2020

Twenty Years of Exceptional Success: The Molecular Education and Research Consortium in Undergraduate computational chemistRY (MERCURY)”

George C. Shields
Furman University

Received: 31 March 2020 | Accepted: 30 April 2020
DOI: 10.1002/qua.26274

FULL PAPER

International Journal of QUANTUM CHEMISTRY WILEY

Twenty years of exceptional success: The molecular education and research consortium in undergraduate computational chemistry (MERCURY)

George C. Shields

Department of Chemistry, Furman University, Greenville, South Carolina

Correspondence
George C. Shields, Department of Chemistry, Furman University, Greenville, SC 29613.
Email: george.shields@furman.edu

Abstract

The molecular education and research consortium in undergraduate computational chemistry (MERCURY) consortium, established in 2000, has contributed greatly to the scientific development of faculty and undergraduates. The MERCURY faculty peer-reviewed publication rate from 2001 to 2019 of 1.7 papers/faculty/year is 3.4 times the rate of the physical science faculty at primarily undergraduate institutions. We have worked with over 1000 students on research projects since 2001, and 75% of our undergraduate research students have been under-represented in chemistry, either female or students of color. Approximately half of our alumni attend graduate school for the purpose of obtaining advanced degrees in STEM fields, and two-thirds are female and/or students of color. We have had more than 1600 attendees at 18 MERCURY conferences, including 111 invited speakers, 61 of whom have been female and/or faculty of color. In this paper, the research accomplishments, transformational outcomes, and scientific productivity of the MERCURY faculty are highlighted.

KEYWORDS

students of color in STEM, consortium, diversity, females in STEM, high-impact practices, inclusion, MERCURY, NSF-MRI, scientific excellence, undergraduate research

1 | INTRODUCTION

The molecular education and research consortium in undergraduate computational chemistry (MERCURY) consortium was formed during the 1999 to 2000 academic year, and a history of the evolution of the consortium has been published.[1] That paper traced how the consortium grew from seven faculty at liberal arts colleges in the Northeast in 2001, when the first National Science Foundation (NSF) Major Research Instrumentation (MRI) grant was received to support the consortium to 27 faculty at predominately undergraduate institutions (PUIs) in 2019. It also detailed the huge impact the annual MERCURY conference has had on the productivity of our undergraduate research groups. In the fall of 2019, we invited more faculty into the consortium, so we are now 38 faculty working with undergraduate research groups at 33 institutions across the country. MERCURY has been supported by five NSF MRI grants, as well as internal funds from Hamilton College, Armstrong Atlantic State University, Bucknell University, and Furman University, to support hosting the shared computational resources and the annual conferences, and by all the colleges and universities in the consortium who have committed to paying for their faculty and students to attend the annual meeting. In this paper, I will outline the scientific productivity, both in terms of research accomplishments and transformational outcomes, that the first five NSF MRI grants enabled, and then highlight the ongoing research efforts of the 38 MERCURY faculty in the consortium today. Research Accomplishments and Transformational Outcomes align with the NSF criteria for grant funding, which are Intellectual Merit and Broader Impacts.

2 | RESEARCH ACCOMPLISHMENTS (INTELLECTUAL MERIT) AND TRANSFORMATIONAL OUTCOMES (BROADER IMPACTS) OF THE FIVE MERCURY NSF MRI PROPOSALS

2.1 | First NSF-MRI Award, August 28, 2001, $400 000, CHE-0116435

"Acquisition of High Performance Computers for the Northeastern Undergraduate Research Chemistry Consortium"

2.1.1 | Research accomplishments

The seven faculty who started the consortium were **Jeffery Greathouse** (*St. Lawrence*, environmental), **Maria Gomez** (*Vassar*, materials), **Carol Parish** (*Hobart & William Smith*, physical organic), **Ramona Taylor** (*Holy Cross*, environmental and materials), **Martha Reynolds** (*Colgate*, bioinorganic), **Marc Zimmer** (*Connecticut*, bioinorganic), and **George Shields** (*Hamilton*, biophysical). Over the 3-year grant period, the seven faculty published 44 research papers in peer-reviewed journals with their students.[2–45] This equates to two published papers per year per faculty member, which is four times higher than the usual productivity of a faculty member at a PUI as documented by Research Corporation.[46] Further, in the first 4 years after the consortium was established, the number of external grant awards received by the faculty more than tripled, and the MERCURY investigators raised more than $4 million to support computational chemistry research involving undergraduate students. The bulk of this funding was used to provide summer stipends, which allowed students to be immersed fulltime in research. Mentoring provided by senior researchers to junior researchers and networking at the national meeting have contributed greatly to the high rate of success in recruiting and retaining students, particularly those from under-represented groups. The seven MERCURY investigators worked with more than 110 undergraduates on research projects during the first 3-year grant period. Marc **Zimmer**'s *Chemical Reviews* article on green fluorescent protein has been cited over 770 times in the Web of Science (WOS) database.[41] Maria **Gomez**'s *PNAS* paper on the hydration and mobility of aqueous OH^- has been cited more than 130 times in WOS.[5] The **Shields** lab's work on pK_a calculations invigorated the field, with two *JACS* papers cited more than 445 times each,[20,24] and two other research papers cited more than 140 times each in WOS.[19,23] Similarly, the lab's *JACS* paper on water clusters in the atmosphere has been cited more than 130 times.[26]

