(OAc)$_2$ Co-catalyzed Saegusa Oxidation Reaction of Unmodified Aldehydes to alpha, beta-Unsaturated Aldehydes" *Adv. Synth. Catal.,* **2009**, *351*, 1229-1232.
52) Li, H.; Zhang, S.-L.; Yu, C. G.; Song, X.-X.; **Wang, W.*** "Synthesis of Chiral Fluorinated Quaternary Carbon Containing β-Ketoesters" *Chem. Commun.,* **2009,** 2136-2138.
53) Gan, X.-W.; Jiang, W.; **Wang, W.;*** Hu, L.-H.* "An Approach to 3,6-Disubstituted 2,5-Dioxybenzoquinones via Two Sequential Suzuki Couplings. Three-step Synthesis of Leucomelone" *Org. Lett.,* **2009,** *11*, 598-592.
54) Li, H.; Zu, L.; Xie, H.; **Wang, W.*** "Organocatalytic Enantioselective Conjugate Addition of 2-Fluoromalonate to Nitroolefins: Direct Synthesis of Chiral Fluorinated γ-Nitro Carboxylic Acid Derivatives" *Synthesis*, **2009**, 1525-1530, invited Special Topics.

55) Luo, G.; Zhang, S.; Duan, W.;* **Wang, W.*** "Chiral Primary Amine Catalyzed Enantioselective Conjugate Addition of *N*-Heterocycles to α, β-Unsaturated Ketones" *Synthesis*, **2009**, 1564-1572, invited Special Topics.

56) Ma, S.; Zhang, S.; Duan, W.;* **Wang, W.*** "An Efficient Enantioselective Synthesis of (+)-(*S*)-[n]-Gingerol via the L-Proline-catalyzed Aldol Reaction" *Bioorg. Med. Chem. Lett.,* **2009**, *19*, 3909-3911. (Invited Special Issue)

57) Song, L; Chen, X.; Zhang, S.-L.;* Zhang, H.; Li, P.; Luo, G.; Liu, W.; Duan, W.-H.;* **Wang, W.*** "An Organocatalytic Approach to the Construction of Chiral Oxazolidinone Rings and Application in the Synthesis of Antibiotic Linezolid and Its Analogues" *Org. Lett.*, **2008,** *10*, 5489-5492.

58) Li, H.; Zu, L.-S.; Xie, H.-X.; Wang, J.; **Wang, W.*** "Highly Enantio- and Diastereoselective Organocatalytic Cascade aza-Michael-Michael Reactions: A Direct Method for the Synthesis of Trisubstituted Chiral Pyrrolidines" *Chem. Commun.*, **2008**, 5636-5638. **This work has been highlighted in *Org. Chem. Highlights as* "New methods for C-N ring construction."** by Organic Chemistry Portal: http://www.organic-chemistry.org/Highlights/2009/27April.shtm.

59) Fu, Z.; Malureanu, L.; Huang, J.; **Wang, W.;** Li, H.; van Deursen, J. M.; Tindall, D. J.;* Chen, J.* "Plk1-dependent Phosphorylation of FoxM1 Regulates a Transcriptional Program Required for Mitotic Progression" *Nature Cell Biol.,* **2008**, *10*, 1076-1082.

60) Xue, F.; Zhang, S.-L.;* Duan, W.-H.;* **Wang, W.*** "A Novel Bifunctional Sulfonamide Primary Amine-Catalyzed Enantioselective Conjugate Addition of Ketones to Nitroolefins" *Adv. Synth. Catal.,* **2008,** *350*, 2194-2198.

61) Zhang,Y.-N.; Zhang, S.-L. Ma, L.; Zhang, Y.; Shen, X.;* **Wang, W.;*** Hu, L.-H.* "Total Synthesis of (+)-Rutamarin" *Adv. Synth. Catal.,* **2008,** *350*, 2373-2379.

62) Wang, J.; Xie, H.-X.; Li, H.; Zu, L.-S.; **Wang, W.*** "A Highly Stereoselective Hydrogen-bond Mediated Cascade Michael-Michael Process through Dynamic Kinetic Resolution" *Angew. Chem. Int. Ed.*, **2008**, *47*, 4177-4179. **This work has been selected as "hot" paper by Angew. Chem. Editors.**

63) Zu, L.-S.; Xie, H.-X.; Li, H.; Wang, J.; Yu, X.-H.; **Wang, W.*** "Chiral Amine Catalyzed Enantioselective Cascade Aza-ene-type Cyclization Reactions" *Eur. Chem. J.,* **2008**, *14*, 6333-6335.

64) Zhou, L.; Wang, W.-J.; Zuo, L.;* Yao, S.-Y.; **Wang, W.**;* Duan, W.* "Selective Debenzylation of Aromatic Benzyl Ethers by Silica-Supported Sodium Hydrogen Sulfate" *Tetrahedron Lett.*, **2008**, *49*, 4876-4878. **This work has been highlighted in *Synfacts.***

65) Liu, G.-X.; Wang, W. "An Update: Diisopropyl 2-Allyl-1,3,2-dioxaborolane-4,5-dicarboxylate" *Encyclopedia of Reagents for Organic Synthesis [EROS]*, **2008**, invited book chapter.

66) Zuo, L.; Yao, S.-Y.; **Wang, W.***; Duan, W.* "An Efficient Method for Demethylation of Aryl Methyl Ethers" *Tetrahedron Lett.*, **2008**, *49*, 4054-4056. **This work has been selected as "*Best Synthetic Methods: Functional Group Protection*" by Organic Chemistry Portal**: http://www.organic-chemistry.org/Highlights/2008/10November.shtm.

67) Xu, H.; Yu, X.-H.* Sun, L.; Liu, J.; Fan, W.; Shen, Y.;* **Wang, W.*** "Microwave-Assisted Three Component Knoevenagel-nucleophilic Aromatic Substitution Reactions" *Tetrahedron Lett.*, **2008**, *49*, 4687-4689.

68) Xie, H.-X.; Zu, L.-S.; Hanine R. Oueis, Li, H.; Wang, J.; **Wang, W.*** "Proline Catalyzed Direct Inverse Electron Demand Diels-Alder Reactions of Ketones with 1,2,4,5-Tetrazines" *Org. Lett.*, **2008**, *10*, 1923-1926.

69) Zu, L.-S.; Xie, H.-X.; Li, H.; Wang, J.; **Wang, W.*** "Highly Enantioselective Aldol Reactions Catalyzed by a Recyclable Fluorous (*S*) Pyrrolidine Sulfonamide on Water" *Org. Lett.*, **2008**, *10*, 1211-1214.

70) Mei, K.; Zhang, S.;* He, S.; Li, P.; Jin, M.; Xue, F.; Luo, G.; Zhang, H.; Song.; L.; Duan, W.;* **Wang, W.*** "(*S*) Pyrrolidine Sulfonamide Catalyzed Asymmetric Direct Aldol Reactions of Aryl Methyl Ketones with Aryl Aldehydes" *Tetrahedron Lett.*, **2008**, *49*, 2681-2684.
71) Yu, X.; **Wang, W.*** "Hydrogen-Bond Mediated Asymmetric Catalysis" *Chem. Asian J.,* **2008**, 3, 516-532 (invited review).
72) Jiang, W.; Fu, Q.-Q.; Fan, H.Y.; **Wang, W.*** "An NBD Fluorophore-Based Sensitive and Selective Fluorescent Probes for Zinc Ion" *Chem. Commun.,* **2008,** 259-261.
73) Zhang, S.; Chen, X.; Zhang, J.; **Wang, W.**;* Duan, W.* "An Enantioselective Formal Synthesis of (*R*)-(+)-α-Lipoic Acid by L-Proline-catalyzed Aldol Reaction" *Synthesis*, **2008**, 383-386.
74) Yu, X.; **Wang, W.*** "Organocatalysis: Chiral Secondary Amine Catalyzed Asymmetric Cascade Reactions" *Org. Biomol. Chem.*, **2008**, *6*, 2037-2046. **The paper is featured as the cover of *Org. Biomol. Chem.***
75) Xiong, Q.-J.; Gao, Z.-B.; **Wang, W.**; Li, M.* "Activation of Voltage-Activated Potassium Channels by Chemical Ligands" *Trends Pharmacol. Sci.*, **2008,** *29*, 99-107.
76) Jiang, W.; Fu, Q.-Q.; Fan, H.-Y.; Ho, J.; **Wang, W.*** "A Highly Selective Fluorescent Probe for Facile Detection of Thiophenols" *Angew. Chem. Int. Ed.*, **2007**, *46*, 8445-8448.
77) Zu, L.-S.; Xie, H.-X.; Li, H.; Wang, J.; **Wang, W.*** "Three Step Synthesis of Chrial Baclofen *via* a Highly Enantioselective Organocatalytic Conjugate Addition of Nitromethane to α, *β*-Unsaturated Aldehydes" *Adv. Synth. Catal.,* **2007,** *349*, 2660-2664.
78) Wang, J.; Li, H.; Xie, H.-X.; Zu, L.-S.; Shen, X.; **Wang, W.*** "Organocatalytic Enantioselective Cascade Michael-Aldol-Dehydration Reactions: Efficient Assembly of Densely Functionalized Chiral Cyclopentenes" *Angew. Chem. Int. Ed.,* **2007**, *46*, 9050-9053. **This article has been selected as a "Hot paper" by *ACIE*.**
79) Xie, H.-X.; Zu, L.-S.; Li, H.; Wang, J.; **Wang, W.*** "Organocatalytic Enantioselective Cascade Michael-Alkylation Reactions. Synthesis of Chiral Cyclopropanes and Investigation of Unexpected Organocatalyzed Stereoselective Ring Opening of Cyclopropanes" *J. Am. Chem. Soc.*, **2007**, *129*, 10886-10894. **This work was highlighted in *Synfacts*.**
80) Zu, L.-S.; Xie, H.-X.; Li, H.; Wang, J.; Jiang, W.; **Wang, W.*** "A Chiral Amine Thiourea Promoted Enantioselective Domino Michael-Aldol Reactions between 2-Mercapto-Benzaldehydes and Maleimides" *Adv. Synth. Catal.*, **2007**, *349*, 1882-1886.
81) Zu, L.-S.; Wang, J.; Li, H.; Xie, H.-X.; Jiang, W.; **Wang, W.*** "Cascade Michael-aldol Reactions Promoted by Hydrogen-Bonding Mediated Catalysis" *J. Am. Chem. Soc.*, **2007**, *129*, 1036-1037. **This work was recognized as the "Most-cited" and a "Hot" paper of *JACS*.**
82) **Wang, W.*** Book Review: "Analogue-Based Drug Discovery" *Drug Dev. Ind. Pharm.,* **2007**, *33*, 803.
83) Zu, L.-S.; Li, H.; Xie, H.-X.; Wang, J.; Jiang, W.; Tang, T.; **Wang, W.*** "Synthesis of Highly Functionalized Chiral Cyclopentanes by Catalytic Enantio- and Diastereoselective Double Michael Addition Reactions" *Angew Chem. Int. Ed.,* **2007**, *46*, 3732-3734. **This work was highlighted in *Synfacts*.**
84) Li, H.; Zu, L.-S.; Xie, H.-X.; Wang, J.; Jiang, W.; **Wang, W.*** "Enantioselective Organocatalytic Double Michael Addition Reactions" *Org. Lett.*, **2007**, *9*, 1833-1835. **This work was highlighted in *Synfacts* and *Org. Chem. Highlights* (http://www.organic-chemistry.org/Highlights/2008/10March.shtm).**
85) Wang, J.; Heikkinen, L. D.; Li, H.; Zu, L.-S.; Jiang, W.; **Wang, W.*** "Quinine-Catalyzed Enantioselective Michael Addition of Diphenyl Phosphite to Nitroolefins: Synthesis of Chiral Precursors of α-Substituted β-Amino Phosphonates" *Adv. Synth. Catal.*, **2007**, *349*, 1052-1056. **This work was recognized as one of the most accessed articles in 05/2007 of *Adv. Synth. Catal.* and highlighted in *Synfacts*.**

86) Li, H.; Wang, J.; Xie, H.-X.; Zu, L.-S.; Jiang, W.; Duesler, E. N.; **Wang, W.*** "Enantioselective Organocatalytic Cascade Reactions: Facile Synthesis of Chiral 1,2-Dihydroquinolines" *Org. Lett.*, **2007**, *9*, 965-968. **This work was recognized as the "Most-cited" and "Hot" paper of *OL.***

87) Li, H.; Wang, J.; E-Nunu, T.; Zu, L.-S.; Jiang, W.; Wei, S.-H.; **Wang, W.*** "One-Pot Approach to Chiral Chromenes *via* Enantioselective Organocatalytic Domino Oxa-Michael-Aldol Reaction" *Chem. Commun*., **2007**, 507-509. **This work was recognized in the top 5 (number 2) of the "Most cited" papers published on *Chem. Commun*. since 2007.**

88) Wang, J.; Zu, L.-S.; Li, H.; Xie, H.-X.; Jiang, W. **Wang, W.* "**Enantioselective Michael Addition of *N*-Heterocycles to Enones Catalyzed by a Bifunctional Cinchona Alkaloid Thiourea" invited to contribute to Special Topics Thiourea in *Synthesis*, **2007**, 2576-2580.

89) Wang, J.; Li, H.; Zu, L.-S.; Jiang, W.; Xie, H.-X.; Duan, W.-H.; **Wang, W.*** "Enantioselective Organocatalytic Conjugate Additions to Enones" *J. Am. Chem. Soc.*, **2006**, *128*, 12652-12653. **This work was recognized as the "Most-cited" and a "Hot" Paper of *J. Am. Chem. Soc.*.**

90) Zu, L.-S.; Wang, J.; Li, H.; Yu, X-H.; **Wang, W.*** "A Recyclable Fluorous (*S*)-Pyrrolidine Sulfonamide Promoted Direct, Highly Enantioselective Michael Addition of Ketones and Aldehydes to Nitroolefins in Water" *Org. Lett.*, **2006**, *8*, 3077-3079. **This work was recognized as a "Hot Paper" in March 2007 and one of the most cited articles (top 6) in 2006 on *Org. Lett.* It was also highlighted in http://www.organic-chemistry.org/abstracts/lit1/320.shtm.**

91) Liu, S.-Y.; Fan, Y.-P.; Peng, X.-X.; **Wang, W.;*** Hua, W.-Y.; Akber, H.; Liao, L.-X.* "A Concise and Enantioselective Approach to the Total Synthesis of (-)-Lasubine I" *Tetrahedron Lett.,* **2006**, *47*, 7681-7684.

92) **Wang, W.;*** Li, H.; Wang, J.; Zu, L.-S.; "Enantioselective Organocatalytic Tandem Michael-Aldol Reactions: One-Pot Synthesis of Chiral Thiochromenes" *J. Am. Chem. Soc.*, **2006**, *128*, 10354-10355. **This work was recognized as the "Most-cited" and a "Hot" Paper of *J. Am. Chem. Soc.* and highlighted in *Synfacts*.**

93) Wang, J.; Li, H.; Zu, L.; Jiang, W.; **Wang, W.*** "Organocatalytic, Enantioselective Conjugate Addition of Nitroalkanes to Nitroolefins" *Adv. Synth. Catal.,* **2006**, *348*, 2047-2050. **This work was recognized as one of the Most Accessed Articles from 6/2006 to 5/2007 of *Adv. Synth. Catal.* and highlighted in *Synfacts*.**

94) Wang, J.; Li, H.; Zu, L.-S.; **Wang, W.*** "Enantioselective Organocatalytic Michael Addition Reactions between *N*-Heterocycles and Nitroolefins" *Org. Lett.,* **2006**, *8*, 1391-1394. **This work was highlighted in *Synfacts*.**

95) Wang, J.; Li, H.; Zu, L.-S.; **Wang, W.*** "Highly Enantioselective Organocatalytic Michael Addition Reactions of Ketones with Chalcones" *Adv. Synth. Catal.,* **2006**, *348*, 425-428. **This work was recognized as one of the Most Accessed Articles in the year of 2006 on *Adv. Synth. Catal*..**

96) Zu, L.-S.; Wang, J.; Li, H.; Yu, X-H.; **Wang, W.*** "Highly Enantioselective Aldehyde-Nitroolefin Michael Addition Reactions Catalyzed by Recyclable Fluorous (*S*) Diphenylpyrrolinol Silyl Ether" *Tetrahedron Lett.*, **2006**, *47*, 5131-5134.

97) Zhang, S.-L.; Duan, W.-H.;* **Wang, W.*** "Efficient, Enantioselective Organocatalytic Synthesis of Trichostatin A" *Adv. Synth. Catal.,* **2006**, *348*, 1228-1234.

98) Li, H.; Wang, J.; Zu, L.-S.; **Wang, W.*** "Organocatalytic Asymmetric Conjugate Addition of Thioacetic Acid to β-Nitrostyrenes" *Tetrahedron Lett.,* **2006**, *47*, 2585-2589.

99) Li, H.; Zu, L.-S.; Wang, J.; **Wang, W.*** "Organocatalytic Asymmetric Conjugate Addition of Thioacetic Acid to Enones" *Tetrahedron Lett.,* **2006**, *47,* 3145-3148.

100) Mei, Y.; Bentley, P. A.; **Wang, W.** "A Selective and Sensitive Chemosensor for Cu^{2+} Based on 8-Hydroxyquinoline" *Tetrahedron Lett.*, **2006**, *47*, 2447-2449.

101) Wang, J.; Li, H.; Lou, B.; Zu, L.-S.; Guo, H.; **Wang, W.*** "Enantio- and Diastereoselective Michael Addition Reactions of Unmodified Aldehydes and Ketones with Nitroolefins Catalyzed by a Pyrrolidine Sulfonamide" *Eur. Chem. J.,* **2006**, *12*, 4321-4332.

102) Wang, J.; Li, H.; Yu, X.-H.; Zu, L-S.; **Wang, W.*** "Chiral Binaphthyl-Derived Amine-Thiourea Organocatalyst Promoted Asymmetric Morita-Baylis-Hillman Reaction" *Org. Lett.,* **2005**, *7*, 4293-4296. **This work was recognized as a *Org. Lett.* Hot Paper and the most cited paper published on *Org. Lett.* in 2005, 2006 and 2007.**

103) Wang, J.; Li, H.; Duan, W.-H.; Zu, L-S.; **Wang, W.*** "Organocatalytic Asymmetric Michael Addition of 2,4-Pentandione to Nitroolefins" *Org. Lett.,* **2005**, *7*, 4713-4716. **This work has been recognized as a *Org. Lett.* Hot Paper and one of the most cited papers published in *Org. Lett.* in 2005.**

104) Wang, J.; Li, H.; Mei, Y.; Lou, B.; Xu, D.; Xie, D.; Guo, H.; and **Wang, W.*** "Direct, Facile Aldehyde and Ketone α-Selenenylation Reactions Promoted by L-Prolinamide and Pyrrolidine Sulfonamide Organocatalysts" *J. Org. Chem.* **2005**, *70*, 5678-5687.

105) **Wang, W.**;* Li, H.; Wang, J. "Pyrrolidine Sulfonamide Promoted Direct, Enantioselective Aldol Reactions of α, α-Dialkyl Aldehydes: Synthesis of Quaternary Carbon-Containing β-Hydroxy Carbonyl Compounds" *Tetrahedron Lett.*, **2005**, *46*, 5077-5079.

106) **Wang, W.**;* Li, H.; Wang, J. "Enantioselective, Organocatalytic Mukaiyama-Michael Addition of Silyl Ethers to α, *β*–Unsaturated Aldehydes" *Org. Lett.*, **2005**, *7*, 1637-1639.

107) **Wang, W.**;* Mei, J.; Li, H.; Wang, J. "A Novel Pyrrolidine Imide Catalyzed Direct Formation of α, *β*–Unsaturated Ketones from Unmodified Ketones and Aldehydes" *Org. Lett.*, **2005**, *7*, 601-604. **This paper is one of the Most Accessed Articles of *Org. Lett.* in the year of 2005.**

108) **Wang, W.**;* Wang, J.; and Li, H. "Direct, Highly Enantioselective Pyrrolidine Sulfonamide Catalyzed Michael Addition Reactions of Aldehydes to Nitrostyrenes" *Angew. Chem. Int. Ed.,* **2005**, *44*, 1369-1371. **This work was recognized as the most cited paper of *Angew. Chem. Int. Ed.* in 2005/2006 and was highlighted in *Org. Chem. Highlights* 2006, January 30. URL: http://www.organic-chemistry.org/Highlights/2006/30JanuaryB.shtm.**

109) **Wang, W.;*** Wang, J.; Li, H. "A Simple and Efficient L-Prolinamide-Catalyzed α-Selenenylation Reactions of Aldehydes," *Org. Lett.,* **2004**, *6*, 2817-2820.

110) **Wang, W.**;* Li, H. "An Efficient Synthesis of the Intrinsic Fluorescent Peptide Labels, (*S*) and (*R*) (6,7-Dimethoxyl-4-coumaryl)alanines *via* Asymmetric Hydrogenations" *Tetrahedron Lett.*, **2004**, *45*, 8479-8481.

111) **Wang, W.**;* Li, H.; Wang, J., Liao, L.-X. "Direct, Organocatalytic alpha-Sulfenylation of Aldehydes and Ketones" *Tetrahedron Lett.,* **2004**, *45*, 8229-8231.

112) **Wang, W.;*** Wang, J.; Li, H., Liao, L.-X. "A Novel Amine Sulfonamide Organocatalyst for Promoting Direct, Highly Enantioselective α-Aminoxylation Reactions of Aldehydes and Ketones", *Tetrahedron Lett.*, **2004**, *45*, 7235-7238. **"Top-50 most cited articles" published in *Tetrahedron Lett.* In 2004-2007.**

113) **Wang, W.;*** Wang, J.; Li, H. "Catalysis of Highly Stereoselective Mannich-Type Reactions of Ketones with α-Imino Esters by a Pyrrolidine Sulfonamide. Synthesis of Unnatural α-Amino Acids," *Tetrahedron Lett.,* **2004**, *45*, 7243-7246. **"Top-50 most cited articles" published in *Tetrahedron Lett.* 2004-2007.**

Before joining UNM (post-doc and graduate work):

114) Zhang, J.; **Wang, W.;*** Xiong, C.; and Hruby, V.J.* "Efficient and Stereoselective Synthesis of *cis*-4-Substittued Proline Analogues" *Tetrahedron Lett.,* **2003**, *44*, 1413-1415.

115) Xiong, C.; Zhang, J.; Davis, P.; **Wang, W.**; Ying, J.; Porreca, F.; and Hruby, V.J. "Stereoselective Synthesis of Individual Isomers of Leu-Enkephalin Analogues Containing Substituted β-Turn Bicyclic Dipeptide Mimetics" *Chem. Commun.,* **2003**, 1598-1599.

116) Zhang, J.; Xiong, C.; Ying, J.; **Wang, W.**; Hruby, V.J. "Stereoselective Synthesis of Dipeptide β-Turn Mimeitcs Targeting Melanocortin Receptors: 4,8-Disubstituted Azabicyclo[4.3.0]nonane Amino Acid Esters" *Org. Lett.,* **2003**, 5, 3115-3118.

117) **Wang, W.**; Yang, J.; Ying, J.; Xiong, C.; Zhang, J.; Cai, C.; Hruby, V.J. "Stereoselective Synthesis of Dipeptide β-Turn Mimetics: 7-Benzyl and 8-Phenyl Substituted Azabicyclo[4.3.0] Amino Acids" *J. Org. Chem.,* **2002**, 67, 6353-6360.

118) **Wang, W.**; Cai, M., Xiong, C.; Zhang, J.; Tevil, D.; Hruby, V.J. "Design and Synthesis of Novel χ^2-Constrained Phenylalanine, Naphthylalanine, and Tryptophan Analogues and their Use in Biologically Active Melanotropin Peptides" *Tetrahedron,* **2002**, *58*, 7365-7374.

119) Zhang, J.; Xiong, C.; **Wang, W.**; Ying, J.; Hruby, V.J. "Stereoselective Bromination-Suzuki Cross-Coupling of Dehydroamino Acids to Form Novel Reverse-Turn Peptidomimetics: Substituted Unsaturated and Saturated Indolizidinone Amino Acids" *Org. Lett.,* **2002**, *4*, 4029-4032.

120) **Wang, W.**; Gao, X.; Wang, B. "Boronic Acid-Based Sensors for Carbohydrates" *Curr. Org. Chem,* **2002**, *6*, 1285-1317.

121) Xiong, C.; **Wang, W.**; Hruby, V.J. "A General Asymmetric Synthesis of *syn* and *anti*-β-Substituted Cysteine and Serine Derivatives" *J. Org. Chem.*, **2002**, *67*, 3514-3517.

122) **Wang, W.**; Zhang, J.; Xiong, C.; Hruby, V.J. "Design and Synthesis of Hydrophobic, Bulky χ^2-Constrained Phenylalanine and Naphthylalanine Derivatives" *Tetrahedron Lett.,* **2002**, *43*, 2137-2140.

123) Xiong, C.; **Wang, W.**; Hruby, V.J. "Regioselective and Stereoselective Nucleophilic Ring Opening Reactions of a Phenyl Substituted Aziridine: Enantioselective Synthesis of β-Substituted Tryptophan, Cysteine, and Serine Derivatives" *J. Org. Chem.*, **2002**, *67*, 1339-1402.

124) **Wang, W**.; Xiong, C.; Zhang, J.; Hruby, V.J. "Practical, Asymmetric Synthesis of Aromatic-Substituted Bulky and Hydrophobic Tryptophan and Phenylalanine Derivatives" *Tetrahedron,* **2002**, *58*, 3101-3110.

125) **Wang, W.**; Xiong, C.; Hruby, V.J. "An Efficient Synthesis of (*2S, 6S*) and *meso*-(*2S, 6R*)-Diaminopimelic Acids via Asymmetric Hydrogenation" *Synthesis,* **2002**, 94-98.