2.1.2 | Transformational outcomes

This proposal requested $780 220 from NSF, matched with $400 000 by Hamilton College and $215 000 from the Consortium Colleges, to support the acquisition of high-end computers for the seven researchers and their students. The consortium purchased two workstations for each institution to serve as local graphics and a 32-processor Origin 300 and an 8-processor Origin 300 located at Hamilton College. In addition, we built a 30-node Beowulf Cluster for the consortium. We used NSF funds to hire a system administrator, and we organized an annual conference for any and all undergraduates to present their work in computational chemistry, to learn from our invited speakers, and to network with other students and faculty in attendance. The consortium has attracted many more women into this traditionally male-dominated research area. Three of our research groups consisted of at least 40% African-American or Hispanic-American students. This proposal had a particularly positive impact on the careers of Maria **Gomez** and Carol **Parish**. **Gomez** moved from Vassar College to Mt. Holyoke College in 2003 and currently occupies the *Elizabeth Page Greenwalt Chair in Physical Sciences*. She was awarded a Henry Dreyfus Teacher-Scholar Award in 2007. She directs the "Passport to Chemistry Adventure Program" supported by Dreyfus. **Parish** moved from Hobart & William Smith Colleges to the University of Richmond in 2005, where she occupies the *Floyd D. and Elisabeth S. Gottwald Chair in Chemistry*. She is the recipient of numerous awards throughout her career, including the Henry Dreyfus Teacher-Scholar Award (2005), the ACS Stan Israel Award for Advancing Diversity in the Chemical Sciences (2011), the Council on Undergraduate Research Goldwater Mentor Award (2016), the ACS Committee on Minority Affairs Zaida C. Morales-Martinez Prize for Outstanding Mentoring of ACS Scholars (2017), and the ACS Award for Research at an Undergraduate Institution (2019).

2.2 | Second NSF-MRI Award, August 3, 2005, $100 000, CHE-0521063

"Acquisition of a Linux Cluster for the Molecular Education and Research Consortium in Undergraduate computational chemistry (MERCURY)"

2.2.1 | Research accomplishments

Undergraduate faculty **Maria Nagan** (*Truman State*, biochemistry), **Glênisson de Oliveira** (*Rhode Island College*, physical), **Wingfeld Glassey** (*Hobart & William Smith*, physical), and **Tricia Shepherd** (*Westminster College*, *Utah*, physical) joined **Gomez**, **Parish**, **Shields**, and **Zimmer**, while Reynolds, Greathouse, and Taylor left the consortium, as did Glassey before the end of the grant period. The Principal Investigator (PI) invited five additional investigators into the consortium during the grant period: **Mauricio Cafiero** (*Rhodes College*, biochemistry), **Kelling Donald** (*University of Richmond*, chemical bonding), **Becky Eggimann** (*Wheaton College*, *IL*, solvation), **Daqing Gao** (*Queensborough Community College of CUNY*, physical organic), and **Eric Patterson** (*Truman State*, physical organic). These MERCURY investigators have published 50 papers,[47–96] which translates to 1.9 publications/faculty/year (seven faculty were in the consortium for 3 years; five were in the consortium for 1 year). This is 3.8 times the national average (0.5 pubs/faculty/year).[46]

2.2.2 | Transformational outcomes

The 12 MERCURY consortium PIs worked with 140 undergraduate students, 13 high school students, 7 high school teachers, and 6 senior scientists at their institutions over the 3-year grant period. Of the 140 undergraduates, 89 were female, 14 were Asian, 13 were Black or African-American, and 12 were Hispanic or Latino. A total of 101 undergraduates were female and/or students of color, which is 72% of the undergraduates trained in our labs. Our students won 20 national or international awards such as Goldwater Scholarships and Fulbright Fellowships during this period. We hosted three more MERCURY conferences in the summers of 2006, 2007, and 2008, with a total of 251 participants. Over 75% of the participants were undergraduates or high school students. Over 50% of the speakers and 50% of the participants were women or students of color.

2.3 | Third NSF-MRI Award, July 15, 2008, $229 000, CHE-0521063, CHE-1044256

> "Acquisition of a High Performance Computer for the Molecular Education and Research Consortium in Undergraduate computational chemistry (MERCURY)"

2.3.1 | Research accomplishments

Both **de Oliveira** and **Gao** left the consortium and Clifford **Padgett** (*Armstrong Atlantic State University*, biochemistry) and **Adam Van Wynsberghe** (*Hamilton*, biochemistry) were invited into the consortium in the second year of the grant. MERCURY faculty published 62 publications during the third MRI grant period,[97–158] that is, an average of 1.7 papers published per investigator per year, a rate 3.4 times the average rate at PUIs.[46] The **Shields** lab's papers on water clusters have been cited over 150 and 190 times,[131,143] and their review article on pK_a calculations has been cited over 130 times.[129]

2.3.2 | Transformational outcomes

This proposal funded $229 000 for an SGI Altix 450. The 13 MERCURY investigators worked with 165 undergraduates over the 3 years of this grant. Of the 13 MERCURY investigators, five are female; and of the 13, three are Hispanic, one is Asian, and one is Black. The diversity of the PIs, as well as their overall commitment to inclusion of all interested students in their work, is reflected in their work with their undergraduate research assistants. A total of 197 personnel worked on this project as a result of this award. This includes three other senior researchers/technicians, five postdoctoral associates (one Asian female, a Black female, and a Black male), 165 undergraduates, three high school students, 11 precollege teachers, and one post-baccalaureate fellow. Of the 165 undergraduates, 92 were female (55%); 26 of the 165 were Asian (16%), 21 were Black (13%), and nine were Hispanic (5%). Of the 92 females, 14 were Asian, 13 were Black, and two were Hispanic. Thus 34% of the undergraduate student researchers were students of color. Including all female and male students, 119 of the 165 were female and/or students of color, which is 72% of the total.

2.4 | Fourth NSF-MRI Award, August 22, 2012, $200 000, CHE-1229354

"MRI: Acquisition of High Performance Computers for the Molecular Education and Research Consortium in Undergraduate computational chemistry (MERCURY)"

2.4.1 | Research accomplishments

Padgett left the consortium, **Gao** (*Central State*) rejoined, and **Kelly Anderson** (*Roanoke College*, physical), **Aimée Tomlinson** (*North Georgia College*, physical), and **Sudeep Bhattacharyay** and **Jim Phillips** (*University of Wisconsin-Eau Claire*, biophysical and physical) joined, bringing the total to 17 MERCURY investigators. We published 79 peer-reviewed papers,[159–237] or 1.5 papers/faculty/year, which is three times the rate for physical science faculty at undergraduate institutions.[46] The **Shields** group's collaboration with Brooks Pate resulted in a *Science* paper on the structures and energetics of the gas-phase water hexamer,[160] which has been cited over 250 times. They showed conclusively that three $(H_2O)_6$ isomers are formed in a low-temperature beam, and that the cage is the lowest energy isomer.[160] **Patterson** published a paper in *Science* on the fate of metabolites of the steroidal growth promoter trenbolone acetate, which is administered to beef cattle. Based on the chemistry, they concluded that predictive models and risk assessment must take into account the transformation products of high-risk environmental contaminants such as endocrine-disrupting steroids.[184] **Parish** and **Donald** published a paper in *JACS* on halogen bonding in DNA base pairs,[169] which has been cited over 70 times in WOS.