126) **Wang, W.**; Xiong, C.; Hruby, V.J. "An Efficient Approach to Asymmetric Synthesis of Dipeptide β-Turn Mimetics: Indolizidinone Amino Acids" *Tetrahedron Lett.,* **2001**, *42*, 3159-3161.

127) **Wang, W.**; Xiong, C.; Yang, J.; Hruby, V.J. "Practical, Asymmetric Synthesis of Aromatic-substituted Bulky and Hydrophobic Tryptophan Derivatives" *Tetrahedron Lett.*, **2001**, *42*, 7717-7719.

128) Springsteen, G., Ballard, C.E., Gao, S.; **Wang, W.**; Wang, B. "The Developemnt of Photometric Sensors for Boronic Acids" *Bioorg. Chem.*, **2001**, *29*, 259-270.

129) Gao, S.; **Wang, W.**; Wang, B. "Building Fluorescent Sensors for Carbohydrates Using Templated-directed Polymerizations" *Bioorg. Chem.*, **2001**, *29*, 308-320.

130) Gao, S.; **Wang, W.**; Wang, B. "A Novel OsO_4-Catalyzed Carbon-Carbon Bond Cleavage Reaction to Give Anthraquinone" *Chemistry Lett.,* **2001**, 48-49.

131) Jiang, J.; **Wang, W.**; Sane, D.C.; Wang, B. "Synthesis of RGD Analogs as Potential Vectors for Targeted Drug Delivery" *Bioorg. Chem.*, **2001**, *29*, 357-379.

132) **Wang, W.**; Borchardt, R.T.; Wang, B. "Orally Active Peptidomimetic RGD Analogs that are Glycoprotein IIb/IIIa Antagonists" *Curr. Med. Chem.*, **2000**, *7*, 437-453.

133) **Wang, W.**; Springsteen, G.; Gao, S.; Wang, B. "The First Fluorescent Sensor for Boronic and Boric Acids with Sensitivity at Sub-micromolar Concentrations" *Chem. Comm.* **2000**, 1283-1284.

134) **Wang, W.**; Camenisch, G.; Sane, D.C.; Zhang, H.; Hugger, E.; Wheeler, G.L.; Borchardt, R.T.; Wang, B."The Use of Prodrug Strategy to Optimize the Oral Absorption of RGD Peptidomimetics" *J. Controlled Release*, **2000**, *65*, 245-251.

135) Shan, D.; Zheng, A.; Ballard, C.E.; **Wang, W.**; Borchardt, R.T.; Wang, B. "A Facilitated Cyclic Ether Formationand its Potential Application in Solid-phase Peptide and Organic Synthesis" *Chem. Pharm. Bull.* **2000**, *48*, 238-244.
136) **Wang, W.**; Gao, S.; Wang, B. "Building Fluorescent Sensors by Template Polymerization: The Preparation of a Fluorescent Sensor for D-Fructose" *Org. Lett.*, **1999**, *1*, 1209-1212.
137) **Wang, W.**; Jiang, J.; Ballard, C.E.; Wang, B. "Prodrug Approaches to the Improved Delivery of Peptide Drugs" *Curr. Pharm. Design*, **1999**, *5*, 265-287.
138) Liao, Y.; **Wang, W.**; Wang, B. "Building Fluorescent Sensors by Template Polymerization: The Preparation of a Fluorescent Sensor for L-Tryptophan" *Bioorg. Chem.*, **1999**, *27*, 463-476.
139) Wang, B.; Nimkar, K.; **Wang, W.**; Zhang, H.; Shan, D.; Gudmundsson, O.S.; Gangwar, S.; Siahaan, T.; Borchardt, R.T. "Synthesis and Evaluation of the Physicochemical Properties of Esterase-Sensitive Cyclic Prodrugs of Opioid Peptides Using Coumarinic Acid and Phenylpropionic Acid Linkers" *J. Peptide Res.* **1999**, *53*, 370-382.
140) Borchardt, R.T.; Camenisch, G.; Hugger, E.; **Wang, W.**; Sane, D.C.; Wheeler, G.L.; Cheng, C.-P.; Wang, B. " Prodrug Strategies to Improve the Oral Absorption of Peptide Mimetics" *Polymer Preprints,* **1999**, *40(1)*, 257-258.
141) Zheng, A.; **Wang, W.**; Zhang, H.; Wang, B. "Two New Improved Approaches to the Synthesis of Coumarin-Based Prodrugs" *Tetrahedron* **1999**, *55,* 4237-4254.
142) Gudmundsson, O.S.; Pauletti, G.M.; **Wang, W.**; Shan, D.; Zhang, H.; Wang, B.; Borchardt R.T. "Coumarin-Based Cyclic Prodrugs of Opioid Peptides that Exhibit Metabolic Stability to Peptidases and Excellent Cellular Permeability" *Pharm. Res.* **1999**, *16*, 7-15.
143) Wang, B.; **Wang, W.**; Camenisch, G.P.; Elmo, J.; Zhang, H.; Borchardt, R.T. "Synthesis and Evaluation of Novel Coumarin-Based Esterase-Sensitive Cyclic Prodrugs of Peptidomimetic RGD Analogs with Improved Membrane Permeability" *Chem. Pharm. Bull.* **1999**, *47,* 90-95.
144) Liao, Y.; **Wang, W.**; Wang, B. "Enantioselective Polymeric Transporters of D-Tryptophan Prepared Using Molecular Imprinting Techniques" *Bioorg. Chem.* **1998**, *26*, 309-322.
145) Camenisch, G.P.; **Wang, W.**; Wang, B.; Borchardt, R.T. "A Comparison of the Bioconversion Rates and the Caco-2 Cell Permeation Characteristics of Coumarin-Based Cyclic Prodrugs and Methylester-Baesd Linear Prodrugs of RGD Peptidomimetics" *Pharm. Res.* **1998**, *15,* 1174-1181.
146) Wang, B.; Zhang, H.; Zheng, A.; **Wang, W.** "Coumarin-Based Prodrugs. Part 3: Structural Effects on the Release Kinetics of Esterase-sensitive Prodrugs of Amines" *Bioorg. Med. Chem.* **1998**, *6*, 417-426.
147) Benbrook, D.M.; Madler, M.M.; Spruce, L.W.; Birckbichler, P.J.; Nelson, E.C.; Subramanian, S.; Weerasekare, G.M.; Gale, J.B.; Patterson, M.K.Jr.; Wang, B.; **Wang, W.**; Lu, S.; Rowland, T.C.; DiSivestio, P.; Berlin, K.D. "Biologically Active Heteroarotinoids Exhibiting Anticancer Activity and Decrease Toxicity" *J. Med. Chem.* **1997**, *40*, 3567-3583.
148) Wang, B.; **Wang, W.**; Zhang, H.; Shan, D.; Smith, T.D. "Coumarin-Based Prodrugs 2. Synthesis and Bioreversibility Studies of an Esterase-sensitive Cyclic Prodrug of DADLE, an Opioid Peptide" *Bioorg. Med. Chem. Lett.* **1996**, *6,* 2823-2826.
149) Wang, B.; Zhang, H.; **Wang, W.** "Chemical Feasibility Studies of a Potential Coumarin-Based Prodrug System" *Bioorg. Med. Chem. Lett.* **1996**, *6,* 945-950.

Articles Appearing in Chapters in Edited Volumes:

1) Zhang, S.-L.; **Wang, W.*** "Proline Derivatives" in "Privileged Chiral Ligands" Ed. by Zhou, Q.-L. Wilely-VCH: New York, **2011,** in press.
2) Zhang, S.-X.; **Wang, W.*** "Organocatalytic α-Sulfenylation and α-Selenenylation" in "Comprehensive Chirality" ed. by Yamamoto, H.; Carreira, E. Elsevier: Oxford, UK**, 2011,** in press.

3) Zhang, S.-L.; **Wang, W.*** “Organocatalytic Enantioselective Conjugate Additions of Heteroatoms to α, β-Unsaturated Carbonyl Compounds” in “Catalyitc Asymmetric Conjugate Reactions” ed. by Cordova, A. Wiley-VCH: New York, page 295-319, **2010**.
4) **Wang, W.**; Zheng, A.; Liu, S.; Wang, B. “Solid Supports, Linkers and Solid-Phase Supported Reagents in Chemical Library Synthesis” in *Combinatorial Approaches to Drug Lead* Discovery, Liu, G.; Xiao, X.; Wang, J. Eds. page 88~122, Science Press, China, **2003**.
5) Gao, S.; **Wang, W.**; Wang, B. “Molecularly Imprinted Polymers as Recognition Elements in Optical Sensors” in *Optical Sensors*, Yan, M.; Ramström, O. Eds., Marcel Dekker, Inc., **2002**, invited book chapter.
6) **Wang, W.**; Xiong, C.; Hruby, V.J. “Two Novel and Efficient Approaches to Synthesis of Enantiopure Dipeptide β-Turn Mimetics: Indolizidinone Amino Acids” In *Peptides: The Wave of the Future: Proceeding of the 16th American Peptide Symposium/2nd International Peptide Symposium*, R.A. Houghten and M. Lebl, Editors. **2001**, 30-31.
7) Cai, C.; **Wang, W.**; Xiong, C.; Soloshonok, V.A.; Cai, M.; Hruby, V.J. “Synthesis of Novel β and γ-Substituted Prolines for Conformation-Activity Relationship Studies of the α-MSH Analogues MT-II” In *Peptides: The Wave of the Future: Proceeding of the 16th American Peptide Symposium/2nd International Peptide Symposium*, R.A. Houghten and M. Lebl, Editors. **2001**, 20-21.
8) Xiong, C.; **Wang, W.**; Cai, C.; Hruby, V.J. “The Novel Asymmetric Synthesis of β-Fuctionalized Phenylalanine Derivatives” In *Peptides: The Wave of the Future: Proceeding of the 16th American Peptide Symposium/2nd International Peptide Symposium*, R.A. Houghten and M. Lebl, Editors. **2001**, 24-25.
9) Xiong, C.; **Wang, W.**; Hruby, V.J. “The General Asymmetric Synthesis of *Syn* and *Anti*- β-Substituted Cysteine and Serine Derivatives” In *Peptides: The Wave of the Future: Proceeding of the 16th American Peptide Symposium/2nd International Peptide Symposium*, R.A. Houghten and M. Lebl, Editors. **2001**, 22-23.
10) **Wang, W.**; Borchardt, R.T.; Sane, D.C.; Wang, B. “Delivering Peptides and Peptidomimetics across Membrane Barriers. A Prodrug Approach” In *Peptides for New Millennium: Proceeding of the 16th American Peptide Symposium*, G.B. Fields, J.P. Tam, G. Barany, Editors. Kluwer Academic Publishers, the Netherlands, **2000**, 214-216.
11) Gudmundsson, O.S.; Bak, A.; **Wang, W.**; Shan, D.; Zhang, H.; Friis, G.J., Wang, B.; Borchardt, R.T. "Prodrug Strategies to Enhance the Permeation of Opioid Peptides through the Intestinal Mucosa" *Peptide and Protein Drug Delivery*, S. Frokjer, L. Christruecrd, P. Krogsgard, Editors. Munksgaard, Denmark, **1998**, p 259-269.
12) Wang, B.; Shan, D.; **Wang, W.**; Zhang, H.; Gudmundsson, O.S.; Borchardt, R.T. "Synthesis of Coumarin-Based, Esterase-Sensitive Cyclic Prodrugs of Opioid Peptides with Enhanced Membrane Permeability and Enzymatic Stability" *Methods in Molecular Medicine* Kazmierski, W.; Walker, J.M. Editors. Humana Press Inc., Totowa, NJ. **1998**, 71-85.

Patents (2 total)

1) **Wang, W.;** Wang, J.; Li, H. “Organocatalysis and Methods of Use in Chemical Synthesis” WO 2006007586 (2006).

2) Fan, Y.; Gao, W.; Gray, N.S.; Hinterding, K.; Lefebvre, S.; Mi, Y.; Nussbaumer, P.; Pan, S.; **Wang, W.**; Zecri, F.; Perez, L. B.; La Montagne, K.R.; Ettmayer, P. (Novartis A.-G., Switz.; Novartis Pharma G.m.b.H.; IRM LLC). “Bis-aromatic alkanols” Patent No. WO 2003099192 (2003).

Invited or Refereed Abstracts and /or Presentations at Professional Meetings:

In Universities and Institutes:

"Organocatalytic Reactions of Ynals" for the following talks:

1) School of Pharmacy, East China University of Science & Technology, Shanghai, China, May 9, 2012.

"Novel Strategies in Cascade Organocatalysis" for the following talks:

2) College of Chemistry and Biotechnology, Hubei Science & Technology University, Xianning, Hubei, China, May 7, 2012.
3) Department of Chemistry, New Mexico Tech, Socorro, NM, Mar 30, 2012.
4) Shanghai Institute of Organic Chemistry, The Chinese Academy of Sciences, Shanghai, China, March 20, 2012.
5) School of Pharmacy, University of Iowa, Iowa City, Feb. 21, 2012.
6) Department of Chemistry, Baylor University, Waco, TX, Jan. 27, 2012.
7) Department of Chemistry, Wuhan University, Wuhan, China, Dec. 22, 2011.
8) Department of Chemistry, Central China Normal University, Wuhan, China, Dec. 23, 2011.
9) Department of Chemistry, East China Normal University, Shanghai, China, Dec. 23, 2011.
10) School of Pharmacy, East China University of Science & Technology, Shanghai, China, Dec. 16, 2011
11) Department of Chemistry, University of Houston, Oct. 13, 2011.

"Powerful Organocatalytic Cascade Reactions for Facile Access to Biologically Important Molecular Architectures" for the following talks:

12) "AnyChem, New Jersey, USA, Jul. 15, 2011.
13) Novartis at Suzhou, China, Jun. 22, 2011.
14) Master Forum, School of Pharmacy, The Second Military Medical University, Shanghai, China, June 15, 2011.

"New Strategies for Development of Anti-cancer Agents - A Case Study of NL-101 by Targeting DNA and HDAC," for the following talks:

15) School of Pharmacy, East China University of Science & Technology, Shanghai, China, March 10, 2011.
16) Department of Chemistry, Shanghai Normal University, Shanghai, China, March 14, 2011.

17) *"Chemical Approaches to Chemical and Biological Problems,"* School of Pharmacy, University of New Mexico, Albuquerque, Feb 15, 2010.
18) *"New Strategies in Developing Organocatalytic Cascade Reactions,"* Department of Chemistry, University of Science & Technology of China, Hefei, China, Jun. 14, 2010.
19) *"New Strategies in Developing Catalytic Cascade Reactions,"* Department of Chemistry, Shanghai Normal University, China, Jun. 22, 2010.
20) "*Development and Application of Organocatalytic Reactions in Drug Discovery, Development and Production,"* School of Pharmacy, East China University of Science & Technology, Shanghai, China, June 1, 2009.

"Powerful Enantioselective Organocatalytic Cascade Reactions" for the following talks:

21) Institute of Chemical and Engineering Sciences, A*Star, Singapore, Aug 18, 2009.
22) Department of Chemistry, National University of Singapore, Singapore, Aug. 13, 2009.

23) Department of Chemistry, Nanyang Technology University, Singapore, Aug. 14, 2009.

24) *"Development and Application of Organocatalytic Reactions in Drug Discovery, Development and Production,"* School of Pharmacy, East China University of Science & Technology, Shanghai, China, June 1, 2009.

"Organocatalytic Enantioselective Cascade Reactions, A Powerful Tool for the Efficient Assembly of Complex Molecular Architectures" for the following talks:

25) Department of Chemistry, Tianjin University, China, May 26, 2009.
26) Department of Chemistry, Nankai University, China, May 27, 2009.
27) Department of Chemistry, Beijing Institute of Technology, Beijing, China, May 25, 2009.
28) Shanghai Institute of Materia Medica, Chinese Academy of Sciences, Shanghai, China, May 18, 2009.
29) Department of Chemical and Chemical Biology, Rutgers, The State University of New Jersey, New Jersey, May 8, 2009.
30) Department of Chemistry, University of Alabama, Oct. 17, 2008.
31) Department of Chemistry, Florida State University, Oct. 16, 2008.
32) Department of Chemistry, University of Nevada, Reno, NV, Oct. 3, 2008.
33) Kunming Institute of Botany, Chinese Academy of Sciences, Kunming, China, July 23, 2008.
34) Department of Chemistry, Shanghai Jiaotong University, Shanghai, China, June 3, 2008.
35) Department of Chemistry and Biological Chemistry, University of Southern California, Los Angeles, CA, May 30, 2008.
36) Department of Chemistry and Biological Chemistry, University of California, Los Angeles, CA, May 29, 2008.
37) Department of Chemistry and Biological Chemistry, University of California, Santa Cruz, CA, May 19, 2008.
38) School of Pharmacy, Sichuan University, Chengdu, China, April 22, 2008.
39) Department of Chemistry, Sichuan University, Chengdu, China, April 21, 2008.
40) Department of Chemistry, University of New Orleans, New Orleans, Louisiana, April 4, 2008.
41) Department of Chemistry, Texas A & M University, College Station, Texas, March 20, 2008.
42) Department of Chemistry, University of Texas at Dallas, Dallas, Texas, March 19, 2008.
43) Department of Biochemistry, University of Texas Southwestern Medical Center, Dallas, Texas, March 18, 2008.
44) Department of Chemistry and Biochemistry, University of Delaware, Newark, Delaware, March 12, 2008.
45) Department of Chemistry, University of Washington, Seattle, Washington, February 25, 2008.
46) Department of Chemistry, Washington State University Pullman, Washington, February 27, 2008.
47) Department of Chemistry & Biochemistry, University of California at San Diego, San Diego, CA, December 3, 2007.
48) Department of Chemistry, University of Colorado, Boulder, Colorado, October 30, 2007.
49) Department of Chemistry, Colorado State University, Fort Collins, Colorado, October 29, 2007.
50) Departments of Chemistry and Medicinal Chemistry, University of Toledo, Toledo, Ohio, October 11, 2007.
51) Department of Chemistry, Wayne State University, Detroit, Michigan, October 10, 2007.
52) Department of Chemistry, University of Arizona, Tucson, October 4, 2007.
53) Department of Chemistry, University of Texas at Austin, Austin, Texas, September 19, 2007.
54) Department of Chemistry, University of Houston, Houston, Texas, September 18, 2007.
55) Department of Chemistry, Peking University, Beijing, China, June 15, 2007.

56) *"Chemical Approaches to Biological Problems,"* Shanghai Institute of Materia Medica, Chinese Academy of Sciences, Shanghai, China, June 7, 2007.

"Organocatalytic Enantioselective Reactions and Their Applications in Organic Synthesis" for the following talks:

57) Department of Chemistry, East China Normal University, Shanghai, China, June 6, 2007.
58) Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, Shanghai, China, June 6, 2007.
59) Department of Chemistry, Central China Normal University, Wuhan, China, May 31, 2007.
60) Department of Chemistry, Shanghai Normal University, Shanghai, China, May 29, 2007.
61) Department of Chemistry, New Mexico State University, Las Cruces, New Mexico, April 19, 2007.
62) Department of Chemistry and Biochemistry, West Virginia University, Morgantown, West Virginia, March 21, 2007.
63) Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, Texas, January 24, 2007.

64) *"Organocatalytic, Enantioselective Approach to Medicinally Interesting Chiral Molecules,"* College of Pharmacy, University of Kentucky, Lexington, Kentucky, October 20, 2006.

"Organocatalytic, Enantioselective Approach to the Preparation of Chiral Molecules" for the following talks:

65) Merck Research Laboratory, Rahway, New Jersey, November 15, 2006.
66) Department of Chemistry, University of Tampa, Florida, March 31, 2006.
67) Department of Chemistry, University of South Florida, Florida, March 30, 2006.

"Biomimetic Approach to Design of Small Organic Molecules as Catalysts for Asymmetric Organic Transformations" for the following talks:

68) Department of Chemistry, Georgia State University, Atlanta, GA, March 25, 2006.
69) Department of Chemistry and Biochemistry, University of Texas at San Antonio, TX, February 24, 2006.
70) College of Pharmacy, Fudan University, Shanghai, China, December 20, 2005.
71) Department of Chemistry, Fudan University, Shanghai, China, December 22, 2005.
72) School of Pharmacy, East China University of Science & Technology, Shanghai, China, June 30, 2005.

"New Strategy in Organic Synthesis. Development of Novel Organocatalysts for Asymmetric Organic Transformations" for the following talks:

73) Shanghai Institute of Materia Medica, Chinese Academy of Sciences, Shanghai, China, December 18, 2004.
74) Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, Shanghai, China, December 20, 2004.
75) Department of Chemistry, Case Western Reserve University, Cleveland, OH, October 11-13, 2004.
76) Department of Chemistry, University of Akron, Akron, OH, October 11-13, 2004.

77) *"Chemical Approaches to Biological Problems,"* College of Pharmacy, University of New Mexico, Albuquerque, NM, March 8, 2004.

"Novel Strategies for Development of Peptide and Peptidomimetic-based Drugs" for the following talks:

78) The Laboratory of Medicinal Chemistry, National Cancer Institutes (NCI), National Institutes of Health (NIH), Frederick, Maryland, January 6, 2003.
79) Department of Chemistry, Northern Illinois University, DeKalb, Illinois, December 2-3, 2002.
80) Department of Chemistry, University of Manitoba, Winnipeg, Canada, November 25-26, 2002.
81) Division of Medicinal Chemistry and Natural Product, College of Pharmacy, University of Iowa, Iowa City, Iowa, November 14-15, 2002.

Invited Talks in Professional Conferences:

1) *"New Strategies in Organocatalysis"* the 1st Japan-US Organocatalysis Symposium, Honolulu, Hawaii, USA, December 15-19, 2012.
2) *"New Strategies in Organocatalysis"* the Cope Symposium, 2012 ACS Rocky Mountain Regional Meeting, Westin Westminster, Westminster, CO, USA, October 17-20, 2012.
3) *"New Strategies in Organocatalysis"* in "Chiral China 2012", August 17-19, Lanzhou, China.
4) *"Oxidative Enamine Catalysis,"* The 2nd International Conference on Molecular and Functional Catalysis, July 30-31, 2012, Singapore.
5) *"New Strategies in Organocatalysis"* Eastern Forum of Science and Technology, June 21-22, 2012, Shanghai, China.
6) *"Oxidative Enamine Catalysis,"* The 7th SINO-American Chemistry Professor Conference, June 28-30, 2011, Guiyang, China.
7) *"Chiral Amine Thioureas Catalyzed Cascade Reactions,"* Pacific Chem 2010, Symposium on Asymmetric Organocatalysis, Hawaii, December 15-20, 2010.
8) *"New Strategies in Developing Powerful Organocatalytic Cascade Reactions,"* International Symposium on Organocatalysis (ISOμ) 2010, July 14-17, 2010, Mülheim an der Ruhr, Germany.
9) *"New Strategies in Developing Powerful Enantioselective Organocatalytic Cascade Reactions,"* The 6th SINO-American Chemistry Professor Conference, June 15-17, 2010, Hangzhou, China.
10) *"Powerful Organocatalytic Enantioselective Cascade Reactions,"* Singapore Catalysis Society Forum, August 17, 2009, Singapore.
11) *"Development of Fluorescence Probes for Chemical and Biological Applications,"* The 6th International Symposium for Chinese Medicinal Chemists (ISCMC-6), Shanghai, China, July 28-August 2, 2008.
12) *"Enantioselective Organocatalytic Cascade Reactions,"* The 10th International Symposium for Chinese Organic Chemists (ISCOC-10) and 7th International Symposium for Chinese Inorganic Chemists (ISCIC), Shanghai, China, July 27-31, 2008.

"Powerful Organocatalytic Enantioselective Cascade Reactions" for the following talks:
13) Gordon Research Conference on Organic Reactions and Processes, Bryant University in Smithfield, Rhode Island, July 13-18, 2008.
14) Gordon Research Conference on Heterocyclic Compounds, Salve Regina University, Rhode Island, June 15-20, 2008.
15) The ACS Rocky Mountain/NW Regional Meeting, Park City, Utah, June 15-18, 2008.
16) The 63rd Southwest Regional American Chemical Society Meeting, Lubbock, Texas, November 4-7, 2007.
17) The 3rd Sino-American Organic Chemistry Symposium, Wuhan, China, June 1-2, 2007.

"Chiral Pyrrolidine Sulfonamide Promoted Enantioselective Organic Reactions" for the following talks:
18) The 2006 Lanzhou International Symposium On Organic Chemistry and Medicinal Chemistry, Lanzhou University, Lanzhou, China, July 9-11, 2006.

19) The 2nd Sino-US Chemistry Professor Conferences, Shanghai, China, July 8-9, 2006.
20) The 16th IUPAC's International Conference on Organic Synthesis (ICOS-16), Mérida, Yucatán, México, June 11-15, 2006.