2.4.2 | Transformational outcomes

During the 3-year period of this grant, the 17 MERCURY investigators worked with 200 undergraduates, and over 75% of them were female and/or from under-represented groups. In addition, 16 high school students, 2 post-baccalaureate alumni, 2 technicians, 4 post-doctoral researchers, and 1 staff research scientist worked with the MERCURY investigators.

2.5 | Fifth NSF-MRI Award, September 1, 2016, $225 000, CHE-1626238, 1662030

"MRI: Addition of High Performance Computers for the Molecular Education and Research Consortium in Undergraduate computational chemistry (MERCURY)"

2.5.1 | Research accomplishments

Undergraduate faculty **George Barnes** (*Siena*, physical), **Chrystal Bruce** (*John Carroll*, physical), **Nick Boekelheide** (*Colby*, biophysical), **JiaJai Dong** (*Bucknell*, biophysics), **Dmitri Kosenkov** (*Monmouth*, physical), **Ashley Ringer McDonald** (*Cal Poly*, biophysical), **Bill Miller III** (*Truman State*, biochemistry), **Juan Navea** (*Skidmore*, physical), **Joshua Schrier** (*Haverford*, Physical), **Isaiah Sumner** (*James Madison*, biochemistry), and **Mychel Varner** (*Iona*, physical) joined the consortium in 2016. **Boekelheide** left in 2017 for family reasons, and in 2017/2018 we added **Heidi Hendrickson** (*Lafayette College*, Physical), **Kedan He** (*Eastern Connecticut State University*, biological), **Aurelia Ball** (*Skidmore College*, biochemistry), and **Joseph Baker** (*The College of New Jersey*, biochemistry). In 2018, Marc **Zimmer**, one of the original senior investigators, retired from the consortium. **Eggimann** and **Gao** left the consortium as well, bringing the total to 27 faculty at 24 different institutions. The faculty published 2 peer-reviewed books,[238,239] 9 peer-reviewed book chapters,[240–248] and 115 peer-reviewed research papers.[249–363] This comes to 1.6 peer-reviewed products/faculty/year during the 3-year grant period, which is 3.2 times the rate of publication for natural science faculty at PUIs.[46]

2.5.2 | Transformational outcomes

Overall, during the 2016 to 2019 grant period we worked with 325 undergraduates, of which 71% were female and/or students of color. In addition, nine high school students, two post-baccalaureate fellows, three master's students, two post-doctoral researchers, and a staff research

scientist worked with the MERCURY investigators. We held four successful conferences, averaged 102 attendees, with an average of 52.5 undergraduate poster presentations. Of our 24 speakers, 16 were female and/or faculty of color. We held pre or post-conference MolSSI programming workshops each summer. **Shields** is on the MolSSI Science & Software Advisory Board. **McDonald** and **Ball** are both MolSSI associates and are well known for their development of undergraduate programming curriculum and MolSSI workshops.

2.6 | Summary of impacts, 2001 to 2019

2.6.1 | Research accomplishments (intellectual merit)

One of the challenges to the overall undergraduate research movement is that the ability of undergraduate research to advance scientific knowledge remains undervalued.[364,365] From 2001, when the first NSF-MRI grant was funded, through the summer of 2019, the MERCURY investigators have published 361 peer-reviewed publications, including 2 in *Chemical Society Reviews*,[104,269] 1 in *Chemical Reviews*,[41] 1 in *Nature Reviews Chemistry*,[328] 3 in *Science*,[160,184,272] 2 in *Nature*,[271,344] 2 in *Angewandte Chemie International Edition*,[199,346] 13 in *JACS*,[20,24,26,36,59,71,84,112,136,169,289,315,336] and 3 in *PNAS*.[5,148,318] We published 44 papers during the first MRI grant period,[2–45] 50 during the second MRI grant period,[47–96] 62 during the third MRI grant period,[97–158] 79 during the fourth grant period,[159–237] and 126 peer-reviewed papers during this fifth grant period.[238–363] Clearly, the impact of undergraduate researchers working with motivated and skilled faculty for the advancement of scientific knowledge is highly significant.

2.6.2 | Transformational outcomes

From 2001, when the first NSF-MRI grant was funded, through the summer of 2019, the MERCURY investigators worked with 888 students on research projects. Without double-counting female students of color, 75% of our undergraduate research students have been female and/or students of color. Approximately half of our graduates attend graduate school for the purpose of obtaining advanced degrees in STEM fields, and approximately two-thirds are female and/or students of color. Since the start of the MERCURY consortium, students mentored by MERCURY faculty have won more than 50 national awards, including 1 Rhodes, 10 Fulbright Fellowships, 21 Goldwater Fellowships, 2 Gates Cambridge Scholarships, and more than 20 national graduate fellowships (NIH, NASA, NDSEG, NSF). We have had more than 1600 attendees at the 18 MERCURY conferences, and 111 speakers, 61 of whom have been female and/or faculty of color.

In terms of operations and maintenance, we have had no major downtime, and usage history reveals that all MERCURY investigators have had adequate computer time on the various HPC clusters we have obtained from MRI funds. PI Shields has invited new investigators into the consortium when others left in order to optimize the use of these clusters. We have demonstrated how to maximize the investment NSF has made in us.

3 | OVERVIEW OF PAST AND CURRENT MAKE-UP OF FACULTY IN THE MERCURY CONSORTIUM

Since 2016, the resources of MERCURY were primarily used by 27 researchers (**Anderson**, **Ball**, **Baker**, **Barnes**, **Bhattacharyay**, **Bruce**, **Cafiero**, **Donald**, **Dong**, **Gomez**, **He**, **Hendrickson**, **Kosenkov**, **McDonald**, **Miller**, **Nagan**, **Navea**,"/> **Parish**, **Patterson**, **Phillips**, **Schrier**, **Shepherd**, **Shields**, **Sumner**, **Tomlinson**, **Van Wynsberghe**, and **Varner**) and their undergraduate students. These 27 research groups kept the clusters fully occupied and used local and national resources as needed (NSF XSEDE and DOE NERSC). Dong has left the consortium, and we added 12 new faculty at the end of 2019, 8 at the Assistant Professor level and 4 at senior levels. This brings the consortium to 38 researchers at 33 institutions.

Involvement in a highly mentored exciting undergraduate research project is the key to cultivating and retaining student interest in the sciences and is therefore an excellent means for increasing the diversity of the chemistry community. It has been conclusively demonstrated that active learning has an outsized impact on retaining female and students of color in STEM fields,[366] and a highly mentored original research project where the student is in charge of his or her own project is the ultimate active learning experience for all students.[365,367,368] The three senior faculty who formed the MERCURY consortium in 2000 are **Maria Gomez** (*Mount Holyoke*, materials), **Carol Parish** (*University of Richmond*, physical organic), and **George Shields** (*Furman*, physical). The 23 faculty who joined in the second, third, fourth, and fifth grant proposals and still remain in MERCURY are **Kelly Anderson** (*Roanoke College*, physical), **Joseph Baker** (*The College of New Jersey*, biochemistry), **Aurelia Ball** (*Skidmore College*, biochemistry), **George Barnes** (*Siena*, physical), **Sudeep Bhattacharyay** (*University of Wisconsin-Eau Clare*, physical biochemistry), **Chrystal Bruce** (*John Carroll*, physical), **Mauricio Cafiero** (*Rhodes*, biochemistry), **Kelling Donald** (*Richmond*, chemical bonding), **Kedan He** (*Eastern Connecticut State University*, biological), **Heidi Hendrickson** (*Lafayette College*, Physical), **Dmitri Kosenkov** (*Monmouth*,

physical), **Ashley McDonald** (*Cal Poly*, biophysical), **Bill Miller III** (*Truman State*, biochemistry), **Maria Nagan** (*Truman State*, biochemistry), **Juan Navea** (*Skidmore*, physical), **Eric Patterson** (*Truman State*, physical organic), **Jim Phillips** (*University of Wisconsin-Eau Clare*, physical), **Joshua Schrier** (*Fordham*, Physical), **Tricia Shepherd** (*Westminster*, physical), **Isaiah Sumner** (*James Madison*, biochemistry), **Aimée Tomlinson** (*North Georgia College*, physical), **Mychel Varner** (*Iona*, physical), and **Adam Van Wynsberghe** (*Hamilton*, biochemistry). **Nagan** and **Patterson** moved to SUNY Stony Brook as lecturers, and they both run productive undergraduate research groups. **Shepherd** has moved to Franklin & Marshall College.

The 12 additional investigators who joined this academic year are **Sarah Arradondo** (*Washington*), **Rob Berger** (*Western Washington*), **Clyde Daly** and **Casey Londergan** (*Haverford*), **Wallace Derricotte** (*Morehouse*), **Jay Foley** (*William Paterson*), **Lindsey Madison** (*Colby*), **Caitlin Scott** (*Hendrix*), **Patricia Soto** (*Creighton*), **Tyler Luchko** (*Cal State Northridge*), **Simbarashe Nkomo** (*Oxford College*), and **Anton Oliynyk** (*Manhattan*), bringing the total number to 38 faculty at 33 different institutions. **Londergan** is Professor and Chair of his department, **Berger**, **Soto**, and **Luchko** are Associate Professors, and the other eight are Assistant Professors. **Scott** is a MERCURY alumna (**Gomez** lab), who joins **Miller** and **Varner** as alumni of MERCURY faculty (**Nagan** and **Parish** labs), and all three attended MERCURY conferences and used MERCURY resources as undergraduates.

The 38 MERCURY investigators now include 11 full Professors, 10 Associate Professors, 15 Assistant Professors, and 2 Lecturers (formerly full Professors). We know from experience that this balance will allow for effective mentoring across the consortium. The success of MERCURY members is in large part due to the network and support of the group.[1] As the consortium has grown, we have formalized the mentoring process to ensure that each member has a small network to which they belong in addition to being supported by the larger consortium. The 12 new members will be assigned to a mentoring group to provide access to the knowledge and strategies of established members and allow a seamless transition into the consortium. Activities for mentoring groups include monthly web meetings, writing groups, pre-submission review of manuscripts and grant proposals, and in-person meetings at conferences. Strategies for improving and balancing teaching, research, and service obligations have been particularly helpful to new faculty. The consortium in general and mentoring groups in particular ameliorate the isolation many computational chemists at PUIs feel. Mentoring networks have been shown to improve career success at all stages of an academic career[369] and are an important contributor to the career satisfaction and productivity of MERCURY consortium members. Chrystal **Bruce**, who is a co-PI on two relevant grants from NSF and the Department of Education totaling $2 293 515 (Advancing STEM Careers by Empowering Network Development; Linked Learning and Early Warning Approach for At Risk Student Success), is responsible for managing and assessing the value of our mentoring groups.

Undergraduate research is the key to cultivating and retaining student interest in chemistry, and we offer as many of these research opportunities as possible to first and second year students.[370,371] MERCURY faculty are well funded to support student stipends, with 17 NSF, 2 NIH, 4 ACS/PRF, 2 Dreyfus, 1 Jeffress Foundation, and 3 Research Corporation grants as PIs to support research ($6.37M) as well as 3 other grants as co-PIs or senior personnel (SP) for research projects ($3.51M). In addition, Schrier is the PI of a DARPA grant worth $7.2M and Bruce is the PI of a DOE grant worth $650 000. All told, as of the 2019/2020 academic year, 22 of the 38 MERCURY faculty hold 41 grants as PIs, worth $14.57M, and are co-PIs/SP on another $3.51M. We expect that the mentoring aspects we have developed over the years will greatly enhance the productivity of our newest members, as it has for others. And the addition of computing resources will enhance our undergraduate research programs. The pictures of the 38 MERCURY faculty are shown below.