Doctoral Advisement:

Five students received PhDs and three student received MS degrees since 08/03

- Jian Wang, graduated on June 6, 2007, now Assistant Professor at Department of Chemistry, National University of Singapore
- Hao Li, graduated on December 12, 2007, now Associate Professor at School of Pharmacy, East China University of Science & Technology, Shanghai, China
- Liansuo Zu, graduated on December 8, 2008, will join School of Life Science, Tsinghua University, Beijing, China in January 2012 as Associate Professor
- Hexin Xie, graduated on February 11, 2009, Post-Doc at School of Medicine, Stanford University
- Wei Jiang, graduated on December 15, 2009, Post-Doc at Department of Chemistry, Stanford University
- Ken Hutt, MS, December 12, 2009
- Ting Wang, MS, June 20, 2011
- Yuan Liu, MS, June 15, 2011

Current Group Members (9 graduate students and 1 post-doctoral fellow)

Graduate Students:

Yanting Cao, Xiaobei Chen, Wenhan He, Chunliang Liu, Aiguo Song, Xixi Song, Weimin Xuan, Xinhuai Zhang, Shihan Zhao

Post-doctoral:

Shilei Zhang

Undergraduate Students Supervised (23 since 08/03)

Nicholas Card, Spring 2004
Jeff Kellgwood, Spring 2005
Timiyin M E-Nunu, Summer 2005
Michael G. Fulton, Summer 2005
Lora D Heikkinen, Summer and Fall 2005
Brandi N. Kimble, Summer 2007
Jordan A. Monteverdi, Summer 2007
Hien D. Vu, Summer 2007
Bernadette R. Aragon, Fall 2007
Hanine R. Oueis, Fall 2007
Hao Qiang, Spring 2008
Athanasios K. Manole, Spring 2008
Kyle R. Tuffli Spring 2008
Athanasios K. Manole, Summer 2008
Devon Reid, Summer 2008
Sengdhaun V. Defibaugh-Chavez, Fall 2008
Devon Reid, Fall 2008
Anna Lee, Spring 2009
Jacob Greenberg, Spring 2009
Devon Reid, Summer 2009
Anna Lee, Fall 2009

Ryan Todd Sterk, Spring 2010
Cynthia Emeanuwa, Spring 2011
Justin J. Aragon, Spring 2012
Ryan Todd Sterk, Spring 2012
Lizcet Ochoa, Spring 2012
Myrna Campos, Spring 2012

Post-doctoral and Visiting Scholars

Current

Shilei Zhang, October 2008 to present (post-doc)

Past

Dr. Qingquan Fu, October 2006 to September 2007 (post-doc)
Prof. Dr. Xinhong Yu, January 2007 to March 2007 (visiting professor)
Dr. Guixia Liu, November 2007 to October 2008 (post-doc)
Dr. Tangzhi Zhang, November 2007 to October 2008 (post-doc)
Mr. Chenguang Yu, August 2008 to August 2010 (visiting student)
Dr. Yinan Zhang, October 2008 to August 2010 (post-doc)
Prof. Dr. Jian Li, June 2009 to September 2009 (visiting professor)
Prof. Dr. Yafei Ji, March 2009 to February 2010 (visiting scholar)

Classroom Teaching

Fall 2008, CHEM 511: Structures and Mechanisms (graduate level), 10 students
Spring 2009, CHEM 514: Organic Reactions and Synthesis (graduate level), 12 students
Fall 2009, CHEM 511: Structures and Mechanisms (graduate level), 20 students
Spring 2010, CHEM 514: Organic Reactions and Synthesis (graduate level), 7 students
Fall 2010, CHEM 511: Structures and Mechanisms (graduate level), 4 students
Fall 2010, CHEM 302: Organic Chemistry II (undergraduate level), 36 students
Fall 2011, CHEM 511:, Structures and Mechanisms (graduate level), 14 students

Reviewing for Journals

Accounts of Chemical Research
ACS Catalysis
ACS Combinatorial Science
Advanced Materials
Arkivoc
Angewandte Chemie International Edition
Asian Journal of Chemistry
Advanced Synthesis & Catalysis
Bioorganic & Medicinal Chemistry
Bioorganic & Medicinal Chemistry Letters
Catalysis Communications
Chemical Biology & Drug Design
Chemical Communications
Chemical Reviews
Chemical Sciences
Chirality
Current Organic Chemistry
Current Organic Synthesis

Drug Design and Chemical Biology
Environmental Science & Technology
European Journal of Chemistry
European Journal of Organic Chemistry
Green Chemistry
Inorganic Chemistry
Journal of the American Chemical Society
Journal of Combinatorial Chemistry
Journal of Medicinal Chemistry
Journal of Organic Chemistry
Journal of Physical Chemistry
Letters in Organic Chemistry
Medicinal Research Reviews
Nature Chemistry
Nucleosides, Nucleotides & Nucleic Acids
Optical Sensors (Book)
Organic & Biological Chemistry
Organic Letters
Organic Process Research & Development
Science of China Chemistry
Supramolecular Chemistry
Synlett
Synthesis
Tetrahedron
Tetrahedron: Asymmetry
Tetrahedron Letters

Department, College and University Level

• Graduate Student Recruitment Committee Member, Department of Chemistry, University of New Mexico, 2003 to present and as Chair, January 2007 to December 2009
• Organic Division Student Seminar Coordinator, Department of Chemistry, University of New Mexico, Fall 2004 to present
• Medicinal Chemistry Faculty Search Committee Member, College of Pharmacy, University of New Mexico, November 2004 to May 2005
• Department Chair Search Committee Member, Department of Chemistry, University of New Mexico, September 2005
• Organic Lecturer Search Committee Member, Department of Chemistry, University of New Mexico, September 2005
• Department Seminar Coordinator, Department of Chemistry, University of New Mexico, Spring 2006 to Fall 2009
• Physical Chemistry Search Committee Member, Department of Chemistry, University of New Mexico, May 2006
• Chemistry Lecturer Search Committee Member, Department of Chemistry, University of New Mexico, September 2006
• Department Chair Search Committee Member, Department of Chemistry & Chemical Biology, University of New Mexico, September 2007
• Chemical Biology Faculty Search Committee Member, Department of Chemistry & Chemical Biology, University of New Mexico, March 2008

• Faculty Review Committee Member, Department of Chemistry & Chemical Biology, University of New Mexico, January 2008 to December 2009
• Advisor, the Chinese Student Friendship Association, August 2003 to June 2009
• Nano-material Faculty Search Committee Member, Department of Chemistry, University of New Mexico, February 2010
• Organic and Biochemistry Faculty Search Committee Member, Department of Chemistry & Chemical Biology, University of New Mexico, October 2010
• Graduate Committee Member, Department of Chemistry & Chemical Biology, University of New Mexico, October 2011 to present

Student Study and Degree Committees:

Zhibing Lu, Ph.D. defense, Sept. 18, 2003; Xiaohua Feng, Ph.D. RP, Sept 25 2003; Jianying Dai, Ph.D. RP, Jan 16, 2004; Ana M. Felix, Ph.D. RP, Oct. 19, 2004; Xiangjie Ling, Ph.D. RP, October 1, 2004; Rui Wu, Ph.D. RP, Nov. 15, 2004; Runtang Wang, Ph.D. defense, March 1, 2005; Raymond Lansing, Ph.D. RP, March 24, 2005; Canhui Wang, RP, March 30, 2005; Weiling Niu, RP, May 5, 2005; Yurong Deng, RP, October 11, 2005; Hexin Xie, RP, October 20, 2005; Jianying Dai, Ph. D. defense, November 1, 2005; Shaorong Yang, Ph.D. defense, December 6, 2005; George Tan, RP, March 8, 2006; Gebhard B. Lulio, RP, March 21, 2006; Jing Yang, Ph.D. defense, April 4, 2006; Jian Cao, RP, May 2, 2006; Zhimin Zhao, Ph. D. defense, April 11, 2006; Jup T Polanams, Ph.D. defense, May 18, 2006, Danqi Chen, RP, May 17, 2007; Benjamin Njus, RP, May 17, 2007; Maozhan Gong, RP, June 20, 2007; Rui Wu, Ph.D. defense, Aug. 27, 2007; Ana M. Felix, Ph.D. defense, Sep. 21, 2007; Ting Shen, RP, Dec. 11, 2007; Caihui Wang, Ph.D. defense, Feb. 4, 2008; Marie Parkes, RP, Feb. 14, 2008; Hua Huang, RP, Jun. 24, 2008; Liansuo Zu, Ph.D. defense, Oct. 28, 2008; Hexin Xie, Ph.D. defense, Nov. 4, 2008; Amanda Heath, MS defense, Nov. 11, 2008; Brian Boro, Ph.D. defense, Jan. 15, 2009; Chao Dong, RP, Apr. 30, 2009; Rurong Deng, Ph.D. defense, Jul. 7, 2009; Jiwen Zou, Ph.D. defense, Jul. 22, 2009; Isaac Acker, MS defense, Aug. 21, 2009; Wei Jiang, Ph.D. defense, Oct. 28, 2009; Xixi Song, RP, Mar. 1, 2010; Abebe Berhane, Ph.D. defense, Mar. 31, 2010; Li Zheng, RP, Apr. 12, 2010; Sihan Zhao, RP, Apr. 12, 2010; Xinshuai Zhang, RP, Apr. 20, 2010; Joseph Sempombe, RP, Aug. 26, 2010; Chao Dong, RP, Aug. 31, 2010; Raymond Lansing, Ph.D. defense, Nov. 11, 2010; Yuan Liu, RP, Nov. 18, 2010; Yanting Cao, RP, Nov.23, 2010; Gebhard Luilo, Ph.D. defense, Dec. 9, 2010; Joseph Sempombe, Ph.D. defense, Mar. 18, 2011; Weimin Xuan, RP, Mar. 24, 2011; Aiguo Song, RP, Apr. 21, 2011; Sara Toew, RP, May 3, 2011; Min Wang, Ph.D. defense, Nov. 10, 2011.

National and Professional Scientific Level

Review scientific manuscripts for journals with average 30-50 papers per year
NSF Peer Review Panel, Organic & Macromolecular Chemistry Program – Synthesis, March/April 2008
NSF grant reviewer
PRF grant reviewer
The European Research Council Advanced/Starting Grant 2010 project proposals reviewer
The City University of New York Research Award Program reviewer
Shanghai Jiaotong University Faculty Recruiting External reviewer
The Chinese "Yong Thousands Talents Program" reviewer
Faculty Senate Grant for Research and Scholarship at West Virginia University reviewer
The Louisiana Board of Regents Research Grants reviewer
External evaluators for tenure and promotion of other Universities

President and Director, The Chinese-American Chemistry & Chemical Biology Professors Association (President: 2011-2012; Director: 2009-2010)
Scientific Advisory Board, the Open Pharma Source <<Yao Yuan>> (homepage: www.yy-w.org)

Student Degree Committee:
Zhibing Lu, Ph.D. defense, Sept. 18, 2003; Xiaohua Feng, Ph.D. RP, Sept 25 2003; Jianying Dai, Ph.D. RP, Jan 16, 2004; Ana M. Felix, Ph.D. RP, Oct. 19, 2004; Xiangjie Ling, Ph.D. RP, October 1, 2004; Rui Wu, Ph.D. RP, Nov. 15, 2004; Runtang Wang, Ph.D. defense, March 1, 2005; Raymond Lansing, Ph.D. RP, March 24, 2005; Canhui Wang, RP, March 30, 2005; Weiling Niu, RP, May 5, 2005; Yurong Deng, RP, October 11, 2005; Hexin Xie, RP, October 20, 2005; Jianying Dai, Ph. D. defense, November 1, 2005; Shaorong Yang, Ph.D. defense, December 6, 2005; George Tan, RP, March 8, 2006; Gebhard B. Lulio, RP, March 21, 2006; Jing Yang, Ph.D. defense, April 4, 2006; Jian Cao, RP, May 2, 2006; Zhimin Zhao, Ph. D. defense, April 11, 2006; Jup T Polanams, Ph.D. defense, May 18, 2006, Danqi Chen, RP, May 17, 2007; Benjamin Njus, RP, May 17, 2007; Maozhan Gong, RP, June 20, 2007

Lisa J. Whalen   Department of Chemistry and Chemical Biology   02/06/2013

Educational History

B.S. *summa cum laude*, July 1999, University of New Mexico, Albuquerque, NM, Chemistry
"Resolution of a Chiral Alcohol by Lipase-Catalyzed Transesterification with Poly(ethylene glycol) in Organic Media," Advisor: Cary J. Morrow

Ph.D. August 2004, University of Colorado, Boulder, CO, Chemistry
"Tools for Studying O-Linked Glycopeptides," Advisor: Randall L. Halcomb

Employment History

Graduate Research Assistant, University of Colorado, May 2000-May 2004
Part-Time Instructor, University of New Mexico, June 2004-August 2004
Postdoctoral Research Associate, The Scripps Research Institute, La Jolla, CA, September 2004-May 2006

Employment History

Consultant, Sigma-Aldrich Corporation, May 2007-November 2007
Consultant, W.W. Norton and Company, Prentice Hall and Wiley, January 2009-present
Summer Faculty, Center for Integrated Nanotechnologies, Sandia National Laboratories, Albuquerque, NM, May-August 2007 to 2010
Summer Research Faculty, University of New Mexico, May-August 2011 and 2012

Honors

Outstanding Adjunct Teacher/Lecturer of the Year, University of New Mexico, 2008-2009
Weber Award for Teaching Excellence, University of New Mexico, 2009-2010
Nominee, Outstanding Adjunct Teacher/Lecturer of the Year, University of New Mexico, 2010-2011

Teaching, Research, and Service Interests

My strongest interest lies in teaching organic chemistry to undergraduates who are preparing for professional careers in the physical sciences, health sciences, or engineering. More specifically, I expect each of the students, regardless of their career choice, to have certain skills upon leaving the two-semester course. These skills include being able to solve problems using multiple layers of data analysis, to manipulate molecules in two dimensions and to describe their three-dimensional structures correctly in two dimensions, to synthesize different types of information to achieve a goal, to predict the reactivity of unknown compounds containing functional groups studied in the course, to understand some basic relationships between reactivity and electronic structure, and to begin to make the connection between the reactivity of functional groups studied in the course to those in biological pathways. These broad learning goals are explored in the context of synthesizing simple organic molecules, interpreting and predicting spectroscopic data (NMR, IR) and learning mechanisms of reactions through patterns and logic. Most recently I have begun exploring the use of collaborative learning in the teaching of large (>50) organic chemistry courses.

Secondary to teaching, I find that it is critical for my well-being to practice the art of organic synthesis and stay current by conducting research full-time in the summer. From 2006-2010, I worked in the lab of Dr. Dale Huber at the Center for Integrated Nanotechnologies. The large variety of projects I was involved in ranged from synthesis and characterization of iron oxide nanoparticles to exploring methods for constructing phase-separated polymer brushes on silicon surfaces. Every summer I supervised and trained undergraduate and high school student interns with an emphasis on teaching organic synthesis techniques and safety. Starting in 2011 I began work in Professor Lorraine Deck's lab making anticancer agents based on a compound that occurs naturally in cotton, gossypol. This position also requires a significant amount of undergraduate student mentoring.

My service has mostly been to the Department of Chemistry and Chemical Biology, where I have been a member of the Undergraduate Studies committee since Fall 2009. Since becoming a faculty member in the BA/MD program I have additional administrative responsibilities that include membership in the Committee on Curriculum and Student Progress and the Basic Sciences Working Group. The Basic Sciences Working Group seeks to find innovative solutions for teaching students with underprepared backgrounds and extend our discoveries to the rest of the University of New Mexico College of Arts and Sciences.

However, administrative duties aside, I find it is much more enjoyable to serve as the Faculty Advisor for the American Chemical Society (ACS) Student Affiliate and participate in their activities as a service to the community. Our main endeavors are selling laboratory notebooks as a fundraiser to send 4-5 students per year to the ACS National Meeting, and spreading interest in chemistry by performing magic shows for younger children.

Teaching Achievements

Classroom Teaching

Summer 2004: Chemistry 301, 87 students
Summer 2006: Chemistry 301, 78 students; Chemistry 303L/304L coordinator
Fall 2006: Chemistry 301, 117 students; Chemistry 303L/304L coordinator, Chemistry 499
Spring 2007: Chemistry 301, 172 students; Chemistry 303L/304L coordinator
Fall 2007: Chemistry 302, 124 students; Chemistry 303L/304L coordinator, Chemistry 499
Spring 2008: Chemistry 301, 193 students; Chemistry 303L/304L coordinator
Fall 2008: Chemistry 302, 167 students; Chemistry 303L/304L coordinator, Chemistry 499
Spring 2009: Chemistry 301, 94 students; Chemistry 425, 40 students; Chemistry 303L/304L coordinator
Summer 2009: Chemistry 303L/304L coordinator

Fall 2009: Chemistry 302, 66 students; Chemistry 425, 30 students; Chemistry 303L/304L coordinator, Chemistry 499
Spring 2010: Chemistry 301, 232 students; Chemistry 496, 2 students; Chemistry 303L/304L coordinator
Fall 2010: Chemistry 302, 198 students; Chemistry 303L/304L coordinator
Spring 2011: Chemistry 301, 235 students; Chemistry 496, 1 student; Chemistry 303L/304L coordinator
Summer 2011: Chemistry 303L/304L coordinator
Fall 2011: Chemistry 302, 177 students; Chemistry 303L/304L coordinator
Spring 2012: Chemistry 302, 35 students; Chemistry 303L/304L coordinator
Fall 2012: Chemistry 301, 134 students; Chemistry 496, 1 student; Chemistry 303L/304L coordinator
Spring 2013: Chemistry 302, 162 students; Chemistry 303L/304L coordinator

Undergraduate Student Mentoring

Jacob Greenberg, January 2012-August 2012, B.A. Chemistry, Synthesis of anticancer agents
Elizabeth Bright, June 2012-present, B.S. Chemistry, Synthesis of benzoxazine ligands
Paul Sandoval, June 2012-August 2012, B.S. Chemistry, Synthesis of anticancer agents

Curriculum Development or Teaching Administrative Positions

Member, BA/MD Committee on Curriculum and Student Progress, 2011-present
Member, BA/MD Basic Sciences Working Group, 2012-present

Service

Chemistry demonstration, UNM Children's Campus, 2006
Member, Department of Chemistry and Chemical Biology Undergraduate Studies Committee, 2009-present
Faculty advisor, American Chemical Society Student Affiliate, 2010-present
Review presentations for tutors, Center for Academic Program Support, 2010-present
Graduate student recruiter, American Chemical Society National Meetings, 2009 and 2010
Career Day, Lowell Elementary School, 2011
Assistant organizer and participant, Mole Day, National Museum of Nuclear Science and History, 2011-present

Articles in refereed journals

Deck, L.M.; Mgami, Q.; Martinez, A.; Martinic, A.; Whalen, L.J.; Vander Jagt, D.L.; Royer, R.E. Synthesis of benzyl substituted naphthalenes from benzylidene tetralones. *Tetrahedron Lett*. **2012**, *53(4)*, 373

Sugiyama, M.; Hong, Z.; Liang, P.-H.; Dean, S.M.; Whalen, L.J.; Greenberg, W.A.; Wong, C.-H. D-Fructose-6-phosphate aldolase-catalyzed one-pot synthesis of iminocyclitols. *J. Am. Chem. Soc.* **2007**, *129*, 14811.

Yu, Z.; Sawkar, A.R.; Whalen, L.J.; Wong, C.-H.; Kelly, J.W. Isofagomine- and 2,5-anhydro-2,5-imino-D-glucitol-based glucocerebrosidase pharmacological chaperones for Gaucher disease intervention. *J. Med. Chem.* **2007**, *50*, 94.

Hanson, S.R.; Whalen, L.J.; Wong, C.-H. Synthesis and evaluation of general mechanism-based inhibitors of sulfatases based on (difluoromethyl)phenyl sulfate and cyclic phenyl sulfamate motifs. *Bioorg. Med. Chem.* **2006**, 14(24), 8386.

Sugiyama, M.; Hong, Z.; Whalen, L.J.; Greenberg, W.A.; Wong, C.-H. Borate as a phosphate ester mimic in aldolase-catalyzed reactions: practical synthesis of L-fructose and L-iminocyclitols. *Adv. Synth. Catal.* **2006**, *348,* 2555.

Whalen, L.J.; Wong, C.-H. Enzymes in organic synthesis: aldolase-mediated synthesis of iminocyclitols and novel heterocycles. *Aldrichimica Acta* **2006**, *39(3)*, 63.

Whalen, L.J.; Halcomb, R.L. Synthesis of an isostere of an *O*-linked glycopeptide. *Org. Lett.* **2004**, *6(19)*, 3221.

Whalen, L.J.; McEvoy, K.A.; Halcomb, R.L. Synthesis and evaluation of phosphoramidate amino acid-based inhibitors of sialyltransferases. *Bioorg. Med. Chem. Lett.* **2003**, *13(1)*, 301.

Whalen, L.J.; Morrow, C.J. Resolution of a chiral alcohol through lipase-catalyzed transesterification of its mixed carbonate by poly(ethylene glycol) in organic media. *Tetrahedron: Asymmetry* **2000**, *11(6)*, 1279.

Articles appearing in chapters in edited volumes

Whalen, L.J.; Greenberg, W.A.; Mitchell, M.L.; Wong, C.-H. Iminosugar-based glycosyltransferase inhibitors. In *Iminosugars: From Synthesis to Therapeutic Applications*, Chapter 7. Compain, P. and Martin, O., Eds. Wiley VCH: Chichester, 2007; pp 153-175.

Works in progress

Deck, L.M.; Weber, W.M.; Whalen, L.J.; Hunsaker, L.A.; Vander Jagt, T.A.; Royer, R.E.; Dang, C.V.; Vander Jagt, D.L. Targeting glutathione S-transferase P1-1 by enone analogs of curcumin, *Bioorg. Med. Chem.*, **2012**, manuscript in preparation.

Deck, L.M.; Weber, W.M.; Whalen, L.J.; Hunsaker, L.A.; Royer, R.E.; Vander Jagt, D.L. Anti-inflammatory activities of trans stilbenes in microglia cells. *J. Med. Chem.* **2012**, manuscript in preparation.

Deck, L.M.; Whalen, L.J.; Hunsaker, L.A.; Vander Jagt, T.A.; Royer, R.E.; Dang, C.V.; Vander Jagt, D.L. Polyphenolic dienone analogs of curcumin as inhibitors of glyoxalase-1. *Bioorg. Med. Chem.* **2012**, manuscript in preparation.

Deck. L.M.; Whalen, L.J.; Heynekamp, J.J.; Wei, J.; Mgani, Q.; Vander Jagt, T.A.; Hunsaker, L.A.; Dang, C.V.; Vander Jagt, D.L.; Royer, R.E. Gossypol analogs as inhibitors of lactate dehydrogenase-A. *J. Med. Chem.*, **2012**, manuscript in preparation.

Lenger, J.; Whalen, L.J.; Ennemann, E.C.; Schröder, M.; Wong, C.-H.; Dierks, T.; Sewald, N.; Hanson, S.R. Development and evaluation of cyclic sulfamates as activity-based probes for sulfatases. Manuscript in preparation, **2011**.

Presentations

Whalen, L.J. Impact of extracurricular review sessions on exam performance in organic chemistry. Presented at UNM OSET Success in the Classroom: Sharing Practices that Work, Albuquerque, NM, February 2011.

Whalen, L.J.; Wong, C.-H. Targeting *E. coli* PBP1b transglycosylase. Presented at the 229th National Meeting of the American Chemical Society, San Diego, CA, March 2005; Poster ORGN 856.

Whalen, L.J.; Halcomb, R.L. Strategies for the synthesis of glycopeptide isosteres. Presented at the 226th National Meeting of the American Chemical Society, New York, NY, September 2003; Paper MEDI 18.

Whalen, L.J.; Halcomb, R.L. Strategies for the synthesis of glycopeptide isosteres. Presented at the 2003 Bristol-Myers Squibb Chemistry Award Symposium, Wallingford, CT, May 2003.

Whalen, L.J.; Halcomb, R.L. Strategies for the synthesis of glycopeptide isosteres. Presented at the 2002 Gordon Research Conference on Medicinal Chemistry, New London, NH, August 2002; Poster 33.

Whalen, L.J.; Halcomb, R.L. Strategies for the synthesis of glycopeptide isosteres. Presented at the 21st International Carbohydrate Symposium, Cairns, Australia, July 2002; PP 185.

Whalen, L.J.; McEvoy, K.A.; Halcomb, R.L. Synthesis and evaluation of phosphoramidate amino acid based inhibitors of sialyltransferases. Presented at the 221st National Meeting of the American Chemical Society, San Diego, CA, April 2001; Paper ORGN 111.

Whalen, L.J.; Morrow, C.J. Resolution of a chiral alcohol by lipase-catalyzed transesterification with poly(ethylene glycol) in organic media. Presented at the 217th National Meeting of the American Chemical Society, Anaheim, CA, March 1999; Paper CHED 293.

Appendix A13. CCB Office Staff Position Descriptions

Department Administrator A3 – (vacant) Oversees and administers programs, strategies, and initiatives designed to develop, enhance, and support the mission of an unusually large, complex, and diverse academic department of the University, as measured by annual revenue and number of faculty and staff. Oversees all internal and external business activities, this includes; accounting and finance, and human resources. Manages and coordinates facility and resource management, information services, and general department administration. As a member of the department's leadership team, the successful candidate will participate with the Chair and senior departmental faculty in strategic and operational decision making.

Administrative Assistant II (vacant**)** The Administrative Assistant is responsible for the management of the departmental office. Routine duties will include answering the telephone; greeting and assisting visitors and students; copying; faxing; maintaining office equipment; distribution of mail; preparing correspondence; typing exams, reports, and research papers; maintaining office supplies for staff and faculty; maintaining staff directory; and other functions that support the teaching and research efforts of the department.

Accountant III (Penn Rabb) Monitors the business activities of the department through the maintenance and control of financial records including restricted and unrestricted accounts, as well as endowments. Performs advanced accounting functions in the management of the department fiscal activities; prepares integrated financial and statistical reports, statements, projections, and recommendations that may have long-term impact on funding for the organization. Supervises the activities of staff, as appropriate to the position. Included in the responsibilities is the processing of a high volume of purchasing and reimbursement documents, journal entries, reconcilliations, payroll, reports, and special projects.

Fiscal Services Tech (Fernando Santillanes) Performs a variety of fiscal and budgetary duties in support of accountant and administrator. Prepares and processes routine financial documents and fund transactions; reconciles financial records; monitors, reconciles and assists with the fiscal administration for the department, including budgets, funding, grants, contracts, payroll, employment, and travel and purchasing. Assists in maintaining records of fiscal and budgetary controls, ledgers, and/or other related transactions, in either direct or indirect support of accountants or administrators.

Coordinator of Program Advisement (Karen McElveny) Provides, oversees, and coordinates undergraduate and a combination of either graduate and/or preprofessional academic and associated student advisement, admission/graduation eligibility assessment, recruitment, financial aid, and associated administrative/liaison activities within a large multi-faceted academic organization. Assists with curriculum planning and program evaluation.

Facilities Service Director (Robert Ortiz) Oversees building scheduling and maintenance, custodial, safety, security, construction, and/or grounds maintenance directly related to Clark Hall and the Science and Math Learning Center (SMLC). Plans and implements capital renewal and replacement projects for the facilities, and develop and implement operating policies and procedures for two seperate diverse buildings.