Anderson

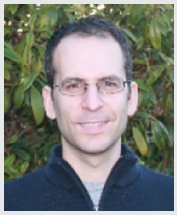

Arradondo

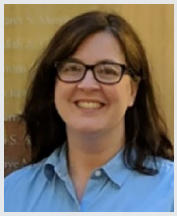

Baker

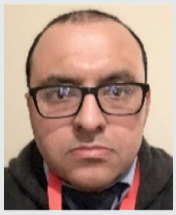

Ball


Barnes


Bhattacharyay

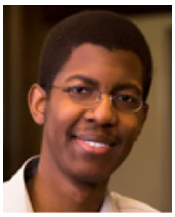

Berger

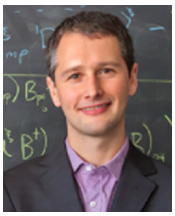

Bruce

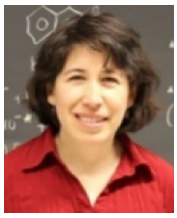

Cafiero


Daly


Derricotte

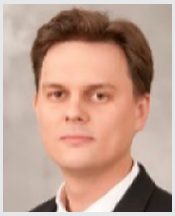

Donald


Foley


Gomez


He


Hendrickson


Kosenkov


Londergan


Luchko


Madison


Miller


Nagan


Navea


Nkomo


Oliynyk


Parish


Patterson


Phillips


Ringer McDonald


Schrier


Scott


Shepherd


Shields


Soto


Sumner


Tomlinson


Van Wynsberghe


Varner

4 | OVERVIEW OF MERCURY FACULTY RESEARCH EFFORTS

MERCURY faculty's research efforts are summarized briefly below, starting with the faculty who have been in the consortium the longest, and proceeding to our newest members.

Maria Gomez's research: The **Gomez group** focuses on charged defect conduction paths with applications to fuel cells. Her earlier work[132,133,167,187,236] showed that there are many possible proton pathways contributing to overall conduction in doped perovskites. Her group showed that, in $BaD_xZr_{1-x}O_{3-y}$ perovskites, an oxygen vacancy[372] near an Al dopant increases the barrier for proton escape from the dopant due to lattice rearrangement, while one near Sc and Y dopant decreases the barrier for proton escape from the dopant, suggesting that the oxygen vacancy can increase proton conduction in some cases. They are exploring how long-range proton conduction pathways change as a result of local structure distortions induced by oxygen vacancies and proton/oxygen vacancy correlation, using extensions of their earlier path-searching techniques[132,167,187,236,372] along with dynamical methods,[373,374] to quantify the effect of a delocalized oxygen vacancy on oxygen vacancy conduction.

Carol Parish's research: The **Parish** group employs the tools of quantum mechanics, conformational searching, and molecular dynamics (MD) simulation to answer questions about the structure, energy, reactivity and/or dynamics of motor proteins, polymerases, damaged DNA, petroleum combustion intermediates, neurosteroids, and ion-gated membrane receptors.[13,15,17,58,59,126,127,169,217,218,220] Current projects include (a) performing highly correlated, multireference quantum chemical calculations on diradical intermediates found in petroleum combustion, and in formation of anti-cancer warhead drugs and fullerene nanoparticles; (b) using highly efficient sampling techniques to study the dynamics of HIV-1 protease flap motions and ionotropic glutamate (iGluR) receptor behavior; and (c) designing novel polyoligomericsilsesquioxane ligands for HIV protease to understand host-guest interactions between iGluR proteins and endogenous ligands. These projects are computationally very demanding and depend on the availability of fast compute cycles with high-speed interconnects.

George Shields' research: The **Shields** group has published a series of papers on accurate relative and absolute calculations of pK_a values, including careful examination of the best theoretical and experimental values for the free energy of hydration of fundamental ions, and the optimum computational procedures for determining deprotonation equilibrium constants in aqueous solution.[19,20,23,24,129,179] An outgrowth of the group's interest in biochemistry[69,71,101,107–109,200,375–378] is understanding the structure of water,[25,26,379–381] leading to accurate calculations of gas-phase water clusters,[28,60,67,102,131,143,144,160,178,199,223,272] which led to research that focuses on modeling the formation of atmospheric aerosols.[287,293,326,349] Understanding this process will yield information about the initial growth of atmospheric aerosols and address the large uncertainty associated with the role of aerosols in global warming.[70,100,130,159,161,162,198,327]

Mauricio Cafieros' research: The **Cafiero** group studies the binding of small molecules to proteins and the conformations of small peptides. They investigate acetaminophen metabolism by a sulfotransferase enzyme (SULT1A3),[197] using an active site model from a crystal structure[382] using DFT and MP2 methods. Working with an experimental collaborator, they expanded this study to how a suite of catecholaminic and catecholic molecules interacts with SULT1A3,[228,229] SULT1A1, catechol-*o*-methyltransferase,[260] phenylalanine hydroxylase,[354] tyrosine hydroxylase,[308] and other enzymes/receptors. They are also working on the discovery of inhibitors for the LpxC enzyme for Gram-negative bacteria.[285,305,383,384]

Kelling Donald's research: In the **Donald** research group, work is focused on (a) halogen bonding and other sigma hole interactions in organic and inorganic systems,[210,278] (b) fluxionality in planar inorganic clusters and the nature and potential control of so-called molecular machines,[208,263] (c) the evolution of structural preferences and thermal stability in metal halide and hydride molecules, clusters, and corresponding extended solids,[322](d) the stability and catalytic applications of structurally interesting or unusual main-group and transition-metal organometallic compounds,[151,231,351,385] (e) the stabilization of unusual bonding arrangements, including planar tetra-coordinate and other unusual coordination environments,[172] (f) quantifying currently qualitative but transferrable concepts in chemical bonding,[233] and (g) aromaticity and analogous phenomena in non-hydrocarbon systems.[338,386] The MRI resources are essential for calculations on large and heavy elemental systems.