Appendix A13. CCB Technical Staff Position Descriptions

Research Facility Director (Dr. Karen Ann Smith) Serves as the designated officer in charge of laboratory facilities and operations for a major, high-tech University laboratory research facility supporting multiple and varied research studies. Manages day-to-day facility operations, and participates in long-range facility planning and decision making with regards to current and future capacity and technology needs. Provides direct and indirect support and guidance to researchers and technical staff using the facility.

Research Scientist II (Ken Sherrell) The position provides analytical support for departmental research faculty, other UNM investigators, and submitters for other state universities who require mass spectrometry evaluation of compounds and proteins. The incumbent processes samples on a fee basis, providing preliminary consultation, sample preparation, mass spectral analysis, protein data processing, result reporting, and data interpretation. The position maintains, troubleshoots, and repairs facility instrumentation; responsible for facility maintenance, schedules, budget, billing, and purchasing of laboratory supplies. The role trains faculty, post-docs, clients, and students in Mass Spec techniques when appropriate to promote the effective use of the instrumentation of the Mass Spec Facility.

Research Engineer II (Fred Fuchs) Under general supervision, independently evaluates, selects, and applies standard engineering research techniques, procedures, and criteria to make minor adaptations and modifications to research assignments. Performs research which involves conventional types of plans, investigations, surveys, structures, or equipment with relatively few complex functions.

Supervisor, Teaching Labs (Gary Bush) Supervises and maintains laboratory facilities for experiments and research in a teaching laboratory. Coordinates and plans laboratory exercises with lecturers; tests and conducts experiments, exercises, and demonstrations. Supervises and provides technical guidance to staff and teaching assistants concerning pre- and post-experiment preparations and processes. Ensures compliance with health and safety standards of laboratory operations.

Teaching Laboratory Technician (James Almand, Nancy Boldt, Sharon Boyd) Prepares chemicals, lab equipment, and student drawers for teaching lab. Maintains laboratory facilities and stockroom for experiments. Plans laboratory exercises with faculty. Tests and conducts experiments, exercises, and demonstrations. Provides technical assistance to staff and teaching assistants concerning experimental preparations and procedures. Ensures compliance with health and safety standards of laboratory operations.

Appendix A14 CCB Scientific Equipment Inventory

Year	Asset Desc	MFG	Asset Amt
1982	ANAEROBIC GLOVE BOX	Forma	$5,712.00
1982	EVAPORATOR FLASH LAB	Cooke	$6,975.00
1982	TEST SET	Tektronix	$8,974.00
1982	CENTRIFUGE ELECT	Beckman	$11,600.00
1983	TANK STORAGE	Cryogenic	$24,825.00
1984	WATER BATH SHAKER	NewBrunswi	$2,851.00
1985	SPEEDVAC CONCENTRATO	Savant	$1,355.00
1986	CHROMATOGRAPH	HewlettPac	$10,850.00
1986	CHROMATOGRAPH	HewlettPac	$11,250.00
1987	INERT GAS SYSTEM	Innovativ	$19,650.00
1988	HEATER LAB	BioRad	$1,600.00
1988	DRYING SYSTEM	BioRad	$2,300.00
1988	HANDI-FREEZE	Fisher	$3,106.00
1988	GENERATOR SWEEP FM	Leader	$3,735.00
1989	POWER SUPPLY	Nikon	$1,172.00
1989	PUMP	Precision	$1,204.00
1989	GENERATOR SWEEP FM	PineInst	$2,485.00
1989	MICROSCOPE	Nikon	$19,228.00
1990	Explosives Refrigerator	LabLine	$1,491.00
1990	STAT CRIT INSTRUMENT	PineInst	$2,485.00
1990	GLOVE BOX ASSEMBLY	Mbraum	$16,600.00
1991	GLOVE BOX ASSEMBLY	UNKNOWN	$32,995.00
1992	CONTROLLER	Mks	$1,726.00
1992	SENSOR	Gastech	$2,263.00
1992	GLOVE BOX ASSEMBLY	VAC	$14,280.00
1994	CIRCULATOR	FisherScien	$1,472.00
1994	TUBE FURNACE	Lindberg	$4,151.00
1994	CHROMATOGRAPH	HewlettPac	$5,688.00
1994	CHROMATOGRAPH	HewlettPac	$7,344.00
1994	SPECTROPHOTOMETER	Shimadzu	$8,166.00
1994	THERMAL ANALYSIS UNT	PerkinElme	$20,978.00
1994	SOURCE, ION	Finnigan	$30,000.00
1994	DIFFRACTOMETER	Siemans	$240,753.00
1995	PUMP SYRINGE	Orion	$1,100.00
1995	GENERATOR SWEEP FM	Wavetek	$4,792.00
1995	TABLE TOP	Newport	$4,862.00
1995	SPECTROPHOTOMETER	Shimadzu	$6,075.00
1995	PUMP VACUUM	Balzers	$8,050.00
1995	LASER ARGON ION	Coherent	$20,070.00
1995	SPECTROMETER	Spex	$20,341.00

1995	RETICLE	Coherent	$25,152.00
1995	SPECTROGRAPH	Spex	$38,112.00
1995	POWER SUPPLY	Oxford	$59,895.00
1995	SPECTROMETER/MASS	Finnigan	$182,758.00
1996	OVEN VACUUM	Fisher	$1,499.00
1996	METER CONDUCTIVITY	Pharmacia	$1,831.00
1996	GENERATOR FUNCTION	HewlettPac	$5,000.00
1996	HEATER LAB	PerkinElme	$5,520.00
1996	TEMPERATURE CONTROL	PerkinElme	$6,287.00
1996	TUBE FURNACE	Lindberg	$7,990.00
1996	CRYOSTAT	Janis	$8,410.00
1996	POTENTIOMETER	Par	$9,000.00
1996	CHROMATOGRAPH	Pharmacia	$9,964.00
1996	MICROSCOPE SYSTEM	MolecImag	$20,700.00
1996	CONTROLLER	MolecImag	$33,038.00
1996	SPECTROPHOTOMETER	Hitachi	$34,500.00
1996	MICROSCOPE SYSTEM	DigitalInst	$41,445.00
1996	MICROSCOPE SYSTEM	DigitalInst	$72,145.00
1997	FRACTION COLLECTOR	Gibson	$1,002.00
1997	ASPIRATOR	ColeParmer	$1,099.00
1997	ASPIRATOR	ColeParmer	$1,099.00
1997	ASPIRATOR	ColeParmer	$1,099.00
1997	ASPIRATOR	ColeParmer	$1,099.00
1997	HOLDER	VWR	$1,125.00
1997	DEIONIZER SYSTEM	VWR	$1,243.00
1997	MICROSCOPE	VWR	$1,713.00
1997	VACUUM SYSTEM	VWR	$1,725.00
1997	PUMP	Rainin	$1,729.00
1997	PUMP VACUUM	VWR	$1,753.00
1997	PUMP VACUUM	VWR	$1,753.00
1997	ICE MACHINE FLAKE	Classic	$1,880.00
1997	LASER HENE	Uniphase	$2,338.00
1997	FRACTION COLLECTOR	Gilson	$2,815.00
1997	FRACTION COLLECTOR	Gilson	$2,815.00
1997	FRACTION COLLECTOR	Gilson	$2,815.00
1997	CELL DISRUPTER	VWR	$2,867.00
1997	EVAPORATOR	Buchi	$3,451.00
1997	EVAPORATOR	Buchi	$3,451.00
1997	PUMP SYSTEM	Rainin	$3,716.00
1997	BENCH CLEAN	Forma	$3,911.00
1997	CAMERA SYSTEM	Chromapro	$3,935.00
1997	ANALYZER	Harrison	$4,258.00
1997	FREEZE-DRYING APPAR	VWR	$5,616.00
1997	PUMP SYSTEM	DYNATech	$6,294.00
1997	SAMPLER AUTO	PerkinElme	$6,588.00

1997	SPECTROGRAPH	Chromapro	$6,761.00
1997	INCUBATOR SHAKER	Forma	$7,186.00
1997	DRYER LAB	Forma	$7,740.00
1997	PROBE	Chromapro	$8,026.00
1997	SPECTROMETER	Paragon	$14,821.00
1997	BIO COMP SYSTEM	NewBrunswi	$20,780.00
1997	SPECTROMETER	PerkinElme	$84,006.00
1997	X-RAY DIFFRACTOMETER	Siemans	$101,211.00
1998	PROBE	Spectra	$1,175.00
1998	SCANNER	Arcus	$1,353.00
1998	TURBIDIMETER	Fisher	$1,358.00
1998	REFRIGERATED TRAP	Savant	$1,755.00
1998	PUMP SYRINGE	HarvardApp	$1,965.00
1998	REACTOR	Raytech	$2,814.00
1998	CENTRIFUGE	VWR	$3,504.00
1998	CENTRIFUGE	VWR	$3,504.00
1998	PUMP SYSTEM	Pharmacia	$5,585.00
1998	CENTRIFUGE	VWR	$5,796.00
1998	CONTROLLER	Pharmacia	$8,488.00
1998	SPECTROPHOTOMETER	Spectra	$8,800.00
1998	MV TRK UNDER 1 TON	Chevrolet	$9,000.00
1998	OPTICAL BENCH	Shimadzu	$9,052.00
1998	SPECTROMETER CONTROL	Bruker	$556,430.00
1999	DATA PROCESSOR/INTEG	SpectraPhy	$1,000.00
1999	VALVE GATE	Lesker	$1,870.00
1999	ISOCRATIC PUMP MODUL	SpectraPhy	$2,000.00
1999	POWER DRIVER	Lesker	$2,290.00
1999	CENTRIFUGE REFRIGERA	SavantInst	$2,374.00
1999	VALVE GATE	Lesker	$2,425.00
1999	VALVE GATE	Lesker	$2,425.00
1999	PUMP GRADIENT DENSIT	SpectraPhy	$2,500.00
1999	PUMP GRADIENT DENSIT	SpectraPhy	$2,500.00
1999	DETECTOR	SpectraPhy	$2,500.00
1999	DETECTOR	SpectraPhy	$2,500.00
1999	TABLE OPTICAL	Newport	$3,153.00
1999	ROLLER MILL LAB	Reliable	$4,950.00
1999	PUMP SYSTEM	Lesker	$7,959.00
1999	ANALYZER	KurtLesker	$9,053.00
1999	SPECTROMETER	Varian	$12,805.00
1999	LASER	Coherent	$66,315.00
2000	STATION COMPUTER	Kachina	$1,106.00
2000	GENERATOR ELECT	Cryo	$1,125.00
2000	SPECTRONIC	ViewTech	$1,282.00
2000	CENTRIFUGE MICRO	VWR	$2,162.00
2000	CENTRIFUGE MICRO	VWR	$2,272.00

2000	POTENTIOSTAT	PineInst	$2,808.00
2000	LIQUID NITROGEN DEWAR	Janis	$4,300.00
2000	UPS SYSTEM	Liebert	$5,750.00
2000	PUMP SYSTEM	AgilentTech	$9,922.00
2000	ELECTRICAL MEASURING	Picoquant	$11,950.00
2000	SPECTROMETER	Nicolet	$65,871.00
2001	VALVE	BioRad	$1,057.00
2001	VALVE	BioRad	$1,196.00
2001	BASE UNIT	BioRad	$1,448.00
2001	FLOWRATOR/BRASS	BioRad	$1,560.00
2001	CLEANER RUG	BioLab	$2,584.00
2001	FLOWRATOR/BRASS	BioRad	$2,730.00
2001	MINICYCLER	MjResearch	$3,019.00
2001	DETECTOR	BioRad	$3,497.00
2001	CONTROLLER	BioRad	$5,537.00
2001	SEPARATOR	Amersham	$6,351.00
2001	POTENTIOSTAT/GALVANOSTAT	PineInst	$6,819.00
2001	Isoelectric Focusing Unit	Amersham	$6,924.00
2001	PROBE	UNKNOWN/OTHER	$9,667.00
2001	HEAT EXCHANGER	Bruker	$15,750.00
2002	LASERJET PRINTER	HewlettPac	$1,080.00
2002	METER P H	Vigor	$1,236.00
2002	ASPIRATOR	VWR	$1,346.00
2002	PUMP SYRINGE	HarvardApp	$1,400.00
2002	SPECTRONIC	ViewTech	$1,605.00
2002	SPECTRONIC	ViewTech	$1,605.00
2002	SPECTRONIC	ViewTech	$1,605.00
2002	SPECTRONIC	ViewTech	$1,606.00
2002	ROTOR CENTRIFUGE	Vigor	$1,923.00
2002	LASERJET PRINTER	HewlettPac	$1,975.00
2002	ANALYZER	Smart	$2,341.00
2002	CYCLER THERMO	VWR	$2,432.00
2002	RECIRCULATOR	VWR	$2,760.00
2002	ICE MACHINE FLAKE	Standard	$3,101.00
2002	GENERATOR WAVEFORM	HewlettPac	$3,840.00
2002	SPECTROPHOTOMETER	Shimadzu	$4,883.00
2002	CRYOSTAT	Janis	$4,926.00
2002	PULSER	BioRad	$5,215.00
2002	DENSITOMETER	BioRad	$10,130.00
2002	KINETIC SYSTEM	VWR	$15,446.00
2002	SPECTROMETER	Nicolet	$16,287.00
2002	CAMERA SYSTEM	Princeton	$44,698.00
2002	MONOCHROMATOR	RoperSci	$46,637.00
2002	SPECTROMETER/MASS	UNKNOWN/OTHER	$282,564.00
2003	MICROWAVE KIT	UNKNOWN/OTHER	$1,250.00

2003	MICROWAVE KIT	UNKNOWN/OTHER	$1,250.00
2003	PUMP VACUUM	VWR	$1,443.00
2003	PUMP	VWR	$1,541.00
2003	PUMP	VWR	$1,541.00
2003	WATER BATH	Varian	$1,590.00
2003	CONTROL UNIT	VWR	$1,613.00
2003	REACTOR	VWR	$1,637.00
2003	BRIDGE	UNKNOWN/OTHER	$2,000.00
2003	STAGE	VWR	$2,128.00
2003	CONDENSER	VWR	$2,209.00
2003	CELL TRANSPORT	VWR	$2,251.00
2003	TRANSPORT EQUIPMENT	VWR	$2,869.00
2003	CYCLER THERMO	MjResearch	$2,950.00
2003	ROTOR CENTRIFUGE	Beckman	$4,260.00
2003	MICROSCOPE	Scientific	$5,035.00
2003	ROTOR VAPOR	VWR	$5,402.00
2003	CELL ASSEMBLY	UNKNOWN/OTHER	$5,696.00
2003	SPECTROPHOTOMETER	Varian	$6,545.00
2003	SPECTROPHOTOMETER	Varian	$8,160.00
2003	SPECTROMETER	UNKNOWN/OTHER	$10,000.00
2003	TESTER	ATLAS	$11,148.00
2003	SPECTROPHOTOMETER	Varian	$17,000.00
2003	SPECTROMETER	Bruker	$19,107.00
2003	PURIFIER	Horizon	$21,010.00
2003	CHROMATOGRAPH	Shimadzu	$21,436.00
2003	SPECTROMETER	Bruker	$22,210.00
2003	CHROMATOGRAPH	MassMicSys	$64,667.00
2003	SPECTROMETER	Bruker	$277,695.00
2004	PUMP AUTO SYRINGE	VWR	$1,222.00
2004	PUMP SYSTEM	VWR	$1,672.00
2004	SOLVENT RECOVERY SYS	Phenomenex	$1,696.00
2004	VACUUM WET-DRY	VWR	$1,980.00
2004	PUMP VACUUM	VWR	$2,227.00
2004	ROTOR VAPOR	VWR	$3,913.00
2004	Test Measurement System	Pxi	$4,111.28
2004	LASER	Coherent	$4,457.00
2004	LASER	Edmund	$6,037.00
2004	Single Zone Furnace	Dynalab	$6,904.83
2004	Cryostat, Liquid He	Janis	$10,829.00
2004	Laser System, Polarized	MellesGrio	$15,218.00
2004	SPECTROPOLARIMETER	Jasco	$125,571.00
2005	Pressure component	MksInstrum	$1,525.02
2005	Pressure cell kit	Bechburhler	$1,635.00
2005	Spectrometer Controller/Photometer	Horiba	$2,813.02
2005	HIGH PRESSURE HOMOGENIZER	FisherScien	$2,941.60

2005	Liquid nitrogen Autofiller	AmerMag	$2,971.83
2005	Centrifuge	VWR	$4,199.25
2005	SYSTEM UPG (EQUIP) FOR AV500	BrukerBio	$6,594.40
2005	Pumping station	Janis	$7,160.00
2005	Spectrometer	Nicolet	$16,711.24
2005	Liquid He Temperature Control System	BrukerBio	$38,930.00
2005	Mass Spectrometry System	Waterscorp	$229,717.69
2005	X-RAY DIFFRACTOMETER	BrukerAxs	$283,200.00
2006	Spectrophotometer	Shimadzu	$8,165.33
2007	Photon Counting Module	PerkinElme	$7,763.50
2007	Photon Counting Module	PerkinElme	$7,763.50
2007	Laser System	MellesGrio	$12,674.57
2007	Microwave Reactor Module	CEMCorp	$13,108.36
2007	Compact diode laser	Edinburgh	$14,075.00
2007	HPLC System	ChromTech	$19,738.90
2007	Nanopositioner	MadCityLab	$24,365.00
2007	Inverted Microscope system	CarlZeiss	$27,713.34
2007	Spectrometer	Princeton	$32,043.83
2007	Spectrograph system	AndorTech	$44,985.00
2008	Laser System	NewPort	$5,185.93
2008	Smart Orbit	ThermoElect	$6,304.98
2008	High Performance Liquid Chromatograph	Shimadzu	$20,354.50
2008	Mass Spec	AgilentTech	$44,236.00
2008	Mass Spectrometer - Discovery System	ApplBioSys	$515,579.79
2009	Monochromator System	Shimadzu	$11,467.22
2009	Fraction Collector	GEHealth	$31,792.58
2009	HPLC System	Shimadzu	$33,613.94
2009	Mettler Toledo DSC1 500C	MettlerTod	$35,129.87
2010	Incubator	Nuaire	$5,880.00
2010	Turbo Pump Helium Leak Detector	Alcatel	$7,298.00
2010	High Power Laser Diode	Phox	$8,310.30
2010	Lock-In Amplifier	Stanford	$8,527.30
2010	Spectrophotometer	ThermoElect	$9,185.00
2010	Bio-Safety Cabinet	Nuaire	$9,330.00
2010	Gel Imaging System	BioRad	$9,763.00
2010	Gas Chromatograph	Agilent	$16,568.65
2010	Gas Chromatograph	Agilent	$16,568.65
2010	Gas Chromatograph	Agilent	$16,568.65
2010	Spectophotometer	Shimadzu	$17,675.24
2010	Spectrometer	BrukerOpt	$18,692.00
2010	Spectrometer.	Bruker	$18,692.00
2010	Spectrometer	Bruker	$18,692.00
2010	Fast Track Microsoft He Cryostat System	OxfordInst	$19,140.88
2010	Micro DAC System	Diacell	$24,004.00
2010	Spectrometer	ApplPhoto	$24,544.00

2010	Beta-RAM - RHPC Detector	LabLogic	$26,553.25
2010	HPLC System	Shimadzu	$31,994.97
2010	Imaging Spectrometer System	Horiba	$33,820.46
2010	Sterilizer	Consolidated	$47,432.80
2010	NMR	Bruker	$196,200.00
2010	NMR	BrukerBio	$300,900.00
2011	Nanopure - Water Purification System	ThermoScien	$5,353.66
2011	Thermal Cycler	BioRad	$5,745.36
2011	HPLC Prep Column	Restek	$6,017.73
2011	Glassware Dishwasher	VWR	$6,133.64
2011	Autoclave Sterilizer 50L	Sanyo	$7,841.40
2011	Centrifuge	Beckman	$7,851.80
2011	Electrochemical Analyzer	CHInstr	$8,770.00
2011	Gel Imaging System	BioRad	$9,345.83
2011	Spectrophotometer	ThermoElect	$9,460.00
2011	Solar Simulator System	Newport	$9,976.09
2011	Tri-Gas Generator	Parker	$10,962.38
2011	Electrochemical Workstation	Bioanaly	$11,180.00
2011	Liquid Chromatograph	Shimadzu	$18,535.81
2011	Spectrofluorophotometer	Shimadzu	$18,775.77
2011	Glovebox Workstation	Mbraun	$28,293.26
2011	Chromotagapher	WatersTech	$36,500.34
2011	Mass Spectrometer	AB Sciex	$86,127.30
2012	Tablet/TF700T	ASUS	$0.00
2012	RecirculatingChiller/NeslabThermoFlex	VWR	$5,106.68
2012	Rotavapor/R-210	VWR	$5,430.98
2012	ThermCycler/S1000	BioRad	$6,005.92
2012	IncubatorShaker/I-24	VWR	$6,683.92
2012	Spectrophotometer/ScanningDoubleBeam	Shimadzu	$6,835.50
2012	Centrifuge/5804R4	VWR	$7,683.40
2012	Spectrophotometer/ScanningDoubleBeam	Shimadzu	$9,403.02
2012	Spectrophotometer/ScanningDoubleBeam	Shimadzu	$9,403.03
2012	GloMaxSystem	Promega	$15,798.00
2012	Spectrometer/FT-IR	Shimadzu	$17,615.50
2012	Titanium HPLC/U3000	Dionex	$36,697.09
2012	SpectrometerSystem	HitachiHiT|Hitachi High Technologie	$48,265.47
2012	Spectrometer/DXRSmartRaman	ThermoElec	$53,875.55

Appendix A15 CCB Annual Report AY 2011-2012

CCB 2011-2012 Academic Year Annual report

Summary sheet

Faculty numbers:	As of June 30, 2012		Change since July 1, 2011
Full professor	8		-1
Associate professor	2		-1
Assistant professor	4		+1
Lecturer	4		none
Staff numbers			
Technical staff	8		none
Administrative staff	5		none
Number of graduate students supported	39.5		+3
Number of peer-reviewed publications			
Faculty	86		+15
Graduate students	46		+3
Number and $ amount of external funding awards	13	$2,473,063	+26%

ANNUAL REPORT

DEPARTMENT OF CHEMISTRY AND CHEMICAL BIOLOGY
July 1, 2011 - June 30, 2012

Stephen E. Cabaniss
Professor and Chair

Submitted to A&S
October 26, 2012

Contents

Executive Summary

The 2011-2012 academic year was academically productive but politically turbulent for the department of Chemistry and Biological Chemistry (CCB). The undergraduate mission of the department moved forward, with CCB teaching ~20,000 student credit hours and graduating a record number of majors while experimenting with a parachute course and designing active-learning pedagogy to improve student success in general chemistry. Departmental research productivity was high on a per-faculty basis and increased from the previous AY, with 86 journal articles published and 21 active research grants totaling nearly $2.5M. On the other hand, retirement of two senior faculty (Deck, Ondrias) and arrival of one assistant professor (Liang) left the department with only 15 tenure track faculty as of June 30, 2012. The small faculty size contributes to decreasing graduate enrollment, which has shrunk by nearly a factor of two in just five years. Faculty disagreements over how to reform the graduate program and other matters led to rising tensions which contributed to the resignation of the chair, David Bear, and his decision to return to his former department in HSC.

Top priorities for the immediate future include improving departmental political climate and function, assessing the effect and expanding the scope of undergraduate course reforms, and re-organizing the graduate program and reversing the decline of graduate enrollment. However, the two greatest needs are also the most resource-intensive: the renovation of Clark Hall (to be financed by $16M in GO bond funds) and the restoration of the research-active faculty to a size capable of sustaining a viable and energetic graduate program (which will require commitments of nearly $1M in start-up funds per year for several years).

I. Significant developments during AY 2011-2012

A. Appointments to the staff

Carol Gislason was appointed Departmental Administrator July 7, 2011, replacing Deborah Moore who departed in February 2011.

Robert 'Bobby' Ortiz was hired as Facilities Services Manager (shared with Mathematics and Statistics) on September 7, 2011.

Erlinda Tribou was hired as an Administrative assistant in February 2011, replacing Tara Solt who departed December 1, 2011.

Buddy Almand was hired as a Teaching Laboratory Technician in March 27, 2011, replacing Steven Shinnick who departed November 11, 2011. (and who in turn replaced Jessica Padilla who departed on August 25, 2011! It is difficult to fill these positions.)

B. Separations from the staff

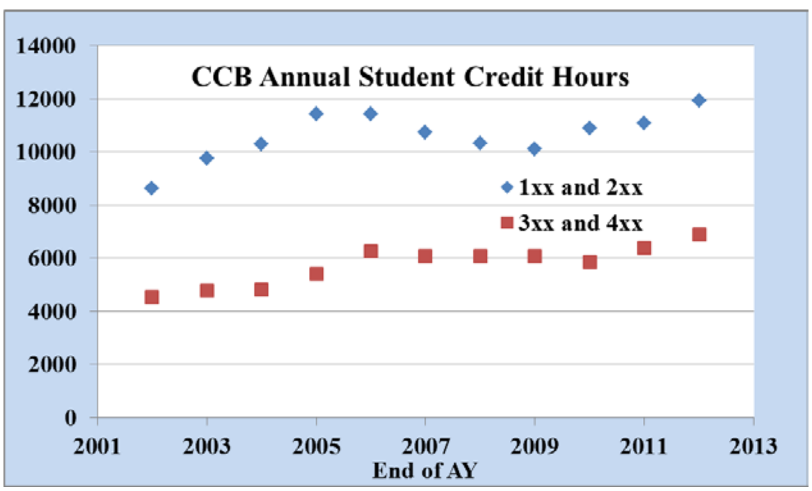
Tara Solt, Administrative Asst II, hired 2/21/11, resigned to accept a promotion to Admin Asst III in ASM Administration on 12/1/2011.