Maria Nagan's research: The **Nagan** group models RNA to understand how chemical functional groups affect structure and biological function. In addition to the standard bases in RNA, there are naturally occurring, post-transcriptionally modified bases. MD studies of human $tRNA^{Lys,3}$ found that the *N6*-threonyl-moiety at position 37 is required for maintenance of the anticodon stair-stepped conformation required for correct codon recognition,[56] and systematic natural bond orbital analysis revealed that strong electrostatic interactions between the backbone and the 34th base are key to retaining the structure.[185] A better force field for nonstandard bases is being developed to match experimental sugar pucker ratios.

Eric Patterson's research: The **Patterson** group explores issues of environmental chemistry via quantum chemical modeling, including the chemistry of steroids that are common contaminants in surface and wastewater. Working with collaborators at Iowa State, they have recently established that trenbolone, a bovine growth hormone, completes an unexpected photochemical hydration/thermal dehydration cycle that prolongs its presence in surface waters.[184]

Tricia Shepherd's research: The **Shepherd** group is studying the transport of water and ions in confined environments because it is central to understanding protein channels in biological systems and material applications involving nanomembrane technology. They plan to build on their

success incorporating the monoatomic water (mW) model[387] and complementary coarse-grained interactions including ions[388] and carbon-based nanoparticles.[166,237,389] They will extend their analysis to study interactions between water and ions under confinement at the hydrophobic nanopore surface.

Adam Van Wynsberghe's research: The **Van Wynsberghe** lab is investigating the kinetics and pathways of ligand association to the influenza viral protein neuraminidase (NA).[136] His group has developed a multi-scale methodology to describe the complete binding trajectories of small molecules binding to either the active or secondary site of NA, by first using Brownian dynamics to compute the distal diffusional approach, and then transitioning to equilibrium MD once the ligand and the protein become proximal, which captures the association dynamics over multiple time scales, followed by post-processing MD trajectories using MM/GBSA to provide insight into the favored pathways of binding. To achieve adequate sampling, they carry out thousands of 5-ns trajectories for this system.

Kelly Anderson's research: The **Anderson** lab uses Monte Carlo molecular simulation techniques to study a variety of complex chemical systems. Currently, their attention is focused on the interactions of multicomponent liquid solutions with solid substrates.[201] Additional work has focused on mixtures of alkanes with other organic species (alkenes, alcohols, perfluoroalkanes).

Sudeep Bhattacharyay's research: The **Bhattacharyay** group studies the chemistry of enzymes, such as the role of dynamics and quantum mechanical tunneling in a flavin-containing enzyme.[390,391] Using extensive MD simulations, they are developing a molecular model of the interplay of dynamics and quantum tunneling in enzyme catalysis,[290,391] and exploring the role of macromolecular crowding on conformational dynamics and enzyme catalysis of bacterial prolyl-tRNA synthetase.[174,195,204,205,332]

James Phillips's research: The **Phillips** group studies condensed-phase effects on the structural properties of molecular complexes: primarily electron donor-acceptor systems (eg, CH_3CN-BF_3),[392,393] and hydrogen-bonded/proton transfer systems.[273] Using low-temperature IR spectroscopy, they assess the extent of structural change across various media via measured frequency shifts. Computations are vital for characterizing gas-phase systems and providing direct insight into the mechanism for medium-induced structural change[181,213,393] and to enable them to identify promising targets and focus their experimental efforts.[181,394,395] Following up on their initial work on group IV halides (MX_4: M = Ti, Si, Ge; X = F, Cl),[211,298,310] they are exploring the nitrile and imine complexes of the monoalkyl analogs (MX_3R) of these acids.

Aimée Tomlinson's research: The **Tomlinson** group studies how the electronic, optical, and structural properties of conjugated oligomer materials vary as a function of conjugation. Using a combination of organic synthesis, theoretical calculations, and physical measurements, they carry out systematic investigations of novel cross-conjugated oligomers based on the benzo[1,2-*d*;4,5-*d*′]bisoxazole (BBO) moiety. This unique electron-deficient ring system with two distinct conjugation axes, namely 2,6-conjugation through the oxazole rings, and 4,8-conjugation through the central benzene ring and spatially segregated frontier molecular orbitals (FMO)s, provides a platform for tuning the LUMO or HOMO by varying the nature of the substituents and their arrangement around the central molecule.[163,164,192,207,396,397]

George Barnes's research: The **Barnes** group studies the reaction dynamics that take place in tandem mass spectrometry systems, in particular, $MS^{[2]}$ techniques for proteomic analysis, which involve the initial separation of an ion of interest (MS step 1), which is then highly energized and dissociates. The dissociation products are then mass-analyzed (MS step 2), which leads to sequencing information. However, the presence of post-translational modifications (PTMs) of peptides, such as methylation, acetylation, phosphorylation, sulfonation, and disulfide bonding, can greatly complicate the identification of the peptide sequence. PTM is a common occurrence in biological systems, and can occur at the N- or C-terminus as well as the side chain of an amino acid. It has been estimated that between 40% and 70% of $MS^{[2]}$ spectra cannot be matched or are misidentified.[398] Because of its utility, there is significant interest in understanding the chemical and physical characteristics of $MS^{[2]}$ systems.[399–407] The Barnes group has studied surface-induced dissociation (SID) of protonated peptides colliding with organic self-assembled monolayer (SAM) surfaces[408–410] as well as reactive landing (RL) of protonated peptides on modified SAM surfaces,[411] which has demonstrated the importance of proton mobility and noncovalent interactions.

Chrystal Bruce's research: The **Bruce** lab focuses on understanding the molecular-level interactions that exist between biologically relevant molecules, specifically small molecule DNA minor groove binders and protein/ligand interactions. Retinoic acid (RA), a form of vitamin A, was originally predicted to reduce the spread of cancer. But in some cases, cancer cell growth has been found to be actually promoted by the introduction of retinoic acid in vivo in rats.[412] This observation was explained by the concentration ratios of two proteins in the specific cell type (FAPB5 and CRABPII). When RA binds to FABP5, a survival pathway is created in the cancerous cells and results in cell proliferation. In the presence of CRABPII, RA is carried to retinoic acid receptors (RAR), which leads to apoptosis and the inhibition of tumor growth. The Bruce group has published the first MD study showing the structure and dynamics of these systems,[312] and are studying small molecules that may promote the natural apoptotic process when bound to FABP5.