Steven Shinnick, Teaching Laboratory Technician departed 11/11/11 to accept a higher paying position with an outside agency.

Dr. Charlotte Mobarak, Director of the Mass Spectrometer Facility and Research Assistant Professor left due to funding issues on June 30, 2012.

Jessica Padilla departed on August 25, 2011.

C. Undergraduate program



Trend in CCB student credit hours over the last 10 years (OIR).

The department of Chemistry and Chemical Biology (CCB) continues to be a major contributor to undergraduate education at UNM, both by teaching 'service' courses for students in other majors and by graduating BA and BS majors in CCB. In AY 2011-2012, CCB taught ~20,000 student credit hours (19,950), or over 3% of the SCH taught on main campus. This represents a ~50% increase over the last 10 years while tenure-track faculty numbers have declined. In AY 2011-2012, CCB graduated 8 B.S. and 36 B.A. students. (Note: the BA number includes all BA double-majors and not just those who listed CCB first on the graduation form, which differs from OIR and A&S statistics).

Course	# of Students Completing Course (Summer 2008, Fall 2008, Spring 2009)	# of Students Completing Course (Summer 2009, Fall 2009, Spring 2010)	# of Students Completing Course (Summer 2010, Fall 2010, Spring 2011)	# of Students Completing Course (Summer 2011, Fall 2011, Spring 2012)
Chem 111 Elements of General Chemistry w/lab	441	484	468	**477**
Chem 212 Integrated Organic Chem & Biochem	105	104	147	**150**
Chem 121/122 General Chemistry	1748	1988	2134	**2252**
Chem 123/124 General Chemistry Lab	1748	1889	1963	**2028**
Chem 301/302 Organic Chemistry	1269	1405	1422	**1548**
Chem 303/304 Organic Chemistry Lab	802	819	827	**868**
Chem 253 Quantitative Analysis	151	135	143	**161**
Chem 315 Physical Chemistry	144	179	131	**148**
Total Number of Students Completing Courses	**6,408**	**7,003**	**7235**	**7632**

Introductory chemistry courses have posed a barrier to student achievement and contributed to low freshman retention, as indicated by historically high W/D/F statistics. To address this problem, the department has implemented and added to the catalog a "parachute" course, CHEM 120, which is available to students struggling in General Chemistry I (CHEM 121). Preliminary results indicate that students who transfer to this course are more likely to eventually pass CHEM 121 than struggling students who do not 'parachute'. CCB faculty also obtained an internal grant to re-design General Chemistry II (CHEM 122) using active-learning, flipped classroom pedagogy.

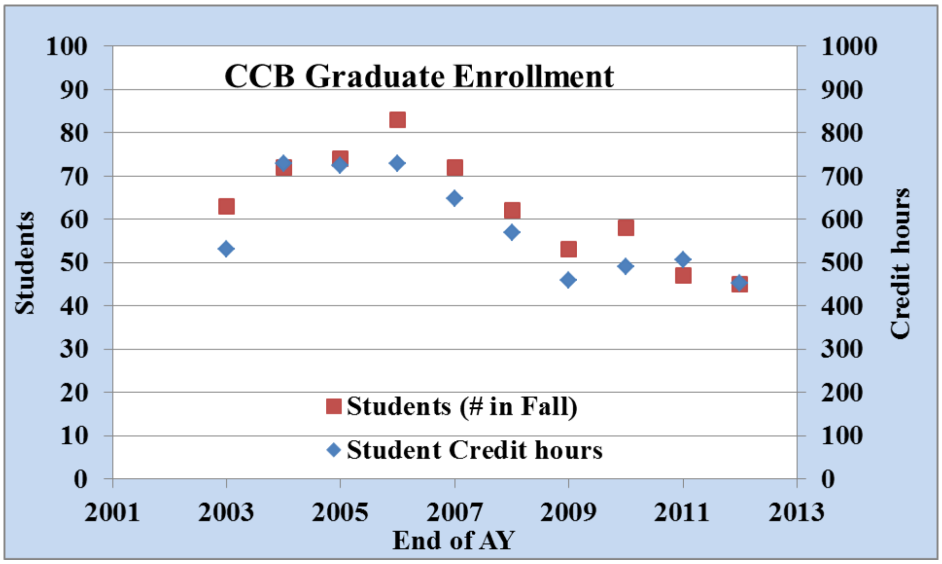
To increase interest in the CCB undergraduate degrees, the department established a set of capstone junior-senior level biological chemistry courses (Chem 421 and 425). As of AY 2011-2012, these courses are now offered every semester and serve over 300 students per year from programs in Chemistry, Biology, Engineering, Pre-Medicine and Pre-Pharmacy who are interested in biological chemistry and chemical biology.

In cooperation with the BA/MD program, CCB developed a set of student-centered active-learning courses to increase success in both general (121 and 122) and organic (301 and 302) chemistry. The department also completed renovation of the organic chemistry teaching laboratory to improve ventilation by adding individual hoods.

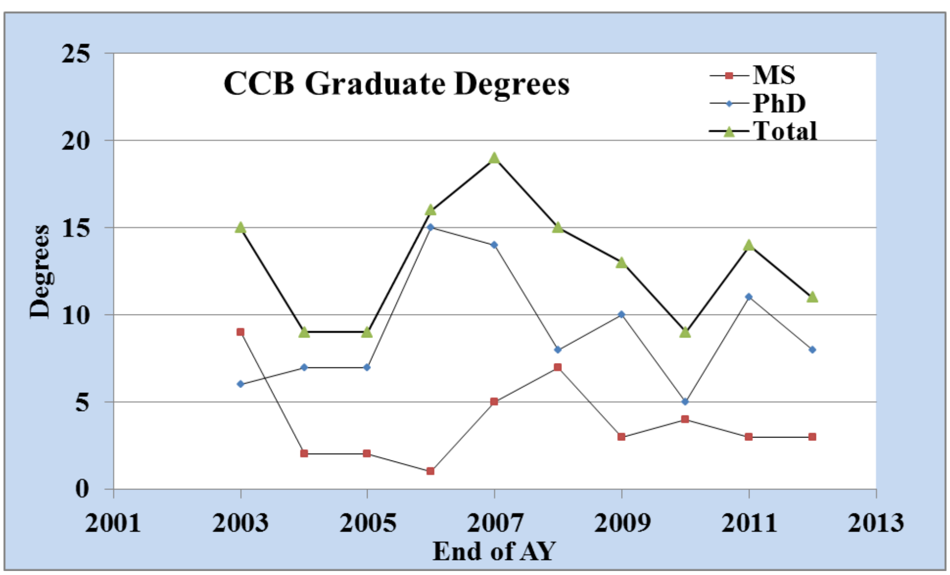
Buoyed by a revenue-sharing financial model, extended university enrollment in CCB courses increased by ~45% from AY 2010-2011 to AY 2011-2012. For the first time, CCB offered an online lab course (CHEM 123L) in the Summer 2012 term.

D. Graduate program

The CCB graduate education program continued to shrink to its smallest size in a decade as defined by numbers of students enrolled (45 in Fall 2011) or by student credit hours taught (453 in AY 2011-2012) (see figure below).

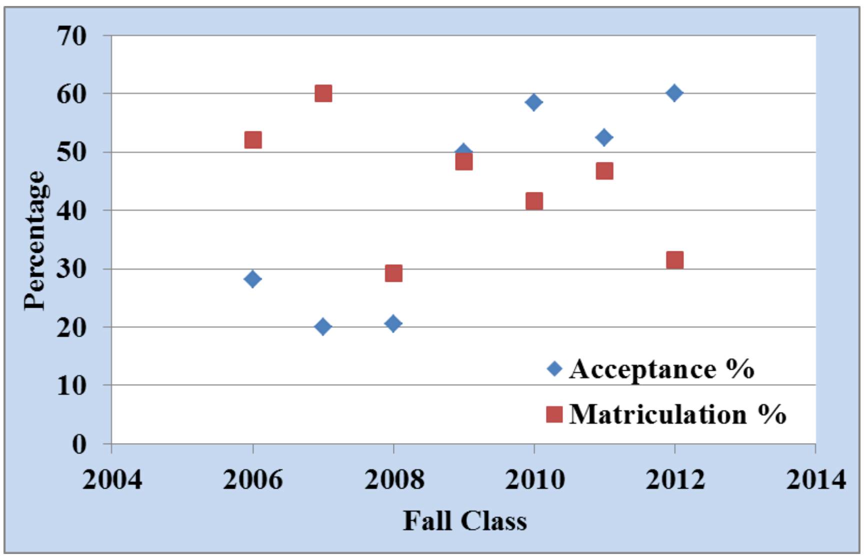


The trend in degrees awarded is less clear, perhaps due to the more stochastic nature of this metric, but also indicates significant shrinking over the last 5 years (see figure below). In 2011-2012, CCB awarded 8 PhD and 3 MS degrees.



As recently as Fall 2007, the department had >60 graduate students, and in 2005 over 80. The number of degrees is approaching the same percentage decrease. In AY 2010-2011, CCB ranked 2nd in A&S in number of PhD degrees awarded, behind History but ahead of all other natural sciences; it is not clear if this will continue over the next few years.

Problematic trends in graduate student recruitment also continue (see figure below). Since 2006, the number of applicants for Fall admission has dropped from ~90 to ~60-65, while the percentage accepted has increased from <30% to >50%. At the same time, the percentage of accepted students arriving at UNM (matriculation % or yield) has dropped (47% in Fall 2011 and 32% in Fall 2012).



Several possible explanations for the shrinkage in the graduate program must be considered. i) As previously argued by David Bear, CCB TA stipends are ~$2000 lower than other flagship universities, ii) The overall decrease in faculty size reduces the number of prospective advisers for new students and the number of RA positions available, iii) the decision not to hire analytical faculty eliminates a popular sub-discipline for prospective students (analytical chemistry is the third largest division of the American Chemical Society), iv) continued reliance on Chinese graduate students at a time when the economy of the PRC has been stronger than that of the USA and v) a graduate education program that fails to excite and attract students. This last possibility has led to several proposals to re-organize the graduate program. Unfortunately, serious disagreements within the faculty have prevented any consensus on the best path forward, and the political fallout from this process has severely undermined departmental morale and cooperation.

E. Research accomplishments

The faculty of the Department of Chemistry and Chemical Biology continued to be among the most prolific publishers on campus on a per capita basis. Twelve research-active professors published a total of 86 peer-reviewed articles, including three in the *Journal of the American Chemical Society*, two in the *Proceedings of the National Academy of Sciences* one in *Science* and one in *Accounts of Chemical Research*. Articles which received special attention include the *Science* article on low-temperature reactivity (H. Guo), a *J. Phys. Chem*. communication modeling a HO + CO reaction surface (H. Guo), and a *Nature* communication on functionalization of aldehydes (W. Wang).

External funding of departmental research increased by ~25% during AY 2011-2012. Faculty brought in $2,473,063 in new research awards from NIH, DoE, NSF and other agencies. Notable awards include a new DTRA grant to David Keller and David Whitten (CBME) and competitive renewals to Kemp (NSF), Paine (DoE), Kirk (NIH), and Wang (NSF).

Significant and worsening problems of conducting research in Clark Hall include electrical power restrictions, unusable fume hoods in many laboratories and repeated plumbing failures which damage experiments and instruments. Perhaps the single most important accomplishment for promoting future research in the department was the designation of the renovation of the Clark/Riebsomer as the number one priority capital project in the State of New Mexico on the General Obligation Bond election ballot for November 2012.

F. Faculty and Administration

Dr. Kuangchiu Joseph Ho: contract reclassified from Sr. Research Scientist I (staff) to Lecturer III effective August 15, 2011 (previously held letter of academic title as lecturer III).

Gary Bush: promoted from Sr. Teaching Laboratory Technician to Supervisor, Teaching Labs effective June 2, 2012.

Wei Wang, promoted from Associate Professor to Professor effective August 13, 2012.

Fu-Sen Liang joined the CCB faculty January 2012, coming from a post-doctoral position at Stanford Medical School with a Ph.D. in organic chemistry from the Scripps Institute. Dr. Liang's background gives him an unusual ability to produce novel compounds for *in vivo* biochemical and medical applications. A search during the 2011-2012 AY led to two junior faculty offers, both of which were accepted. Dr. Ramesh Giri (synthetic chemistry) and Dr. Terefe Habteyes (electron transport) joined the department in August 2012.

Prof. Lorraine Deck retired July 31 of 2011 and Prof. Mark Ondrias retired June 30 of 2012; both remain at UNM as 0.25 FTE retirees, Deck teaching organic chemistry and conducting research and Ondrias continuing to oversee the A&S advising program.

Prof. David Bear decided at the end of the Spring term 2012 to resign as chair of CCB, citing personal and professional issues. Bear had served as chair for three years, and in that time oversaw the hiring of five junior faculty and overdue renovations in Clark/Riebsomer. He returned to his faculty position at HSC but will continue to teach CHEM 421 for the 2012-2013 AY. In June 2012 the Dean of A&S appointed Steve Cabaniss to succeed Bear, beginning July 16, 2012.

II. Plans and recommendations for the future

A. Faculty governance- new departmental handbook and mentoring structure

CCB has operated for the past 20+ years without a written set of governance policies. We are in the process of discussing a faculty handbook, drafted over the summer, which will establish rules on voting rights and procedures, faculty meeting guidelines, committee memberships and duties, chair's duties, etc. While in many cases this written handbook will simply codify past practice, several significant changes to recent practice will include:

a. Requiring a 2/3 majority vote for substantive departmental decisions
b. Requiring that agendas and summaries for faculty meetings be distributed in a timely fashion
c. Re-instituting an elected faculty advisory committee
d. Establishing a formal mentoring committee for each assistant professor which includes a senior faculty member from outside of the department.
e. Establishing consistent, written standards for tenure and promotion within the department.

Historically, mentoring of junior faculty in CCB has not been consistently successful. The percentage of new hires who are still retained at UNM after 7 years has been disappointingly low; of the 6 new assistant professors hired between 2000 and 2005, only one remains on the faculty. Two of the five who left did not apply for tenure, while three others left UNM within a year of receiving tenure. In addition to establishing mentoring committees, the department will actively monitor junior faculty progress through regular meetings with the chair and reviews by senior faculty. Although it is unrealistic to think that all new hires will remain with the department, our goal is a 10-year faculty retention rate of ~2/3.

B. Faculty hiring- senior hires in energy, materials, biological chemistry

The department needs enough senior faculty to provide departmental leadership, university service and mentoring for junior faculty, especially in our research focus areas of biological chemistry, catalysis and energy. The energy area presently has no tenured faculty, and current projections are that three of the 8.5 full professors will retire within three years. Consequently, the hiring plan for AY 2012-2013 focuses on senior scientists; we hope to bring in at least two senior faculty, including one related to energy.

In the longer term, departmental teaching and research must be built principally by hiring junior faculty at the assistant and associate levels. Specific, short-term needs are for a biomolecular mass spectrometrist (biological focus area), a separation scientist (biological focus) and a chemical education specialist (see below). Anticipated retirements will create openings for faculty specializing in reaction kinetics and metal complexation in any of the focus areas. Funding permitting, we plan two junior faculty hires per year in AY 13-14, 14-15, and 15-16, which should allow us to attain a target faculty size of ~20 tenure-track and ~5 lecturers by Fall of 2016.

The ACS refers to chemistry as "the central science", and UNM has faculty in a variety of departments (Earth and Planetary Science, Biology, Physics, Biochemistry, Chemical Engineering, Biomedical Engineering, Pharmacy) engaged in chemically-oriented research and teaching. Previous arrangements regarding secondary appointments in CCB have not attracted many of these faculty. In order to take better advantage of this resource, we plan to revise the arrangements and extend offers of secondary appointments to faculty who teach classes of interest to chemistry graduate students (or which would qualify as restricted electives for senior BA and BS majors) and who are interested in potentially advising chemistry graduate students.

C. Undergraduate program- new course for non-majors, advising system, pedagogy

".....ignorance of chemistry poses a barrier to the democratic process. Ordinary people must be empowered to make decisions - on genetic engineering, on waste disposal sites, and on dangerous and safe power plants. They can call on experts to explain advantages and disadvantages, the options, benefits and risks. But experts do not have the mandate; the people and their representatives do." Roald Hoffmann (1989 Nobel Laureate, Chemistry)

University science departments have an obligation not simply to educate scientists, but the public at large. Chemistry departments are uniquely well-situated to promote science literacy relevant to issues of public policy, since so many key problems- energy production, public health and medication, environmental degradation- have a chemical basis. We are currently designing a course to teach fundamental chemistry to non-science majors using a "newspaper topic" approach which should directly promote science literacy in the public arena. The course, which we plan to offer in the 2013-2014 academic year, will use the American Chemical Society's textbook Chemistry in Context and a 'repeated exposure' instructional approach which differs significantly from that used in our courses for science majors.

Designed to improve graduation rates, the new Arts and Sciences advising model will provide a shared CCB/Biochemistry advisor and drive other program changes. We are currently designing mandatory orientation sessions for new majors scheduled to begin next month. In the longer term, we expect these sessions to become a resource for majors and minors in Chemistry and Chemical Biology. Combining undergraduate advising for CCB and Biochemistry in a single individual should improve the quality of course and major level advising for students in both departments and help to decrease time to degree. We plan to improve pre-professional and career advising by increasing participation of tenure-track faculty.

Introductory chemistry courses are often an obstacle to potential science majors and contribute to low freshman retention rates. Possible causes of the problem include inadequate student preparation, poor math skills, and inappropriate pedagogy. To address inherent difficulties in using a lecture-based pedagogy to teach problem-oriented material, we are implementing a course re-design of CHEM 122 to use flipped-classroom, active learning pedagogy. Assuming favorable results for the test sections, we plan to expand this pedagogy to other sections of CHEM 122 and to initiate a re-design of CHEM 121. Preliminary efforts to employ this type of pedagogy in organic chemistry (CHEM 301 and 302) are underway in Dr. Whalen's BA/MD sections and may be the basis for future changes in those courses as well.

In keeping with state and UNM policy, CCB would like to facilitate transfer of students from CNM and other colleges in New Mexico. We are working with the Dean of Science (Richard Calabro) and faculty at CNM to improve coordination between UNM and CNM versions of general and organic chemistry courses; the resulting sets of course objectives and standards should help to establish a level playing field for 2- and 4-year colleges throughout the state. A degree-level articulation agreement with CNM for the Title V STEM UP program should be completed by summer 2013.

D. Graduate Program- Program reorganization and chemical education

The structure of the graduate program has been a highly contentious issue within the CCB faculty; last year's attempts to find common ground were unsuccessful and ultimately divisive. For AY 2012-2013 the chair has imposed temporary waivers to accommodate students caught in the disagreement, but a long-term solution with widespread faculty support must be found if the graduate program is to progress. Curricular options which have been suggested include i) completely separate 'tracks' for students in chemical biology and students in chemistry, ii) a sequence of required core courses for all students and iii) a 'menu' from which students select a small number (2-4) of core courses. Other options include creation of research areas to replace divisions for graduate training and changes in the written exam program. Some combination of these options should be in place by Fall 2013.

Although the CCB graduate program has awarded more Ph.D. degrees than all but two other departments in the college of Arts and Sciences over the last 4 years, the number of graduate students in the incoming class and in the program overall has been decreasing. As the numbers of junior faculty increase, this trend must be reversed. Our short-term (4 year) goal is to attract 20-25 new graduate students each year (up from 14 in Fall 2011 and 13 in Fall 2012). As funds allow, we plan to improve graduate student recruitment through a more aggressive internet presence (social media, improved website), more direct recruitment of US undergraduates (visits, conferences), and increased stipends in the first year to offset relocation expenses. However, increasing the number of research-active faculty will also be required.

STEM education at the university and college level is an increasingly important topic at the state and university level. Research on science teaching and learning indicates that in many cases the standard 'lecture mode' is not the most effective pedagogy, but given the variety of student audiences and types of material, and the financial constraints of large student numbers, it is not always clear how to improve. Several CCB faculty and others across campus are engaged in discipline-based educational research (DBER) aimed at improving our STEM teaching. We are beginning discussions with faculty in other departments about how STEM-DBER might be formalized in a research or graduate program. One possibility is to add chemical education as a research area in the CCB graduate program so that our faculty could advise students in this field.

E. Research- Renovating labs, increasing instrument access, facilitating grant activity

The CCB laboratory space in Clark/Riebsomer has multiple and serious deficiencies rendering much of it unusable for modern chemical research. Passage of the upcoming general obligation bond C on Nov. 6 should provide $16M for building renovations. We have begun initial discussions with the capital improvement, campus development and architects' offices on how to manage these renovations. The current timetable calls for the project scope to be delineated by the end of Fall 2012 term, architects to be hired during the following Spring 2013, bids finished by roughly the beginning of Fall term 2013 and construction activities to commence shortly thereafter. We hope to modernize all building utilities and Riebsomer wing lab space, convert some of the older Clark wing labs into offices and meeting rooms, and convert remaining Clark wing labs into computer or 'dry lab' space. The construction will cause considerable disruption in the next two academic years, but should eventually provide UNM with competitive chemistry lab space and an improved learning environment for our students.

Researchers in CCB and related departments in A&S and in Engineering have occasional use for analytical instrumentation not available (due to cost and/or complexity) in their own labs or departments. Currently, shared instrumentation facilities for elemental analysis and electron microscopy maintained by E&PS are both extensively used and fiscally solvent. CCB has similar facilities for molecular analysis by NMR and mass spectrometry, although the latter is not solvent and has not met the goals for which it was established. Additionally, modern analytical instruments purchased by CCB principally for educational research are typically used only ~2 months of the year, but are not readily available for researchers in CCB (and hardly available at all to others) due to the absence of staff for maintenance and operations. We are discussing the possibility of establishing a molecular analysis facility to ensure researcher access to mass spectrometry and other techniques by providing staff and a viable administrative framework. This facility should aid students and faculty in CCB and other departments, both directly by providing instrument time and/or analyses and indirectly by freeing up funds which might otherwise be spent purchasing and operating duplicative instrumentation.

CCB has had recurring problems with financial statements and grant expenditures which are detrimental to the departmental research effort. Additionally, our junior faculty require considerable assistance in submitting proposals and managing grants. We are considering a fiscal staff re-organization to address these issues, possibly by creating a position for a grants and contracts specialist. Any fiscal/grants re-organization would coincide with the changes in the advising structure prompted by A&S decisions, scheduled for early Spring 2013.

III. Faculty Publication list

The faculty of the Department of Chemistry and Chemical Biology FY 2012 publication record continued to be among the most prolific on campus. Eleven research-active faculty published a total of 86 peer-reviewed articles, including three in the *Journal of the American Chemical Society*, two in the *Proceedings of the National Academy of Sciences* one in *Science* and one in Accounts of Chemical Research. Articles which received special attention include the Science article on low-temperature reactivity (H. Guo), a *J. Phys. Chem*. communication modeling a HO + CO reaction surface (H. Guo), and a *Nature* communication on functionalization of aldehydes (W. Wang).

Stephen Cabaniss

Klammler, H.; Hatfield, K.; da Luz, J.A.G.; Annable, M.D.; Newman, M.; Cho, J.; Peacock, A.; Stucker, V.; Ranville, J.; Cabaniss, S.E.; Rao, P.S.C. "Contaminant discharge and uncertainty estimates from passive flux meter measurements" 2012, Water Resources Res. 48 Article Number: W02512 DOI: 10.1029/2011WR010535.

Leavitt, J.J.; Howe, K.; Cabaniss, S.E. "Equilibrium modeling of U(VI) speciation in high carbonate groundwaters: Model error and propagation of uncertainty" 2011, Appl. Geochem. 26 (2011), pp. 2019-2026.

Debra Dunaway-Mariano

Rational design, synthesis and evaluation of first generation inhibitors of the Giardia lambliafructose-1,6-biphosphate aldolase.Li Z, Liu Z, Cho DW, Zou J, Gong M, Breece RM, Galkin A, Li L, Zhao H, Maestas GD, Tierney DL, Herzberg O, Dunaway-Mariano D, Mariano PS. J Inorg Biochem. 105, 509-17 (2011).

Regioselectivity of enzymatic and photochemical single electron transfer promoted carbon-carbon bond fragmentation reactions of tetrameric lignin model compounds. Cho DW, Latham JA, Park HJ, Yoon UC, Langan P, Dunaway-Mariano D, Mariano PS. J Org Chem. 76, 2840-52 (2011).

Homo sapiens Dullard Protein Phosphatase Shows a Preference for the Insulin-Dependent Phosphorylation Site of Lipin1. Wu R, Garland M, Dunaway-Mariano D, Allen KN. Biochemistry 50, 3045-7 (2011).

Divergence of Chemical Function in the Alkaline Phosphatase Superfamily: Structure and Mechanism of the P-C Bond Cleaving Enzyme Phosphonoacetate Hydrolase. Kim A, Benning MM, Oklee S, Quinn J, Martin BM, Holden HM, Dunaway-Mariano D. Biochemistry. 50, 3481-94 (2011).

Divergence of Structure and Function in the Haloacid Dehalogenase Enzyme Superfamily: Bacteroides thetaiotaomicron BT2127 Is an Inorganic Pyrophosphatase. Huang H, Patskovsky Y, Toro R, Farelli JD, Pandya C, Almo SC, Allen KN, Dunaway-Mariano D. Biochemistry 50, 8937-49 (2011).

The Enzyme Function Initiative. Gerlt JA, Allen KN, Almo SC, Armstrong RN, Babbitt PC, Cronan JE, Dunaway-Mariano D, Imker HJ, Jacobson MP, Minor W, Poulter CD, Raushel FM, Sali A, Shoichet BK, Sweedler JV. Biochemistry 50, 9950-62 (2011).

A Thioester Substrate Binds to the Enzyme Arthrobacter Thioesterase in Two Ionization States; Evidence from Raman Difference Spectroscopy. Jian Dong, Zhihao Zhuang, Feng Song, Debra Dunaway-Mariano and Paul R. Carey Journal of Raman Spectroscopy 43, 65-71 (2012).

Investigation of the Catalytic Mechanism of the Hotdog-Fold Enzyme Superfamily Pseudomonas sp. Strain CBS3 4-Hydroxybenzoyl-CoA Thioesterase. Zhuang Z, Latham J, Song F, Zhang W, Trujillo M, Dunaway-Mariano D. Biochemistry. 51, 786-794 (2012).

Human brown fat inducible thioesterase variant 2 cellular localization and catalytic function. Chen D, Latham J, Zhao H, Bisoffi M, Farelli J, Dunaway-Mariano D Biochemistry 5, 6990-6999 (2012).

The Catalytic Mechanism of the Hotdog-fold Enzyme Superfamily 4-Hydroxybenzoyl-CoA Thioesterase from Arthrobacter sp. Strain SU. Song F, Thoden JB, Zhuang Z, Latham J, Trujillo M, Holden HM, Dunaway-Mariano D Biochemistry 51, 7000-7016 (2012).

Correlation of Structure and Function in the Human Hotdog-fold Enzyme hTHEM4. Zhao H, Lim K, Choudry A, Latham JA, Pathak MC, Dominguez D, Luo L, Herzberg O, Dunaway- Mariano D. Biochemistry 51, 6490-2 (2012).

John Grey

(* corresponding author, † undergraduate student)

Wise, Adam J.; Grey, John K.* "Resonance Raman studies of excited state displacements of conjugated polymer donor/acceptor charge transfer complexes" Physical Chemistry Chemical Physics (2012) 14, 11273-11276.

Niles, Edwards T.; Roehling, John D.; Yamagata, Hajime; Wise, Adam J.; Spano, Frank C.; Moule, Adam J.; Grey, John K.* "J-Aggregate behavior in poly(3-hexylthiophene) nanofibers" Journal of Physical Chemistry Letters (2012) 3, 259-263.

Gao, Jian; Grey, John K.* "Spectroscopic studies of energy transfer in fluorene co-polymer blend nanoparticles" Chemical Physics Letters (2012) 522, 86-91.

Wise, Adam J.; Precit, Mimi R.;† Papp, Alexandra M.;† Grey, John K.* "Effect of fullereneintercalation on the conformation and packing of poly-(2-methoxy-5-(3′-7′-dimethyloctyloxy)-1,4-phenylenevinylene)" ACS Applied Materials and Interfaces (2011) 3, 3011–3019.

Hua Guo

S. Lin, D. Xie, and H. Guo, J. Phys. Chem. C., 115, 20583 (2011). Pathways of methanol steam reforming on PdZn and comparison with Cu.

C. Xie, A. Li, D. Xie, and H. Guo, J. Chem. Phys., 135, 164312 (2011), State-to-state quantum dynamics of the $N(^4S) + OH(X^2\Pi) \rightarrow H(^2S) + NO(X^2\Pi)$ reaction.

G. K. Smith, Z. Ke, H. Guo, and A. C. Hengge, J. Phys. Chem. B., 115, 13713 (2011), Insights into the phosphoryl transfer mechanism of cyclin-dependent protein kinases from ab initio QM/MM free-energy studies.

P. W. Thomas, M. Zheng, S. Wu, H. Guo, D. Liu, D. Xu and W. Fast, Biochem., 50, 10102 (2011), Characterization of purified New Delhi metallo-β-lactamase-1 (NDM-1).

J. Daranlot, M. Jorfi, C. Xie, A. Bergeat, M. Costes, P. Caubet, D. Xie, H. Guo, P. Honvault, K. M. Hickson, Science, 334, 1538 (2011), Revealing atom – radical reactivity at low temperature through the N + OH reaction. (Featured in Science and C&E News, Dec, 2011)

J. Ma, D. Xu, H. Guo, V. Ting, M. E. Kellman, J. Chem. Phys., 136, 014304 (2012), Isotope effect in normal-to-local transition of acetylene bending modes.

B. Jiang, D. Xie, and H. Guo, J. Chem. Phys., 136, 034302 (2012), State-to-state photodissociation dynamics of triatomic molecules: H_2O in its B band.

J. Li, Y. Wang, B. Jiang, J. Ma, R. Dawes, D. Xie, J. M. Bowman, and H. Guo, J. Chem. Phys., 136, 041103 (2012), Communication: A chemically accurate potential energy surface for the HO + CO → H + CO_2 reaction. *(Top 20 most read article on J. Chem. Phys., January and February 2012)*

H. Guo, Theo. Chem. Acc., 131, 1077 (2012), Theoretical characterization of reaction dynamics in the gas phase and at interfaces (Editorial, 50^{th} anniversary issue).

H. Guo, Int. Rev. Phys. Chem., 31, 1 (2012), Quantum dynamics of complex-forming reactions (invited review, featured on cover, and one of the most read articles in 2012).

S. Lin, D. Xie, and H. Guo, J. Mole. Catal. A, 356, 165 (2012), First-principles study of the methyl formate pathway of methanol steam reforming on PdZn(111) with comparison to Cu(111).

J. Li, C. Xie, J. Ma, Y. Wang, R. Dawes, D. Xie, J. M. Bowman, H. Guo, J. Phys. Chem. A, 116, 5057-5067 (2012), Quasi-classical dynamics of the HO + CO → H + CO_2 reaction on a new ab initio based potential energy surface.

X. Zhu, J. Ma, D. R. Yarkony, and H. Guo, J. Chem. Phys., 136, 234301 (2012), Computational determination of $\tilde{A}$ state absorption spectrum of NH_3 and ND_3 using a new quasi diabatic representation of the $\tilde{X}$ and $\tilde{A}$ states and full six dimensional quantum dynamics.

B. Jiang, X. Ren, D. Xie, and H. Guo, Proc. Natl. Acad. Sci. USA., 109, 10224 (2012), Enhancing dissociative chemisorption of H_2O on Cu(111) via vibrational excitation.

C. Xie, J. Li, D. Xie, and H. Guo, J. Chem. Phys., 137, 024308 (2012), Quasi-classical trajectory studies of the H + CO_2 → HO + CO reaction on a new ab initio based potential energy surface.

J. Ma, J. Li, and H. Guo, Phys. Rev. Lett., 109, 063202 (2012), Tunneling facilitated dissociation to H + CO_2 in $HOCO^-$ photodetachment.

J. Ma, H. Guo, R. Dawes, Phys. Chem. Chem. Phys., 14, 12090 (2012), Low temperature rat constants for the N + CN → N_2 + C reaction: two-dimensional quantum capture calculations on an accurate potential energy surface.

J. Ma, J. Li, H. Guo, J. Phys. Chem. Lett., 3, 2482 (2012), Quantum dynamics of the HO + CO → H + CO_2 reaction on an accurate potential energy surface.

J. Li, R. Dawes, and H. Guo, J. Chem. Phys., 137, 094304 (2012), An ab initio based full-dimensional global potential energy surface for FH_2O (X^2A') and dynamics for the F + H_2O → HF + HO reaction.

David Keller

Kumud Poudel, David Keller, and James Brozik. Single-Particle Tracking Reveals Corralling of a Transmembrane Protein in a Double-Cushioned Lipid Bilayer Assembly. Langmuir **27**, 320-327 (2011).

Richard Kemp

D.A. Dickie and R.A. Kemp, "Formation of an Intramolecular Main Group-CO_2 Adduct", *Inorg. Chem.*, **50**, 11288 (2011).

G.R. Fulmer, A.N. Herndon, R.A. Kemp, and K.I. Goldberg, "Hydrogenolysis of Pd(II)-OR Complexes", *J. Am. Chem. Soc.*, **133**, 17713 (2011).

C.A. Stewart, D.A. Dickie, B. Moasser, and R.A. Kemp, "Reactions of CO_2 and Related Heterollenes with CF_3-Substituted Aromatic Silylamines of Tin", *Polyhedron,* **32**, 14 (2012).

B.M. Barry, D.A. Dickie, A.E. Wetherby Jr., W.E. Barker IV, C.A. Larsen, R. Waterman, W.E. Geiger, and R.A. Kemp, "CO_2 Interactions with Main Group Compounds Directed Towards Preparing Useful Organic Compounds", *Prepr. Pap. - Am. Chem. Soc. - Fuel Chem.*, **57**, 294 (2012).

D.A. Dickie, K.B. Gislason, and R.A. Kemp, "Formation of Phosphino-substituted Isocyanate by Reaction of CO_2 with Group 2 Complexes Based on the (Me_3Si)(*i*-Pr_2P)NH Ligand", *Inorg. Chem.*, **51**, 1162 (2012).

A. Mrutu, W. William, and R.A. Kemp, "Synthesis and Characterization of Molybdenum and Tungsten Complexes Containing Tris(diphenylphosphino)methane", *Inorg. Chem. Comm.,* **18**, 110 (2012).

A.M. Felix, D.A. Dickie, Giang Page, Ian S. Horne, and R.A. Kemp, "Addition of Aluminum and Gallium Species to Aromatic and Alkyl-substituted 1,4-Diaza-1,3-butadiene Ligands", *Inorg. Chem.*, **51**, 4650 (2012).

A.M. Felix, B.J. Boro, D.A. Dickie, Y. Tang, J.A. Saria, B. Moasser, C.A. Stewart, B.J. Frost, and R.A. Kemp, "Insertion of CO_2 into Divalent Group 2 and 12 Amides", *Main Group Chem.*, **11**, 13 (2012).

C.A. Stewart, D.A. Dickie, and R.A. Kemp, "Investigation of Metal Cyclam Complexes as Potential Catalysts for the Production of Dimethylcarbonate", *Inorg. Chim. Acta*, **392**, 268 (2012).

L.A. Steele, R.A. Kemp, and T.J. Boyle, "Lanthanide Alkoxides with CO_2", *Polyhedron*, doi: 10.1016/j.poly. 2012.05.021 (2012).

Martin Kirk

K. P. O'Halloran, C. C. Zhao, N. S. Ando, A. J. Schultz, T. F. Koetzle, P. M. B. Piccoli, B. Hedman, K. O. Hodgson, E. Bobyr, M. L. Kirk, S. Knottenbelt, E. C. Depperman, B. Stein, T. M. Anderson, R. Cao, Y. V. Geletii, K. I. Hardcastle, D. G. Musaev, W. A. Neiwert, X. K. Fang, K. Morokuma, S. X. Wu, P.

Koegerler, C. L. Hill, Revisiting the Polyoxometalate-Based Late-Transition-Metal-Oxo Complexes: The "Oxo Wall" Stands. *Inorg. Chem.* **2012**, *51*, 7025-7031. DOI: 10.1021/ic2008914.

M. L. Kirk, D. A. Shultz, E. C. Depperman, D. Habel-Rodriguez, and R. D. Schmidt. Spectroscopic Studies of Bridge Contributions to Electronic Coupling in a Donor-Bridge-Acceptor Biradical System, *J. Am. Chem. Soc.* **2012**, *134,* 7812-7819. DOI: 10.1021/ja300233a

R. A. Rothery, B. Stein, M. Solomonson, M. L. Kirk, J. H. Weiner, Impact of Pyranopterin Conformation on Molybdenum and Tungsten Enzyme Function. *PNAS.* **2012**, *109 (37)* 14773-14778. doi:10.1073/pnas.1200671109.

J. Sempombe, B. Stein, and M. L. Kirk. Spectroscopic and Electronic Structure Studies Probing Covalency Contributions to C-H Bond Activation and Transition State Stabilization in Xanthine Oxidase, *Inorg. Chem.* **2011**, *50*, 10919-10928.

R. P. Mtei, E. Perera, B. Mogeesa, P. Basu, and M. L. Kirk. A Valence Bond Description of Dizwitterionic Dithiolene Character in an Oxomolybdenum-bis(dithiolene), *European Journal of Inorganic Chemistry, EuroJIC,* **2011**, *36,* 5467-5470.

J. Sempombe, M. G. I. Galinato, B. O. Elmore, W. Fan, J. G. Guillemette, N. Lehnert, M. L. Kirk, C. Feng, Mutation in the Flavin Mononucleotide Domain Modulates Magnetic Circular Dichroism Spectra of the iNOS Ferric Cyano Complex in a Substrate-Specific Manner. *Inorg. Chem.* **2011**, *50*, 6859-6861. DOI: 10.1021/ic200952c

C. M. Zaleski, S. Tricard, E. C. Depperman, W. Wernsdorfer, T. Mallah, M. L. Kirk, V. L. Pecoraro. Single Molecule Magnet Behavior of a Pentanuclear Mn-based Metallacrown Complex: Solid State and Solution Magnetic Studies. *Inorg. Chem.* **2011**, *50,* 11348-11352.

K. G. Matz, R. Mtei, R. Rothstein, M. L. Kirk, and S. J. Nieter Burgmayer. A Study of Mo(4+)(Quinoxalyl-Dithiolenes) as Models for the Non-Innocent Pyranopterin in the Molybdenum Cofactor. *Inorg. Chem.* **2011**, *50,* 9804-9815.

R. P. Mtei, G. Lyashenko, B. Stein, N. Rubie, R. Hille, and M. L. Kirk. Spectroscopic and Electronic Structure Studies of a DMSO Reductase Caltalytic Intermediate: Implications for Electron and Atom Transfer Reactivity, *J. Am. Chem. Soc.* **2011**. *133*, 9762–9774. **DOI:** 10.1021/ja109178q

H. Sugimoto, H. Tano, K. Suyama, T. Kobayashi, H. Miyake, S. Itoh, R. P. Mtei, and M. L. Kirk, Chalcogenidobis(ene–1,2–dithiolate)molybdenum(IV) Complexes (Chalcogenide E = S, Se): Probing Mo≡E and Ene–1,2–dithiolate Substituent Effects on Geometric and Electronic Structure, *Dalton Trans.,* **2011**, *40*, 1119-1131. DOI: 10.1039/c0dt00871k

Fu-Sen Liang

Liang, F. -S., Ho, W. Q. & Crabtree, G. R. "Engineering the ABA Plant Stress Pathway for Regulation of Induced Proximity" Sci. Signal. 2011, 4, rs2. Highlighted in: Sci. Signal. 2011, 4, pe13. and Nat. Struct. Mol. Biol. 2011, 18, 403.

Patrick Mariano

"Rational Design and Evaluation of First Generation Inhibitors of the Giardia lamblia Fructose-1,6-biphosphate Aldolase," Zhimin Li, Zhengang Liu, Daewon Cho, Jiwen Zou, Maozhen Gong, Robert M. Breece, Andrey Galkin, Ling Li, Hong Zhao, Gabriel D. Maestas, David L. Tierney, Osnat Herzberg, Debra Dunaway-Mariano, Patrick S. Mariano, J. Inorg. Biochem. (2011), 105, 509-516

"Photochemical Approach to the Preparation of Lariat Crown Ethers Containing Peptide Sidearms" Dae Won Cho, Ung Chan Yoon, Patrick S. Mariano, Bull. Kor. Chem. Soc. (2011), 32, 503-509.

"Studies Leading to the Development of a SET-Photochemical Strategy for Syntheses of Macrocyclic Poly-Ethers, -Thioethers, and –Amides" Dae Won Cho, Ung Chan Yoom, Patrick S. Mariano, Acc. Chem. Res. (2011), 44, 204-215.

"Regioselectivity of Enzymatic and Photochemical Single Electron Transfer Promoted Carbon-Carbon Bond Fragmentation Reactions of Tetrameric Lignin Model Compounds" Dae Won Cho, John A. Latham, Hea Jung Park, Ung Chan Yoon, Paul Langan, Debra Dunaway-Mariano, Patrick S. Mariano, J. Org. Chem. (2011), 76, 2840–2852

"Exploration of Photochemical Reactions of N-Trimethylsilylmethyl-Substituted Uracil, Pyridone, and Pyrrolidone Derivatives", Dae Won Cho, Chan Woo Lee, Jong Gu Park, Sun Wha Oh, Nam Kyoung Sung, Hea Jung Park, Kyung Mok Kim, Patrick S. Mariano, Ung Chan Yoon, J. Photochem. Photobiol. (2011), 10, 1169-1180.

"A Strategy for the Preparation of Cyclic Polyarenes Based on Single Electron Transfer Promoted Photocyclization Reactions", H. J. Park, J. H. Choi, B. N. Park, U. C. Yoon, D. W. Cho and P. S. Mariano, Res. Chem. Intermed. (2012), 38, 847-862.

Robert T. Paine

S. Pailloux, C.E. Shirima, E.N. Duesler, K.A. Smith and R.T. Paine "Synthesis and lanthanide coordination chemistry of 2[(phosphinoyl)methyl]-4,5-dihydrooxazole and 2-[(phosphinoyl)methyl)benzoxazole ligands" *Polyhedron* , **30**, 2746 (2011).

T. Chen, E.N. Duesler, H. Nöth, and R.T. Paine "Synthesis and reactivity of a zirconocene bis-(aminoborylphosphane)" *Main Group Chem*. **10**,279 (2011).

M. Chakravarty, S. Pailloux, E.N. Duesler, K.A. Smith, R.T. Paine, N.J. Williams and R.D. Hancock "Synthesis and metal coordination chemistry of (phenyl)(pyridine-2-ylmethyl)phosphinodithioic acid, [2-C_5H_4N]$CH_2P(S)(SH)(Ph)$" *Polyhedron*, 33, 327 (2012).

D. Rosario-Amorin, E.N. Duesler, R.T. Paine, B.P. Hay, L.H. Delmau, S. Reilley, B.L. Scott and A. J. Gaunt "Synthesis and Coordination Chemistry of Phosphino Oxide Decorated Dibenzofuran Platforms" *Inorg. Chem.,51,6667* (2012).

Yang Qin

"Photo-Cross-Linkable Azide-Functionalized Polythiophene for Thermally Stable Bulk

Heterojunction Solar Cells.” Nam, C.-Y.; Qin, Y.; Park, Y. S.; Hlaing, H.; Lu, X.; Ocko, B. M.; Black, C. T.; Grubbs, R. B. Macromolecules, 2012, 45, 2338-2347.

“Self-Assembly of Borane End-Functionalized Polystyrene Through Tris(1-pyrazolyl)borate (Tp) Iron(II) Linkages.” Qin, Y.; Shipman, P. O.; Jäkle, F. Macromol. Rapid Commun. 2012, 33, 562-567.

Wei Wang

Zhang, X.-S.; Song, X.-X.; Li, H.; Zhang, S.-L.; Chen, X.-B.; Yu, X.-H.; Wang, W.* “An Organocatalytic Cascade Approach toward Polysubstituted Quinolines and Chiral 1,4-Dihydroquinolines–Unanticipated Effect of *N*-Protecting Groups” *Angew. Chem. Int. Ed.,* 2012, 51, 7282-7286.

Song, X.-X.; Zhang, X.-S.; Zhang, S.-L.; Li, H.;* Wang, W.* “Direct Transformation of Simple Enals to 3,4-Disubstituted Benzaldehydes under Mild Reaction Conditions via an Organocatalytic Regio- and Chemo-selective Dimerization Cascade” *Chem. Eur. J.,* 2012, *18*, 9770-9774.

Xuan, W.; Chen, C.; Cao, Y.; He, W.; Jiang, W.; Liu, K.-J.;* Wang, W.* “Rational Design of a Ratiometric Fluorescent Probe with a Large Emission Shift for the Facile Detection of Hg^{2+}” *Chem. Commun.,* 2012, *48*, 7292-7294.

Wang, H.; Yang, W.; Liu, H.; Wang, W.;* Li, H.* “$FeCl_3$ Promoted Highly Regioselective [3+2] Cycloaddition of Dimethyl 2-Vinyl and Aryl Cyclopropane-1,1-dicarboxylates with Aryl Isothiocyanates” *Org. Biomol. Chem.,* 2012, ***10****,* 5032-5035.

Xuan, W.-M. Sheng, C.-Q.;* Cao, Y.-T.; He, W.-H.; Wang, W.* “Emerging Fluorescent Probes for the Detection of Hydrogen Sulfide in Biological Systems” *Angew. Chem. Int. Ed.,* 2012, *51,* 2282-2284 (Highlights).

Liu, L.; Wu, D.; Li, X.; Wang, S.; Li, H.; Li,* J.; Wang, W.* “Organocatalytic Enantioselective Conjugate Addition of Ketones to Isatylidine Malononitriles” *Chem. Commun.,* 2012*, 48*, 1692-1694.

Zhu, J.; Yu,* S.; Lu, W.-C..; Deng, J.; Li, J.; Wang, W.* “Direct Oxidative Conversion of 3-Aryl Propionaldehydes to 3-Aryl Acroleins Promoted by SOMO Catalysis” *Tetrahedron Lett.,* 2012*, 53*, 1207-1209.

Deng, J.; Wang, F.; Yan, W.-Z.; Zhu, J.; Jiang, H.-L.; Wang, W.;* Li, J.* “Synthesis of 3-Substituted 1,5-Aldehyde Esters via an Organocatalytic Highly Enantioselective Conjugate Addition of New Carbonylmethyl 2-Pyridinylsulfone to Enals” *Chem. Commun*., 2012, *48*, 148-150. Invited for “the joint ChemComm–Organic & Biomolecular Chemistry ‘Organocatalysis’ web themed issue.”

Xie, H.-X.; Zhang, S.-L.; Li, H.; Zhao, S.-H.; Xu, Z.-A.; Song, X.-X.; Yu, X.-H.;* Wang, W.* “Total Synthesis of Polyene Natural Product Dihydroxerulin by Mild Organocatalyzed Dehydrogenation of Alcohols” *Chem. Eur. J.* 2012, *18*, 2230-2234.

Zou, Z.-Q.; Deng, Z.-J.; Yu, X.-H.;* Zhang, M.-M.; Zhao, S.-H.; Lou, T.; Yin, X. Xu, H.; Wang, W.* “A New Facile Approach to *N*-Alkylpyrroles from Direct Redox Reaction of 4-Hydroxy-L-proline with Aldehydes” *Science China – Chemistry,* 2012, *55*, 43-49 (invited paper).

Liu, L.; Wu, D.; Zheng, S.; Li, T.; Li, X.; Wang, S.; Li, J.; Li, H.;* Wang, W.* "Synthesis of Highly Functionalized Chiral 3, 3'-Disubstituted Oxindoles via an Organocatalytic Enantioselective Michael Addition of Nitroalkanes to Indolylidene-cyanoacetates" *Org. Lett.,* 2012*, 14*, 134-137.

Zhang, F.; Yang, X.-S.; Zhu, F.-X.; Huang, J.-L.; He, W.-H.; Wang, W.*; Li, H.-X.* "Highly Active and Reusable Organometallic Catalysts Covalently Bonded to an Ordered Mesoporous Polymer" *Chem. Sci.,* 2012, ***3,* 476-484**.

Song, X.-X.; Song, A.-G.; Zhang, F.; Li, H.-X.;* Wang, W.* "Direct Stereoselective β-Arylation of Unmodified Enals Using an Organocatalytic Cross-coupling-like Reaction" *Nature Commun.,* 2011, *2*, 524, doi:10.1038/ncomms1541. This work has been highlighted in *Synfacts*.

Xie, H.-X.; Zhang, Y.-N.; Zhang, S.-L.; Chen, X.-B.; Wang, W.* "Bifunctional Cinchona Alkaloid-thiourea Catalyzed Highly Efficient, Enantioselective Aza-Henry of Cyclic Trifluoromethyl-Ketimines and Application in Synthesis of Anti-HIV Drug DPC 083" *Angew. Chem. Int. Ed.,* 2011, *50,* 11773-11776. This work has been highlighted in *Synfacts*.

Zhang, S.-L.; Xie, H.-X.; Song, A.-G.; Wu, D.-Y.; Zhu, J.; Zhao, S.-H.; Li, J.;*, Yu, X.-H.;* Wang, W.* "Efficient Preparation of *trans*-α, β-Unsaturated Aldehydes from Saturated Aldehydes by Oxidative Enamine Catalysis" *Science China – Chemistry,* 2011, *54*, 1932-1936 (invited for special issue of International Year of Chemistry).

Zhang, S.-L.; Xie, H.-X.; Zhu, J.; Li, H.; Zhang, X.-S.; Li, J.;* Wang, W.* "Organocatalytic Enantioselective α-Functionalization of Aldehydes via Oxidation of Enamines and Their Application in Cascade Reactions" *Nature Commun.,* 2011, *2,* 211, DOI: 10.1038/ncomms1214. This work has been highlighted in *C&EN News* (March 7, 2011 issue on page 9) as "News of the Week" and *Synfacts*.

IV. External professional outreach activities

Joe Ho obtained a $10,000 grant to obtain and operate a mobile laboratory for high school outreach. He also continues to lead a summer workshop for secondary chemistry teachers and maintain a website for their use.

Steve Cabaniss organize a community Teach-In on the Albuquerque aquifer jet fuel plume originating from Kirtland AFB. He also maintains the "Student's Guide to Free Chemistry Software" (https://sites.google.com/site/chemistryfreeware/home).

Rick Kemp and members of his research group participated in the Sandia NL "Dognapping" event on forensic science. (http://cenblog.org/the-editors-blog/2011/01/csi-dognapping-at-sandia/)

V. External funding 2011-2012

During AY 2011-2012 CCB faculty held 21 research grants from NSF, NIH, DoE and external agencies totaling xxx$. New awards during this time included…$2,473,063

Cabaniss, Steve (co-PI)
DoE Subaward from University of Florida $132,288
Novel Sensor for the In Situ Measurement of Uranium Fluxes

Deck, Lorraine
Arizona State University $756
Synthesis of Therapeutic Analogues for Cancer

Dunaway Mariano, Debra
NIH $485,998
Enzymes: Structure, Mechanism, Function, Inhibition

Dunaway Mariano, Debra
NIH $183,096
A Collaborative Center for an Enzyme Function Initiative

Grey, John
NSF $245,000
CAREER: Understanding Structure-Function Relationships in Polymeric Semiconductor Materials from a Top-Down and Bottom-up Perspective.