Dmitri Kosenkov's research: The **Kosenkov** lab is studying fundamental interactions of electronic excited states of organic chromophores used as molecular sensors (eg, pyridinium *N*-phenolate betaine dyes and boron-dipyrromethene) in organic solvents to obtain detailed atomistic-level knowledge of mechanisms of energy transfer,[413] and to continue to enhance their expertise in modeling intermolecular interactions,[414–416] fragmentation EFP and FMO methods,[234,417,418] and hybrid QM/MM methodologies that interface electronic structure methods for electronic excited states with EFP.[419]

Ashley Ringer McDonald's research: The **McDonald** group studies molecular interactions in complex macromolecular systems using correlated electronic structure techniques and molecular simulations to computationally characterize ligand/aptamer binding to understand the structural

and energetic changes that occur in molecular recognition events involving DNA and RNA aptamers. They are also developing a computational model of MEK1, a key protein involved in the RAF-MEK-ERK cascade, which is activated in many tumor cell lines and in the tumors of cancer patients,[356] which they will use to screen small molecule inhibitors of MEK1. This project is not feasible without MERCURY's resources.

Bill Miller III's research: The **Miller** group studies problems in biochemistry using MD, including studies on DNA-binding proteins.[218,220,274,294,295,299,303,329,331,352] Current work includes designing an isoflavanone derivative for aromatase inhibition to treat endometriosis and inhibiting the aggregation of amyloid beta proteins found in the brains of patients with Alzheimer's disease (AD). Specifically, they are studying a class of molecules called polyphenols that have shown promising experimental results for AD.

Juan Navea's research: The **Navea** group investigates problems in physical chemistry of interfaces. This includes how tropospheric gases bind to atmospheric aerosols, leading to various coordination modes between the surface (aerosol) and the substrate (adsorbed trace gases).[420–424] Among the components of aerosols are semiconductor compounds, such as TiO_2, that can trigger photo-induced heterogeneous reactions on the substrate.[425–427] They are modeling the nitrate-TiO_2 interface using computational chemistry methods. In addition, they investigate the substrate's vibrational frequency shifts resulting from the co-adsorption of water and nitrates on TiO_2 active sites.[428–430] Modeling the aerosol interaction with trace atmospheric gases will add to our understanding of the indirect effects of atmospheric aerosols on climate change. Moving from computational studies using PC workstations to the MERCURY resources has been essential to increase the computational efficiency of our surface-substrate models.

Joshua Schrier's research: The **Schrier** group uses simulations and machine learning to understand and design organic-inorganic hybrid materials for energy and environmental problems. In particular, they are interested in understanding the role of noncovalent interactions in controlling inorganic topologies,[343] the role of reaction conditions and reagent properties on reaction outcome,[330] and how human biases in experimental decision making hinder progress in machine learning using those datasets.[344] Current computational work will contribute to understanding molecular interactions in the formation of precursor solutions and electrolyte solution properties.

Isaiah Sumner's research: The **Sumner** group uses classical MD, ab initio molecular dynamics (AIMD) and electronic structure theory to study enzyme mechanisms. The transfer of an acetyl group or ubiquitin to a target protein are two examples of a process called protein post-translational modification (PTM), which allows cells to rapidly respond to internal and external stimuli. Despite the importance of acetyl and ubiquitin transferases,[431,432] there are currently no studies that conclusively show the enzymes' reaction pathways.[433–435] The group aims to determine and compare the reaction pathways for representative members of the acetyl and ubiquitin transfer family of enzymes using AIMD and QM/MM electronic structure calculations.[301,345] MERCURY resources are crucial to the success of this project.

Mychel Varner's research: The current research of the **Varner** group concerns reactions of neonicotinoid insecticides with atmospheric species and collaboration with a synthetic organic chemist, requiring high-level ab initio calculations on small complexes. They also investigate new particle formation (NPF) in the atmosphere,[436,437] and have shown that although amines typically have concentrations 1 to 3 orders of magnitude lower than that of NH_3 in the atmosphere, they still play an important role in driving NPF.[255]

Sarah Arradondo's Research: The **Arradondo** lab characterizes various noncovalent interactions within interesting systems using ab initio methods and density functionals in conjugation with large, robust basis sets.[438–441] They are currently investigating the different configurations within several room-temperature ionic liquids along with the hydrogen-bond networks that these materials have with water and how these interactions may affect the materials' bulk-phase properties when including a co-solvent.

Joseph Baker's research: The **Baker** group uses MD simulations to investigate the biomechanical properties of type IV pilus (T4P) filaments and the interactions of ionic liquid/deep eutectic solvents with proteins and membranes. They use a comprehensive, multi-scale computational approach, including both all-atom and coarse-grained MD simulations, to characterize the T4P structural ensemble, identify the most important inter-monomer interactions for T4P stability and strength, and develop a coarse-grained model to accurately describe the force-transitioned state of a T4P filament.[442,443] They also investigate the influence of ionic liquids and deep eutectic solvents on the conformation of proteins and small peptides including Trp-cage and insulin,[281,444]and also how these solvents embed in the lipid bilayer[340] and impact the permeability of lipid bilayers to small molecules.

Aurelia Ball's research: The **Ball** group aims to understand how intrinsically disordered proteins interact with and influence more structured proteins in order to perform their function as part of different cellular and disease processes,[251] including studying how the disordered HIV protein Vif interacts with human proteins to protect the virus from antiviral defenses,[333] and characterize the binding pathway for a proline-rich disordered peptide that binds an SH3 domain to pass information in cellular signaling.