Grey, John (Co-PI)
DTRA $1,500,000
Controllable Adhesion, Detection, and Release of CBW Agents by Multifunctional "SMART" Nanoscale Surfaces

Guo, Hua
NSF (Co-PI), 2010-2013, $435,077 (equipment only)
MRI: Acquisition of a GPU-Accelerated Parallel Supercomputer for Computational Science and Engineering Research at the University of New Mexico

Guo, Hua
NSF $130,555
Dynamic Effects in Heterogeneous Catalytic Reactions

Guo, Hua
DOE $ 120,000
Wave Packet Based Statistical Approach to Complex-Forming Reactions

Guo, Hua
DTRA $148,919

Modeling Case-Enhanced Explosives with Coupled Chemistry Hydrocodes

Keller, David
DTRA $270,123
Controllable Adhesion Detection & Release of CBM Agents by Multifunctional “Smart” Nanoscale Surfaces

Kemp, Richard
National Science Foundation $145,000
Heteroallenes as Building Block for Synthesis and Sequestration

Kemp, Richard
Department of Energy $250,000
Direct Epoxidations Using Molecular Oxygen

Kemp, Richard
ACS-PRF $100,000
π-Bonded Cationic Ligands as Catalysts and Precursors

Kirk, Martin
National Institute of General Medical Sciences/NIH/DHHS $282,355
Spectroscopic Studies of Molybdoenzymes and Models

Kirk, Martin
National Science Foundation $193,700
Acquisition of a Low-field NMR Spectrometer for Research and Training

Kirk, Martin
NSF $298,400
Nanoscale Electron Correlation and Ferromagnetic Exchange in Donor-Acceptor Biradical Systems: Relationship to Molecular Electronics”

Paine, Robert
Washington State University $100,000
Advanced Aqueous Separation Systems for Actinide Partitioning

Paine, Robert
Department of Energy $282,355
Preorganized and Immobilized Ligands for Metal-Ion Separations

Wang, Wei
West Virginia University HSC $75,009
Phosphodiesterase-2 and Mood Disorders: Target Validation and Drug Discovery

Wang, Wei
NSF $175,000
Oxidative Enamine Catalysis in Organic Synthesis

VI. Appendices:

Appendix A. Major equipment purchases

Zeiss fluorescence microscope Axio Observor D1 (Liang Lab, startup funds)

Dionex HPLC Titanium U3000 (Liang lab, start-up funds)

Thermo DXR SmartRaman Raman spectrometer (senior teaching lab, teaching funds)

Appendix B. Enrollments by degree

Number of Students Enrolled in Degree Plans – By Semester

Semester	Minor	BA	BS	MS	PhD
SU 09	356	139	174	3	44
FA 09	374	143	168	4	43
SP 10	392	156	187	4	47
SU 10	328	141	162	1	45
FA 10	279	129	156	1	46
SP 11	328	136	150	1	39
SU 11	174	83	34	1	29
FA 11	446	170	129	0	45
SP 12	499	186	127	1	43

Appendix C. Teaching schedules by term

Summer 2011 Teaching Schedule

COURSE	TITLE	DAYS	TIMES	ROOM	INSTRUCTOR
CHEM 121 001	General Chem with Lab	MTWRF	0920-1020	DSH 120	Yang, S
CHEM 122 001	General Chem with Lab	MTWRF	0920-1020	CLARK 101	Ho, K
CHEM 253 001	Quant Analysis with Lab	MTWRF	1250-1350	CLARK 101	McBride, J
CHEM 301 001	Organic Chemistry	MTWRF	1030-1130	WOOD 101	Bellew, D
CHEM 302 001	Organic Chemistry	MTWRF	1140-1240	CLARK 101	Bellew, D

Fall 2011 Teaching Schedule

COURSE	SEC	TITLE	DAYS	TIMES	ROOM	INSTRUCTOR
CHEM 111	001	Elem of Gen Chem w/lab	MWF T T	1000-1050 1230-1345 or 1400-1515	CLARK 101	Paine
CHEM 111	002	Elem of Gen Chem w/lab	MWF R R	1300-1350 1230-1345 or 1400-1515	CLARK 101	Ray
CHEM 121	001	Gen Chem w/lab	MWF	0900-0950	WOOD 101	Ray
CHEM 121	002	Gen Chem w/lab	MWF	1000-1050	WOOD 101	TBA
CHEM 122	001	Gen Chem w/lab	MWF	1100-1150	NTHP 122	McBride
CHEM 122	002	Gen Chem w/lab	MWF	0900-0950	WOOD 149	McBride
CHEM 122	003	Gen Chem w/lab				
CHEM 122	004	Gen Chem w/lab				
CHEM 122	005	Gen Chem w/lab	ARR	ARR	ARR	Bellew
CHEM 131L	001	Gen Chem w/lab	MWF	1100-1150	DSM 328	Mariano/Ho
CHEM 192	001	Concepts for Chem	MWF	0900-0950	MITCH 221	Knottenbelt
CHEM 192	002	Concepts for Chem	MWF	1000-1050	MITCH 221	Knottenbelt
CHEM 192	003	Concepts for Chem	MWF	1700-1750	MITCH 221	SET ASIDE
CHEM 212	001	Integ Org Chem/Bioch	MW F	1600-1715 1600-1650	CLARK 101 DSH 120	Ray
CHEM 253	001	Quant Analysis w/lab	TR	0930-1045	CLARK 101	McBride
CHEM 301	001	Organic Chem	MWF	0800-0850	MITCH 101	Holder
CHEM 301	002	Organic Chem	MWF	1000-1050	DSH 125	Mariano
CHEM 301	003	Organic Chem	TR	1700-1815	CLARK 101	Deck
CHEM 301	004	Organic Chem	ARR	ARR	ARR	Bellew
CHEM 301	005	Organic Chem	MWF	1100-1150		SET ASIDE
CHEM 301	006	Organic Chem	TR	0900-1015	MITCH 101	Bellew
CHEM 302	001	Organic Chem	MWF	0900-0950	CLARK 101	Whalen
CHEM 302	002	Organic Chem	MWF	1100-1150	CLARK 101	Whalen
CHEM 302	003	Organic Chem	MWF	0900-0950	DSH 325	Bellew
CHEM 302	004	Organic Chem	MWF	1200-1250	CLARK 101	CANCELLED
CHEM 302	005	Organic Chem	TBA	ARR	ARR	Bellew
CHEM 311	001	Physical Chem	MWF M	1400-1450 1500-1550	CLARK 101	Guo
CHEM 315	001	Intro Physical Chem	TR F	1100-1215 1100-1215	EDUC 101A	Keller
CHEM 411L	001	Lab Methods In Physical Chem	M T W	1200-12250 1230-1520 1200-1450	MITCH 213 Clark 109 Clark 109	Ho
CHEM 421	001	Biological Chem	TR	1230-1345	SMLC 102	Bear

CHEM 425	001	Biological Pathways	MWF	0900-0950	DSH 123	Melancon
CHEM 431	001	Adv Inorganic Chem	TR	1100-1215	CLARK 101	Kemp
CHEM 471	001	T: Environ Chem	TR	1530-1645	DSH 226	Cabaniss
CHEM 471	002	T: Polymer Chem	TR	1400-1515	MITCH 120	Qin
CHEM 471	010	T: Charac Meth Nanostructure	TR	1100-1215	MECH 214	Grey
CHEM 500	001	Chemistry Teaching Methods	F	1300-1350	SMLC 120	Ho
CHEM 500	002	Chemistry Teaching Methods	F	1300-1350	SMLC 120	Ho
CHEM 511	001	Molecular Structure Theory	MWF	0900-0950	DSH 332	Wang
CHEM 521	001	Biological Chemistry	TR	1230-1345	SMLC 120	DDM
CHEM 537	001	Physical Methods Inorganic	TR	1400-1515	MITCH 214	Kirk
CHEM 545	001	T: Environ Chem	TR	1530-1645	DSH 226	Cabaniss
CHEM 545	002	T: Polymer Chem	TR	1400-1515	MITCH 120	Qin
CHEM 545	004	T: Biological Pathways	MWF	0900-0950	DSH 123	Melancon
CHEM 567	003	T: Charac of Nano Materials	TR	1100-1215	MECH 214	Grey
CHEM 623	004	Research Colloquium	F	1500-1600	CLARK 101	Bear
CHEM 625	001	Sem: Nat Prod Chem Biology	TBA	ARR	ARR	Melancon
CHEM 625	002	Sem: Inorganic	M	1200-1250	BANDE 105	Kirk
CHEM 625	003	Sem: Organic	F	1200-1250	MITCH 107	Wang
CHEM 625	004	Sem: Physical	W	1200-1250	BANDE 105	Guo
CHEM 625	005	Sem: Bio	F	1300-1350	DSH 234	DDM

Spring 2012 Teaching Schedule

COURSE	SEC	TITLE	DAYS	TIMES	ROOM	INSTRUCTOR
CHEM 111	011	Elem of Gen Chem w/lab	MWF T	1000-1050 1230-1345	CLARK 101 CLARK 101	Paine
CHEM 111	012	Elem of Gen Chem w/lab	MWF T	1000-1050 1400-1515	CLARK 101 CLARK 101	Paine
CHEM 111	013	Elem of Gen Chem w/lab	MWF R	1300-1350 1230-1345	CLARK 101 CLARK 101	Ray
CHEM 111	014	Elem of Gen Chem w/lab	MWF R	1300-1350 1400-1515	CLARK 101 CLARK 101	Ray
CHEM 121	001	Gen Chem w/lab	MWF	0900-0950	WOOD 101	Yang
CHEM 121	002	Gen Chem w/lab	MWF	1100-1150	WOOD 101	Sorensen
CHEM 122	001	Gen Chem w/lab	MWF	1000-1050	WOOD 101	Yang
CHEM 122	002	Gen Chem w/lab	MWF	1100-1150	NTHP 122	Cabaniss
CHEM 122	003	Gen Chem w/lab	TR	1700-1815	DSH 123	Yang
CHEM 122	005	Gen Chem w/lab	MWF	1100-1150	DSH 224	Knottenbelt
CHEM 132L	011	Principles of Chemistry	MWF T	1100-1150 0900-1150	DSH 234 SMLC 280	Mariano/Ho
CHEM 132L	012	Principles of Chemistry	MWF R	1100-1150 1530-1820	DSH 234 SMLC 280	Mariano/Ho
CHEM 192	001	Concepts for Chem	MWF	0900-0950	MITCH 329	Knottenbelt
CHEM 192	002	Concepts for Chem	MWF	1100-1150	MITCH 329	Knottenbelt
CHEM 212	001	Integ Org Chem+Bioch	MTWF	0900-0950	WOOD 149	DDM
CHEM 253L	011	Adv. Inorg. Lab	TR M	0930-1045 1200-1600	CLARK 101 CLARK 116	McBride
CHEM 253L	012	Quant Analysis w/Lab	TR T	0930-1045 1400-1800	CLARK 101 CLARK 116	McBride
CHEM 253L	013	Quant Analysis w/Lab	TR W	0930-1045 1400-1800	CLARK 101 CLARK 116	McBride
CHEM 253L	014	Quant Analysis w/Lab	TR R	0930-1045 1230-1630	CLARK 101 CLARK 116	McBride
CHEM 253L	015	Quant Analysis w/Lab	TR M	0930-1045 1700-2100	CLARK 101 CLARK 116	McBride
CHEM 301	001	Organic Chem	MWF	0900-0950	CLARK 101	Fu-Sen

CHEM 301	002	Organic Chem	MWF	1100-1150	CLARK 101	Bellew
CHEM 301	003	Organic Chem	MWF	1100-1150	DSH 123	Qin
CHEM 301	004	Organic Chem	ARR	ARR	ARR	Bellew
CHEM 302	001	Organic Chem	MWF	0800-0850	MITCH 101	Holder
CHEM 302	002	Organic Chem	MWF	1000-1050	SMLC 102	Mariano
CHEM 302	003	Organic Chem	TR	1700-1815	CLARK 101	Deck
CHEM 302	004	Organic Chem	MWF	1000-1050	DSM 224	Whalen
CHEM 302	005	Organic Chem	ARR	ARR	ARR	Bellew
CHEM 302	006	Organic Chem	M	1410-1700	UNMW	Bellew
CHEM 302	007	Organic Chem	TR	0900-1015	DSH 123	Bellew
CHEM 312	001	Physical Chem	MWF M	1400-1450 1500-1600	MH 102 MH 102	Grey
CHEM 315	001	Intro Physical Chem	MWF M	1300-1350 1400-1450	DSH 123 DSH 123	Keller
CHEM 326	001	ST: Intro to NMR	W	1000-1050	TBA	Smith
CHEM 421	001	Biological Chem	TR	1230-1345	EDUC 103	Bear
CHEM 425	001	Biological Pathways	MWF	0900-0950	DSH 229	Melancon
CHEM 432L	001	Adv. Inorg. Lab	TR T	1230-1520 1100-1150	CLARK 109A CLARK 117A	Bellew
CHEM 453L	001	Analytical Chemistry	MW MW	1000-1050 1500-1750	CLARK 109 CLARK 109	McBride
CHEM 471	001	Chem & Phys Nanoscale	TR	0930-1045	DSH 128	Evans
CHEM 500	001	Chemistry Teaching Mthds	F	1300-1350	SMLC 356	Ho
CHEM 500	002	Chemistry Teaching Methods	ARR	ARR	ARR	Ho
CHEM 501	001	Molecular Struc Thry	TR	0900-1015	CLARK 166	Guo
CHEM 536	001	Syn Mech Inorg Chem	TR	1100-1215	CAST 51	Kirk
CHEM 537	001	T: Indust Chem & Catalysis	W	1600-1820	MITCH 109	Kemp
CHEM 545	001	T: Simulation	TR	1400-1515	MITCH 218	Guo/Keller/Grey
CHEM 545	003	T: Biological Pathways	MWF	0900-0950	DSH 229	Melancon
CHEM 567	001	T: Mechanistic Enzymology	F	1000-1200	TBA	DDM
CHEM 623	001	Research Colloquium	F	1500-1600	CLARK 101	Bear
CHEM 625	001	Sem: Inorganic	M	1200-1250	BANDE 105	Kemp
CHEM 625	002	Sem: Organic	F	1200-1250	CLARK 101	Qin
CHEM 625	003	Sem: Physical	W	1200-1250	BANDE 105	Keller
CHEM 625	004	Sem: Biochem	F	1400-1450	BANDE 105	Melancon
CHEM 625	005	Sem: Nat Prod Chem Biology	ARR	ARR	ARR	Melancon
CHEM 625	006	Sem: The World of Enzymes	ARR	ARR	ARR	DDM
CHEM 627	001	ST: Intro to NMR	W	1000-1050	TBA	Smith

Appendix D. Enrollments by course

Graduate Courses	**Fall**	**Spring**
	2011	**2012**
Chem 501 001: Molecular Struc Thry (Guo)	NO	5
Chem 504	NO	NO
Chem 511 Mechanisms Org Chem (Wang)	14	NO
Chem 514	NO	NO
Chem 521 Biological Chemistry (Dunaway-Mariano)	14	NO
Chem 536 002: Syn Mech Inorg Chem (Kirk)	NO	3
Chem 537 001: Industrial Chem & Catalysis (Kemp)	NO	7
Chem 545 001: Simulation (Guo, Keller, Grey)	NO	8
Chem 545 001: Environ Organic Chem (Cabaniss)	1	NO
Chem 545 002: Polymer Chem (Yang)	11	NO
Chem 545 004: Biological Pathways (Melançon)	1	8
Chem 567 010: Charac Methods Nanostructures (Grey)	2	NO
Chem 567 001: Mechanistic Enzymology (Dunaway-Mariano)	NO	11

Undergraduate Courses	Summer 2011	Fall 2011	Spring 2012
Chem 111L	NO	243	234
121 Enrollment	54	806	538
# of Sections	1	3	2
123L Enrollment	40	735	473
# of Labs	3	33	23
122 Enrollment	62	356	509
# of Sections	1	3	4
124L Enrollment	52	287	441
# of Labs	3	14	20
Chem 131L	NO	26	NO
Chem 132L	NO	NO	18
Chem 212	NO	75	80
Chem 253	11	72	78
Chem 311	NO	34	NO
Chem 312	NO	NO	41
Chem 315	NO	61	87
Chem 331L	NO	NO	NO
Chem 332L	NO	NO	NO
Chem 351L	NO	NO	NO
Chem 352	NO	NO	NO
Chem 411L	NO	7	NO
Chem 412	NO	NO	NO
Chem 415	NO	NO	NO
Chem 421	NO	48	83
Chem 425	NO	39	51
Chem 431	NO	21	NO
Chem 432	NO	NO	1
Chem 433	NO	NO	NO
Chem 454	NO	NO	NO
Chem 471 Grey	NO	NO	NO
Chem 471 Evans	NO	3	16
Chem 471 Cabaniss	NO	11	NO
Chem 471	NO	NO	NO
301 Enrollment	99	427	336
# of Sections	2	6	4
302 Enrollment	73	282	321
# of Sections	2	4	7
303L Enrollment	46	276	176
# of Labs	3	16	10
304L Enrollment	38	144	202
# of Labs	3	8	12

Appendix E. Degrees awarded

Undergraduate Degrees

NAME	DGR	SEM
Camplain, Ricky L.	BA	Fall 2011
Charley, Ericka L.	BA	Fall 2011
Davis, Danae J.	BA	Fall 2011
Esquibel, Kathleen N.	BA	Fall 2011
Powers, Brett J.	BA	Fall 2011
Schwartz, Thais M.	BA	Fall 2011
Vega, Andrew J.	BA	Fall 2011
Conklin, Laura M.	BS	Fall 2011
Miller, Michael R.	BS	Fall 2011
Rice, Vanessa A.	BS	Fall 2011
Dominguez, Dennis R.	BA	Spring 2012
Endres, Andrew L.	BA	Spring 2012
Greenberg, Jacob A.	BA	Spring 2012
Lopez, David A.	BA	Spring 2012
Speer, Kelly A.	BA	Spring 2012
Villanueva, Charles J.	BA	Spring 2012
Warden, Christina L.	BA	Spring 2012
Aragon, Franchelle M.	BA	Spring 2012
Bryant, Estefania	BA	Spring 2012
Esquivel, Stephen B.	BA	Spring 2012
Fuentes, Raymond S.	BA	Spring 2012
Gladysz, Jessica S.	BA	Spring 2012
Lavezo, Laura A.	BA	Spring 2012
Malone, D'Eldra R.	BA	Spring 2012
Martin, Matthew R.	BA	Spring 2012
Munoz, Oscar	BA	Spring 2012
Rodriguez-Shotland, Sarah R.	BA	Spring 2012
Rojo, Manuel R.	BA	Spring 2012
Salazar, Terry C.	BA	Spring 2012
Salgado, Victor R.	BA	Spring 2012
Sanchez, Lia E.	BA	Spring 2012
Smith, Christopher D.	BA	Spring 2012
Sterk, Ryan T.	BA	Spring 2012
Terrell, Whitney B.	BA	Spring 2012
Doan, Thu Q.	BS	Spring 2012
Hoppe, Sarah M.	BS	Spring 2012
Martinez, Andrea M.	BS	Spring 2012
Ortiz, Amber L.	BS	Spring 2012
Starkey, Alexander B.	BS	Spring 2012
Cuna, Elizabeth	BA	Summer 2011
Friedman, Jessica K.	BA	Summer 2011
Rabinowitz, Jon R.	BA	Summer 2011
Rogers, Craig T.	BA	Summer 2011
Yazzie, Shihomi	BA	Summer 2011

Graduate Students

LAST NAME	FIRST NAME	DRG	CHAIR	MEMBER 1	MEMBER 2	MEMBER 3	GR YR
Latham	John	PhD	Debra Dunaway-Mariano	Mariano	Melançon	Bear	Sp 12
Li	Xichen	MS/CW	Wang	Melançon	Keller		Sp 12
Zhang	Xinshuai	PhD	Wang	Guo	Mariano	Feng	SP 12
Parkes	Marie	PhD	Kemp	Kirk	Wang	Bear	SP 12
Song	Xixi	PhD	Wei Wang	Mariano	Feng		SP 12
Huang	Hua	PhD	Debra Dunaway-Mariano	Mariano	Kirk	Allen	FA 11
Liu	Yuan	MS	Wang	Mariano	Qin		FA 11
Wang	Min	PhD	Debra Dunaway-Mariano	Mariano	Wang	Allen	FA 11
William	Wilson	PhD	Bear	Ho	Watkins	Cabaniss	SU11
Wang	Ting	MS/CW	Wei Wang	Keller	Melançon		SU 11
Breece	Robert	PhD	Martin Kirk	Guo	Tierney	Timmins	SU 11

Appendix F. Graduate Student recruitment

Graduate Recruitment Report Fall 2011/Spring 2012

COUNTRY	OFFERS	ACCEPTED	DECLINE	NO RESP	ENROLLED
CHINA	22	9	13	0	9
FRANCE	1	1	0	0	1
USA	10	5	3	2	4

New Graduate Students Fall 2011 and Spring 2012

LAST	FIRST	DEGREE	COUNTRY
Thomas	Alan	PhD	USA
Kooser	Ara	PhD	USA
Chang	Fei	PhD	China
Hu	Keda	PhD	China
Yang	Guoshun	PhD	China
Yang	Jianzhong	PhD	China
Bleier	Grant	PhD	USA
Loch	Aruny	PhD	France
He	Jingxuan	PhD	China
Huang	Shijie	PhD	China
Sun	Lin	PhD	China
Wright	Catherine	MS	USA
Wu	Yajun	PhD	China
Zhang	Jie	PhD	China

Appendix G. Graduate Assistantships

SEMESTER	TA	RA
SU 09	10	26
FA 09	33	13
SP 10	29	15
SU 10	10	30
FA 10	24	17
SP 11	12	22
SU 11	12	22
FA 11	30	11
SP 12	28	10

Appendix H. Departmental Colloquium schedule

Fall 2011

August 26, 2011	David Whitten, UNM, Center for Biomedical Engineering (Qin)
September 3, 2011	Gregory Cook, North Dakota State Univ, (Grad students)
September 9, 2011	Graeme Henkelman, UT-Austin (Guo)
September 16, 2011	Jeff Miller, Argonne Natl. Lab, (NSMS/Chemistry)
September 23, 2011	Chris Cheatum, U of Iowa (Grey-ACS Student Chapter)
September 30, 2011	Gregory Reinhart, Texas A & M (DDM)
October 7, 2011	Richard Armstrong, Vanderbilt (DDM)
October 14, 2011	Fall Break
October 21, 2011	Frieder Jaekle, Rutgers - Newark (Qin)
October 28, 2011	Alex Kornienko, NM Tech (Melançon)
November 4, 2011	Masahiro Terada, Tohoku University, Japan (Wang)
November 11, 2011	Mike Barnes, U of Mass, Amherst (Grey)
November 18, 2011	Larry Sklar, UNM Dept. of Pathology (Melançon)
November 25, 2011	Thanksgiving break
December 2, 2011	Harry Gray, Cal Tech: **Riley Schaeffer Endowed Lecture**

Spring 2012

Jan. 20, 2012	Fu-Sen Liang, New Faculty
Jan. 27, 2012	Kirk Schanze, U of Florida (Qin)
Feb. 3, 2012	Pieter Dorrestein, UCSD (Melançon)
Feb. 10, 2012	Chris Bardeen, U of California, Riverside (student series)
Feb. 17, 2012	So-Jung Park, UPenn (Grey)
Feb. 24, 2012	Hang (Hubert) Yin, U of Colorado, Boulder (Wang)
Mar. 2, 2012	Jiong Yang, Texas A & M (Wang)
Mar. 9, 2012	Mike Heagy, NM Tech (Melançon)
Mar. 16, 2012	SPRING BREAK
Mar. 23, 2012	Sam-Shajing Sun, Norfolk (Qin)
March 30, 2012	Jeremy Smith, NMSU (Kemp)
April 6, 2012	Zhihao Zhuang, U. of Delaware (DDM)
April 13, 2012	Wenshe Liu, Texas A & M (Wang)
April 20, 2012	Frank Raushel, Texas A & M (DDM)
April 27, 2012	Wei You, UNC (Qin)

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Appendix A16. CCB Strategic Plan 2008

Departmental Strategic Plan

Department of Chemistry and Chemical Biology
The University of New Mexico
January 18, 2008

SUMMARY

This document outlines the long-range and strategic plan for the Department of Chemistry and Chemical Biology at The University of New Mexico. The Departmental Strategic Planning Committee has, in conjunction with the Faculty at large, developed a list of major goals for the department over the next five year period, and these are to (1) to increase the research posture of the Department among peer institutions and increase national and international visibility, (2) recruit and retain excellent faculty, building on the research strengths of the department, (3) improve the Departmental infrastructure and research environment, (4) maintain our status as the best institution in New Mexico for educating undergraduate Chemistry majors, and (5) continue to develop an undergraduate program that is recognized for its quality of instruction.

The achievement of these goals will require the Department to build bridges and develop mutually strong relationships with Los Alamos and Sandia National Laboratories, and allied departments on the UNM campus (Biology, Biochemistry, Engineering, Pharmacy, CHTM, HSC, etc.), support and enhance strong programs currently in residence and develop new research thrusts in emerging areas where funding levels are high (e.g. Sustainable Energy, Nanotechnology), improve faculty governance, organize current space to maximize research efficiency and work with the Administration to secure new and modern research facilities, continue to pursue extramural funding to upgrade departmental facilities and equipment, increase graduate research assistant (RA) numbers, and increase the number of undergraduate majors and educational service to the University community.

The key goals presented in this strategic plan will be met by a number of specific objectives. Although the current resources available to the Department will be strategically used to meet these objectives, additional support from the University administration is essential to ensure the Department increases its national and international stature. Garnering this additional administrative support is imperative, as Chemistry plays a vital role in the education of undergraduate and graduate students at high-quality research universities in the US. As such, a strong Chemistry and Chemical Biology Department at UNM will play a fundamental role in advancing the University toward membership in the Association of American Universities (AAU), a stated goal of President Schmidly. This long-range and strategic plan is intended to guide the Department moving forward toward its stated goals and objectives during the five-year period 2008-2012. The faculty is unified in their commitment to meet each of these goals, thereby increasing the Department's posture among peer institutions and developing into one of the universally recognized strong research departments in the US.

MISSION STATEMENT

The mission of the Department of Chemistry and Chemical Biology is to provide quality education to traditional and nontraditional graduate and undergraduate students in the College of Arts and Sciences, and to the University at large. The Department provides a robust educational environment that fosters the acquisition of chemical knowledge and the use of chemical principles to give students deeper insight into understanding how Chemistry will play a fundamental role in molecular science discovery and the development of new technologies in the 21^{st} century. Therefore, we view Chemistry as the central science, and the Department as a community of scholars whose research and educational activities focus on understanding the fundamental properties of materials, and chemical and biological reactions at the molecular level. The faculty is committed to the development of a nationally and internationally recognized and prominent graduate research program. This program will be fully engaged in efforts to ensure success of the mission. To this end, the Department will actively seek mutual partnerships with the University community, the National Laboratories in New Mexico, and the greater national and international scientific communities in order to fully contribute to the fundamental molecular science needs of our society.

RESEARCH

Goal: Increase the research posture of the Department among peer institutions, increase national and international visibility, and develop into a top-50 tier Department in the US.

Background. The present faculty is thirteen in number, and four are labeled as "part time". This small group is responsible for providing class room/laboratory chemistry instruction to a large undergraduate population of science majors. Our current faculty size is ~100% smaller than that at peer institutions of similar size. The small number of faculty demands a faculty course load of 2 undergraduate classes per semester, and this course load does not include the courses that support the graduate program. Two courses per semester is a reasonable course load for a faculty member that has elected not to direct a large research group. It is not possible for a faculty member that has the responsibility to direct a large research group to teach two courses per semester. This is because the one-on-one training of a graduate student is very time consuming. It involves a day-to-day interaction regarding experimental design, results and interpretation for ~5 years, assistance in seminar preparations, thesis preparation, assistance with obtaining a postdoctoral position, assistance with obtaining a job, and moving from one job to the next. A research active lab consists of 3-17 graduate students. Such a lab also serves undergraduates who require credits in research in order to graduate with a BS degree, and undergraduates who wish to prepare themselves for graduate school by carrying out an undergraduate research project.

We can identify ten members of our faculty who fit into the category of “research active”. Three are senior faculty who are still active in research, but are not accepting new graduate students, and will be winding down their involvement in research over the next several years. In the years between closing shop and retirement these faculty are eligible for increased teaching loads. Three individuals among this group of seven faculty members have elected to dispense with research and take on upper administrative duties outside of the Department. These individuals, while performing an important service to the University as a whole, have taxed the Department's teaching and research capabilities. One is close to retirement, the other two are not. The seventh member, who has not been able to assemble and direct a group of graduate students, is able to teach undergraduate courses. It is our expectation that this faculty member will assume this responsibility.

The faculty classified as invested in future research and research training (criteria being age and tract record) are only seven in number. These faculty represent the classical subdisciplines: Organic (1), Inorganic (3), Physical (2), Biochemical (1). Analytical chemistry as of 2008 has no faculty representation, and the Chemistry Department faculty is presently exploring alternative ways to offer analytical chemistry courses as required for a certified BS degree in Chemistry.

The radical drop in Departmental faculty correlates with the enormous drop in the number of applications for graduate admission (>100 applications is now down to ~20) and a corresponding drop in the quality of the applicants. This sets up a downward spiral in recruiting research active faculty and graduate students. Moreover, the young research active faculty that are working towards tenure are compromised. They face the question of whether to stay in hopes that next year will be better or move to a different University so that their research program might survive. The recently tenured faculty have proven their ability to be successful under the most resource poor conditions. They have successfully competed for federal research grants, have a proven track record and they are horribly underpaid compared to their peers in neighboring State Universities. We must ask "how can the Department retain these successful individuals?" The University has no policy for retention under these conditions. Other universities are trolling for such faculty because in a time of funding crisis a funded, proven investigator and an experienced classroom teacher is a very safe hire.

Objectives. The Department faculty must undertake an ever more aggressive commitment to improving research productivity, raising external research funds, enhancing faculty quality, and improving student and postdoctoral quality.

Strategies. Strategies to Increase Research Activity in the Department:

1. The people
Faculty: Recruiting and Retention:

I. Create a better balance in faculty work loads and allow faculty to focus their efforts in the area of their career focus (research education or undergraduate classroom education)

1. Optimize efficiency of faculty performance by focusing the effort of research active faculty on research related tasks. This will mean a maximum teaching load of one course a semester, with both courses at the upper level undergraduate level and graduate level. These faculty will serve on one or more of the following committees: (1) undergraduate major/graduate student recruiting committee (new), (2) graduate admissions committee, (3) graduate advising committee, (4) instrument and training grant application committee (new), and (5) shared instrumentation committee.
2. Optimize the undergraduate teaching program by focusing efforts of faculty who have

chosen the undergraduate education track, on classroom instruction and curriculum development. This will mean a course load of 2 classes per semester and service on one or more of the following committees: (1) undergraduate advising committee (new), (2) undergraduate awards committee, (3) undergraduate curriculum committee (new).

II. Create an equitable salary structure within the Department that is comparable to other regional State Universities. The 3 levels (Assistant, Associate, and Full) should have a non-overlapping salary range. Promotion to the next level should carry with it an immediate salary adjustment. Salary increases should be based on effort and merit.

III. Create a "semester off" policy for the two faculty members assigned to head the undergraduate major graduate student recruiting committee. These 2 faculty will alternate semesters off from teaching during which they will spend full time on recruiting efforts (lecturing at neighboring institutions and participating in high school career days; entertaining prospective students; hosting faculty from neighboring institutions; overseeing the application process (contact applicants); preparation and distribution of recruitment materials).

IV. Hire 7 new research active faculty over the next five-year period (this includes ongoing searches).

V. Add a Lecturer position

VI. The time scale to reach a *research active* faculty size of 25 should occur over a 10 year period. The impact of the proposed hires should have no effect on the lecturers that are already in place or are to be hired. The numbers of lecturers are not anticipated to be reduced as the number of tenure track research faculty reaches the target goal of 25.

Metrics. Double faculty publications and research grant support per year. Increase visibility among peer institutions as measured by national and international awards, national offices held, positions on journal editorial boards, invited seminar presentations, organizing national and international meetings, etc.

TEACHING

Goal: Maintain our status as an outstanding institution in New Mexico for Chemical education at the undergraduate level and continue to develop and expand our undergraduate program to be recognized for its quality of instruction and preparation of its students entering the workforce or continuing on to professional or graduate school.

Over the last five years, the Chemistry Department has significantly revamped the undergraduate curriculum for all degrees offered. Several courses at the 400- level have been developed that focus on Biological Chemistry and Nanotechnology. Both the Chemistry minor degree and the B.A. major degree offer several specialized tracks where students are able to choose from a variety of electives that most suit their needs. These range from programs appropriate for entry to Chemistry graduate school and degrees with a strong pre-medical bias. The B.S. program has been significantly streamlined through the creation of a highly coordinated laboratory and lecture sequence.

Objective. Future goals will be to complete the curriculum restructuring by the creation of a set of documents that outline the learning objectives and assessment strategies for all courses offered as part of our undergraduate program. Assessment of our program will focus on the objectives outlined in the State of New Mexico HED student learning outcomes for the Natural Sciences. Special emphasis will be given to the introduction of active learning and technology (clickers, etc) into our classrooms, and the overall preparedness of our graduating students. Additionally, we will make every effort to provide and maintain state of the art instructional laboratories.

Strategy. The Undergraduate Curriculum Committee will be responsible for obtaining course outlines from each appropriate Division in the Department. The Committee will be responsible for ensuring that each course fits into a well-coordinated undergraduate program, and that each course fulfills the main learning and training objectives of our degree program. In addition, an Undergraduate Teaching Committee will be established to provide detailed statistics and assessment of our freshman and sophomore courses. Develop an annual evaluation and assessment report to provide evidence of teaching effectiveness as well as strategies for continuous improvement (similar to what has been outlined by the Provost's office for the university's accreditation by the North Central Association's Higher Learning Commission). Regarding instructional laboratories, significant efforts we will develop a cohesive and comprehensive laboratory curriculum that provides the necessary exposure to modern instrumentation and the practice of chemistry as a profession.

Metrics: A compendium of Course Outlines should be assembled within the next year for all courses offered at the undergraduate level. Detailed assessment of statistical data from the lower-division classes will begin this year, and meaningful data should be assembled within the next three years. An assessment exam for the core courses has been developed to help evaluate student learning. Faculty who coordinate CHEM 111 and 121 will each be responsible for performing and evaluating their course's assessment and writing an annual report. The reports will be reviewed separately each June by the undergraduate committee for comment on the teaching strategies and assessment, before being sent to the Provost's office before the start of the fall term.

Objective. Offer on-line and hybrid chemistry courses which allow us to serve students in more diverse communities in NM and provide more flexibility of faculty assignments.

Strategy. The idea can be evaluated by first implementing a pilot hybrid course in general chemistry lab as an alternative for students. An assessment will be given to evaluate student's performance from both formats (regular and hybrid) of the lab, and will be used in the consideration of offering more on-line or hybrid courses in the future.

Metrics. The proposed hybrid lab course of general chemistry should be implemented first. The outcome of the pilot hybrid lab can provide a basis for further discussion of whether more hybrid or on-line courses will be offered by the Department and the identification of these courses.

Objective. Streamline the undergraduate lab courses and keep the pedagogy of lab activities current with the need of 21st century chemical education.

Strategy. (1) Reconsider the current lab experiments to include more non-recipe type of lab activities to promote critical thinking and scientific inquiry. (2) Form a committee with teaching faculty to reconsider the placement of experiments in all level of the labs.

Metrics. (1) Much efforts have been sought to integrate the upper-level labs. The first of the three integrated lab courses will be implemented as early as fall 2008. The new general chemistry labs will also be implemented in fall 2008 which include elements of inquiry-based activities. (2) The effectiveness of the inquiry-based experiments to our students should be assessed.

Objective. Explore the use of new instructional technologies to modernize our undergraduate instructions.

Strategy. Establish a forum to advocate and share experience of using iClicker, WebCT, and other instructional technologies. Make example videos and tutorials available to help faculty to prepare their own videos and promote the use of Departmental video production equipment.

Metrics. Lecture and lab videos for general chemistry are in production. More courses and chemistry subjects should be considered to be added to the targeted audiences. The distribution and publication of these videos will be sought. The Department should have a provision to include the budge for the supporting staff, student helpers and the maintenance of the AV equipment.

Objective. Department establishes a guidance of course contents for undergraduate core courses to ensure these courses are taught in the way they were designed and the key concepts are covered in the proper sequence

Strategy. Faculty who teaches undergraduate core courses (CHEM 121/122/253… etc) should write learning objectives (key concepts, attainable learning outcomes, etc) for each course. The learning objectives will be discussed by a teaching committee to generate a departmental guidance.

Metrics. A departmental guidance is generated as the result of the committee's recommendations. The guidance must be followed by the faculty, including temporary and part-time faculty assigned to teach these courses.

INFRASTRUCTURE

Goal: Improve the Departmental infrastructure and environment for research and education.

Objective. A significant amount of new and improved space will be needed to accommodate a proposed research active faculty size of 25.

Strategies. An aggressive committee will be formed that will formulate plans to secure additional and renovated space. This will allow growth to the target of twenty-five research active faculty and the retention of current faculty. The new Math and Sciences Learning Center is in the initial stages of planning, with ground-breaking expected in late Fall 2008 or Spring 2009. Van H. Gilbert, Architect, has been selected but negotiations must still take place for the cost of design and construction. It is expected that it will take one year to draw the building plans, and two years to construct, so occupancy may be possible in Fall or Spring 2011. Four of the major service lab courses taught by Chemistry will move to this building, the General and Organic Chemistry labs. The rooms vacated by the departure of these courses from Clark and Reibsomer need to be renovated for new research-active faculty. Clark Hall 109, 109A, 150, and 207 will be converted into quality laboratory research space and offices for this purpose. Clark 180, currently a teaching assistant office, may be converted into office space for new staff.

Metrics. Marked progress toward renovation of Clark 109, 109A, 150, 180 and 207 should be well underway at the end of the 5-year period and efforts to obtain new and modern research space for the increased activity of this larger and more productive faculty should be in place. The new Math and Sciences Learning Center should be ready for occupancy by Fall 2011.

Objective. Obtain increased allocations for materials and services that meet inflationary pressures, and obtain significant allocations for instrumentation matching funds in order to upgrade existing facilities.

Strategies. Funds for upgrading instruments and for the purchase of major new instrumentation can be found through the National Science Foundation's Cyber infrastructure and Research Facilities (CRIF:CRF)**,** Major Research Instrumentation (MRI), EPSCoR Research Infrastructure Improvement, and Instrumentation for Materials Research (IMR) grant programs, which all have deadlines in early 2008. Some letters of intent are due in December 2007. Additional matching funds, if necessary, may be acquired from the College of Arts and Sciences. Instrument user fees, which should be reasonable but meet inflationary pressures, may be another source of funds.

Metrics. In keeping with our research mission to focus on the areas of materials and biological chemistry, we should expect to obtain funds for one major instrument every three years, and user fees should change accordingly with the rate of inflation. Upgrading of current instrumentation should take place at the rate of one instrument every two years.

Objective. Increase and improve Chemistry staff support so that it approaches that of peer research active institutions.

Strategies. Hire new support staff for the Department that meets the needs of the research faculty. The lack of support for proposal submission and technical writing means that research-active faculty loses valuable time negotiating the submission process rather than focusing on the science and proposal body. Hiring a technical writer who has experience with proposal submission will greatly improve the ability of the Department to submit proposals smoothly to funding agencies. At least two more administrative assistants are needed in the Department to assist research-active faculty with manuscript submission and other duties. These assistants would be assigned to faculty along divisional lines and it would be ideal if they had experience with chemistry drawing software, such as ChemDraw, as well as knowledge of the manuscript submission process.

Metrics. The acquisition of a technical writer should be accomplished within the next year to two years as office space becomes available in Clark Hall. As more space becomes available, two administrative assistants should be hired.

HIRING PLAN

Note: The hiring plan is one of the major issues that will need to be addressed early in the tenure of the new department chair.

Goal: Recruit new and retain existing faculty to enhance our core research areas and teaching missions, and allow for expansion into new, emerging areas of research.

Objective. Commence with an aggressive 5-year hiring plan to bring the research active faculty size to 17 in five years.

Strategies. We have developed the following hiring plan that will allow growth in core and emerging research areas and allow for comprehensive coverage of graduate and undergraduate educational programs. As we see it, the core of the current faculty that will be driving the graduate program over the span of this five-year plan consists of Professors Kirk, Kemp, Guo, Dunaway-Mariano, Tierney, Wang and Grey. The remaining faculty (Professors Paine, Mariano, Deck, Keller, Evans, Ondrias and Holder) are unlikely to support a significant number of new graduate students. The hiring plan outlined below will more than double the number of research active faculty in the Dept., going forward from the end of this five-year plan. The details that follow reflect a desire to build a balanced Department that continues to support our biological thrust, through establishment of a bioorganic component, and develops a more meaningful thrust in Nanoscience and materials chemistry.

EXAMPLE FIVE-YEAR FACULTY HIRING PLAN

Search Year	Level	Probable field	Possible Retirements
2007-2008	Assistant Prof. (underway)	Biological	Cary Morrow
	Professor/Chair (underway)	Open	
.	Assistant Prof. (offer rejected)	Analytical	
2008-2009	Assistant Prof.	Organic	Lorraine Deck
	Assistant Prof.	Physical/Materials	
	Lecturer/Visiting Assistant Prof.	General, Analytical or Organic	
2009-2010	Assistant Prof.	Organic	Richard Holder

	Assistant Prof.	Biophysical	
	Lecturer/Visiting Assistant. Prof	General, Analytical or Organic	
2010-2011	Assistant Prof.	Organic	Pat Mariano
	Lecturer/Visiting Asst. Prof	General, Analytical or Organic	
2011-2012	Assistant Prof.	Biological	Bob Paine Mark Ondrias

Details and Rationale. The seven core research faculty in the current Department consist of three inorganic (all experimental), two physical (one experimental, one computational), one organic and one biological research group. In order for a graduate program in chemistry to thrive, it must have an active organic chemistry component. For this reason, we have chosen to front load the hiring plan to add junior faculty in organic chemistry, as well as in physical/materials chemistry to further our commitment, as demonstrated in the hiring of Prof. Grey, in developing a more meaningful materials thrust.

In chronological order, we envision the seven Assistant Professor hires will resemble the following:

1) An organic chemist with an emphasis in organometallic catalysis as a tool for organic synthesis. A hire of this type will complement Prof. Wang's research, with potential overlap with Prof. Kemp.
2) An experimental physical chemist with an emphasis on materials fabrication and application development. This hire will interact heavily with other Departments, including CINT, as well as complement Prof. Grey's program.
3) An organic chemist with an emphasis on natural product chemistry, synthesis and isolation, and drug discovery. This hire will likely interact with the College of Pharmacy (CoP), and complement Prof. Wang and Position #1 (above).
4) A biochemist with an emphasis on the genetic and enzymatic manipulation of natural product biosynthesis. This hire will interact with Prof. Dunaway-Mariano and the faculty member hired in the 2007 search, as well as with the organic faculty, and potentially CoP.
5) An experimental physical chemist with an emphasis in biophysics, in an area such as bioimaging and/or single molecule spectroscopy.
6) A biochemist with an emphasis on structural biology, such as macromolecular crystallography.
7) An organic chemist, with an emphasis in an emerging growth area, such as glycochemistry.

With the addition of three senior hires and the successful recruitment of an external chair in 2007, in five years, accounting for retirements, the Chemistry Department would house 18 externally-funded, research active faculty, 2 tenured teaching faculty, and approximately 5 non tenure-track teaching faculty, for a total of 25 (72 % of whom are supporting the graduate program).

Metrics. Have a research active faculty size of 17 at the end of this 5-year planning period.

<u>Objective.</u> Hire aggressively in the emerging area of Nano Chemistry.

Fabricating and characterizing nanoscale materials has emerged as a critical research area that encompasses many important aspects of the basic sciences. Many top academic institutions across the country have recognized the need to establish nanoscience research centers to facilitate collaborative efforts to tackle complex problems facing our society. Because chemistry (synthetic and experimental) plays a central role in this exciting new research, it is now imperative that UNM Chemistry seek to hire several outstanding new faculty members that can make contributions in this area of research and participate in collaborative projects with existing faculty.

UNM is in an advantageous position for nanoscience research owing to the close proximity of national labs (Sandia and Los Alamos) as well as the newly constructed outreach facility in Albuquerque, the Center for Integrated Nanotechnologies (CINT). Several other UNM departments have established specific research thrusts in nanoscience (Chem. Eng., Physics, ECE, etc.) which have been used successfully used to recruit top new faculty members. Because nanoscience is multi-disciplinary in nature, there is an urgent need for upper echelons of administration to facilitate inter-department and external collaborations, joint department hires, and sharing of essential facilities.

Strategies.
Several new faculty hires are needed in nanoscience research in order to establish UNM Chemistry in this field. The following are target research areas for future hires with physical, biological or materials chemistry backgrounds related to nanoscience.

1) Energy.
Developing and characterizing new functional materials (such as donor/acceptor and energy harvesting systems) and device strategies for efficient conversion, transport and storage of energy are of great interest. In order to maximize the potential impact in this area, new faculty research interests should complement existing faculty. Current needs are: i) synthesis and functionalization of carbon nanotubes, quantum dots, conjugated polymers, and metal nanoparticles; ii) fabrication and characterization of devices using electrochemical, optical, and/or high energy spectroscopic techniques; iii) development of new computational techniques for modeling novel processes important for energy conversion in complex nanostructured materials and devices.

2) Biophysics.
Biomolecules often possess complex structure that is intimately related to the functionality of the molecule. Research directed toward elucidating biological structure-property relationships and development of new methods to track biological processes is essential. Specific thrusts include: i) synthesis of new biological labels such as fluorescent markers; ii) characterization of protein and nucleic acid folding and reactions; iii) development of new model systems for complex biological systems.

Metrics.

Because of the multidisciplinary nature of nanoscience it is crucial that new hires complement research interests and activities of existing faculty. These faculty should also be able to utilize the numerous resources available both on and off campus for their research which should also negate costly startup expenditures and facilitate collaborative research. Joint appointments are also an effective means to augment startup packages in addition to increasing the visibility of faculty research programs.

Appendix I

Model for hiring jointly with other Departments.

Broad Outline of Chemistry/Pharmacy MedChem Hiring Plan

A "search committee" comprised of an equal number of Chemistry and Pharmacy faculty members should be established to begin a broad search for a medicinal chemistry faculty member.

(a) The search should be for a person at any faculty level but should concentrate on finding a senior medicinal chemist with broad experience in either the pharmaceutical industry or academia.

(b) Emphasis should be given to finding a person who can establish a strong, independent research program and who can participate in graduate and undergraduate teaching programs in Pharmacy and Chemistry.

The committee, with input from the Pharmacy and Chemistry faculty, should reach joint agreement on a short list of people to interview.

The invitees should meet with members of the Chemistry and Pharmacy faculties and deliver (1) a joint Chemistry/Pharmacy seminar, focusing on work they have completed, and (2) a "future research seminar" in which they describe their proposed research programs.

Selection of a person to whom an offer is made will be based on input from the Pharmacy and Chemistry faculties, negotiated by the "search committee," and decided finalized by votes of faculty in Chemistry and Pharmacy.

The conditions of the offer and faculty appointment should be as follows:

The appointment should be 50% Arts and Sciences and 50% Pharmacy.

Whether or not the appointment is made with "tenure' should be based on a consideration of the person's background and teaching experience.

A requirement of the 50% appointment in Chemistry should be that the medicinal chemist will teach one Chemistry course annually at either the graduate or undergraduate level.

Start up funds for this position should derive 50% from Chemistry and 50% from Pharmacy.

Research space will be in a location (*i.e.,* Pharmacy or Chemistry) chosen by the new faculty member.

Overhead return on grants obtained by the new faculty member should be distributed on a 1:1 basis to Pharmacy and Chemistry.

Updated planning considerations, October 2012:

People- The 10-year target scenario is a tenure-track faculty size of 25 with 5 non-tenured lecturers. In an average chemistry department, this would correspond to ~20 active research groups with ~100 graduate students and perhaps 10-20 post-doctoral associates.

In this scenario, the department should have 6-7 front office (non-technical) staff (currently 5) and 6-7 technical staff (currently 3).

We have no reliable data on undergraduate enrollment projections. Given that online enrollment has been booming, we could conceivably see a drop in face-to-face undergraduate teaching. However, demographic projections suggest that level face-to-face enrollments are more likely in large courses.

If we succeed in doubling or tripling the number of BS chemistry majors from the current level (~10 BS degrees awarded per year), this will double or triple the enrollment in 3 upper-level lab courses (analytical, physical and synthesis labs), but will have little or no effect in lower-level labs and lectures due to the much higher numbers of non-majors in those classes.

Research- CCB currently has formal areas of research concentration in biological chemistry and in energy/materials chemistry. Over the next 10 years, we plan to expand these two areas and perhaps add chemical education as a third.

Teaching- We plan to add a non-science-majors course (CHEM 101) which we anticipate to have a high enrollment (300+ students per term). No other major changes in curriculum are planned in the near future.

Space distribution- While it is desirable that all CCB faculty have an office in Clark Hall, it is not necessary or desirable that all of their research space be located in Clark. Currently, four CCB faculty have all or part of their research effort in other buildings (Guo in Bandelier, Habteyes in CHTM, Kemp at the AML, and Cabaniss in Centennial Engineering), and this practice may well continue after renovation. However, it is desirable to keep most (>75%) of the departmental research effort within Clark/Riebsomer. At the same time, faculty from other departments may benefit from access to lab space in Clark/Riebsomer (previously provided for ChNE faculty, for example).

Teaching Space- The vast majority of our lecture classes are currently taught in other buildings- in Clark Hall, only room 101 is designated a lecture classroom. However, we are currently expanding the number of class sections that use active learning and collaborative pedagogy. Providing one or two classrooms (50 to 100 students) suitable for this type of pedagogy will be necessary moving forward.

While General Chemistry labs are currently taught in the SMLC, Organic Labs (303L and 304L) are still taught in antiquated Clark 150 with overflow sections in Clark 109. If the SMLC bump-out is funded by the severance bond proposal, these teaching labs will move to the new SMLC space.

Upper division laboratory courses (analytical, physical, synthesis) will continue to be taught in Clark Hall. Currently, each class has a total enrollment of 10 or fewer students per year, reflecting the number of BS chemistry required to take the sequence. However, regardless of enrollment (up to ~30), the space requirements for the first two are the same: an "instrument room" to hold the various spectrometers, etc. (currently in Clark 107) and a "prep room" with one or two fume hoods, bench space and sinks. The synthesis class requires more specialized fume hoods and bench space. Dr. Joe Ho oversees the instructional labs and will be an important contact for these class issues.

CCB currently has two small conference rooms (117 and 166) with minimal IT capabilities and a slightly larger meeting room (214), but will need at least one more as the faculty size increases.

Office space- We need to have individual offices for all faculty (including lecturers), advisors, and fiscal staff. It is highly desirable to have (smaller) offices for all post-docs and for visiting scientists (2-5 per year). Graduate students may share office space, although placing graduate student desks in 'wet' chemistry labs is no longer considered a safe practice.

Research space- Unfortunately**,** this most critical need is also quite difficult to predict. Although some of the problems in Clark Hall are obvious and visible- recurring water leaks, dangerous flooring, worn and broken fixtures, etc., - much of the problem is hidden behind the walls in the form of antiquated plumbing, a 'maxed-out' electrical system and inadequate ventilation. We can be certain the department will require a mixture of instrument rooms (NMR, ESR, MS, etc.), synthesis space (fume hoods), and flexible lab benches. We will also need a mixture of 'core facility' shared space and individual PI spaces. We will also need special-purpose spaces, including constant-temperature rooms, 'clean' space, and low noise/vibration space.