Robert Berger's research: The **Berger** group uses DFT to study the relationship between the structure and properties of crystalline materials, primarily for solar energy conversion. Most projects focus on predicting and understanding the effects of structural tunability (via doping, substitution, temperature-controlled distortions, and/or strain) on the electronic band structure and band gap of light-absorbing perovskite compounds. These perovskites include both halide photovoltaics (eg, $CH_3NH_3PbI_3$)[445] and oxide photocatalysts (eg, $SrTiO_3$).[446,447] They use the VASP code, and MERCURY resources will facilitate the computation of larger-unit-celled structures (eg, layered and/or doped perovskite superstructures).

Clyde Daly's research: The **Daly** research group will use computations of vibrational spectroscopy to investigate the dynamics and structure of complex condensed-phase systems,[448–454] and use nonequilibrium MD to investigate nanomaterials. Specific projects include (a) using machine learning techniques to build more accurate maps between QM calculations of vibrational frequencies for single reporters and classical

simulations of their condensed phase dynamics, (b) simulating the spectroscopy of CO_2 and water in mixtures of ionic liquids,[448,449,451,453] (c) describing the sequestration behavior of acyl carrier proteins using Raman spectroscopy of attached alkyl probes,[450] and (d) determining the interaction between biomolecules and nanomaterials using nonequilibrium MD simulations. These projects require a wide range of computing resources and software, so the MERCURY resources are essential.

Wallace Derricotte's research: The **Derricotte** group focuses on studying the effect of noncovalent interactions on reaction mechanisms with a new method that involves decomposing the reaction force using symmetry-adapted perturbation theory (SAPT).[455] They have developed a free open-source Python package, PYREX (PYthon Reaction Energy eXtension), that implements their SAPT reaction force method and numerous other techniques that provide novel insight into the chemical and physical driving forces of chemical reactions (https://github.com/WDerricotte/pyrex). They are investigating a series of antioxidant molecules to quantify the effect of noncovalent interactions between the antioxidant and various reactive oxygen species. This project absolutely requires the MERCURY computing resources.

Jonathan Foley's research: The **Foley** lab leverages multi-scale theoretical and computational approaches, bridging quantum mechanical and electrodynamics methods, to study fundamental aspects of light-matter interactions and to enable the design of materials to control light, heat, and chemical reactivity. Key scientific outcomes so far include the discovery of an emergent optical phenomenon in composite nanoparticles known as "scattering-mediated absorption",[456–458] and the development of an open-source software package, WPTherml, for designing materials for harnessing heat.[459,460]

Kedan He's research: The **He** group has expertise in electronic structure methods,[461] and is currently developing machine learning algorithms for fast mining to extrapolate meaningful information from databases of chemical structures to discover and design molecules with important biological properties, such as (a) ligand and structure-based virtual screening to discover novel EGFR inhibitors, and (b) virtual screening and identification of potential illegal synthetic cathinones.

Heidi Hendrickson's Research: The **Hendrickson** lab uses computational methods to (a) utilize and develop multiscale computational approaches (DFT, QM/MM, MD) to model charge transfer and transport properties in semiconducting polymeric materials,[277] (b) utilize computational methods (protein-ligand docking, QM/MM, MD, protein network analysis) to identify and characterize protein-ligand interactions in G-protein coupled receptors,[318] and (c) utilize electronic structure calculations to characterize highly absorbing species in atmospheric brown carbon aerosols.[339]

Casey Londergan's research: The **Londergan** group uses all-atom simulations of proteins with artificial "vibrational probe" functional groups to better understand the experimental data associated with IR and Raman spectra of those probe groups. They conduct well-sampled MD simulations in explicit solvents to understand the protein's overall conformational distribution; then they include the probe groups explicitly and use fragment-potential-based frequency calculations[462] to directly simulate the spectra.

Tyler Luchko's research: The **Luchko** lab uses computational methods to study the solvation of small molecules and biomolecules at the molecular scale. They are actively developing the 3D reference interaction site model (3D-RISM) of molecular solvation,[463] which uses statistical physics to predict the molecular distribution of explicit, all-atom solvent models around solute molecules and calculate the solvation thermodynamics from these distributions.[464] Using 3D-RISM, they can predict properties of the solute molecules, such as solvation free energy, enthalpy and entropy,[465] hydrophobicity,[466] protein-drug binding affinities,[467] and the distribution of water and ions around solutes.[468–471]

Lindsey Madison's research: The **Madison** group studies vibrational motions of clathrate hydrates, a naturally forming crystalline phase of water characterized by the presence of nonpolar, small molecules such as carbon dioxide or methane.[472,473] Better understanding of this material can advance knowledge about the role clathrate hydrates play in global climate change,[474] the unintentional and disastrous formation in pipelines,[475,476] and their relevance in astrochemical reactions.[477] More fundamentally, clathrate hydrates are a unique host-guest system because the relatively weak intermolecular forces that hold the lattice together result in an extremely flexible host.[478–480] The group studies the vibrational wave function of these materials to predict the complete vibrational spectrum and compare them to classical MD simulations,[480,481] as well as electronic structure calculations of small and medium-sized clusters.[482–485]

Simbarashe Nkomo's research: The **Nkomo** research group,[486–489] working in collaboration with an experimental organic synthesis group, uses computational methods to study the stability properties of cyclobutadiene derivatives and uses the information to propose synthetic routes for highly conjugated target molecules such as 10,11diphenylcyclobuta[5,6]pyrazino[2,3f][1,10]phenanthroline.

Anton Oliynyk's research: The **Oliynyk** group studies intermetallic compounds and combines machine learning methods with experimental research.[490–495] They study the inorganic chemistry of intermetallic materials with focus on energy-converting materials and mechanical properties such as hardness and wear resistance.[493] The materials are synthesized directly from elements by high-temperature methods, including arc-melting and sintering. A cutting-edge machine learning-driven approach[492] is utilized to guide the discoveries of novel materials and screen chemical space for potential compounds, and computational methods are used for structure prediction from first principles.

Caitlin Scott's research: The **Scott** lab[496–501] uses computational tools to predict the structures of G-protein-coupled receptors (GPCRs) at various stages of activation for structure-based drug design.[502–504] Approximately one-third of drugs approved by the FDA target this family of proteins.[505] Unfortunately, GPCRs are quite flexible and dynamic, and despite the recent advances in protein crystallography, the conformations of GPCRs at various activation states remain unknown. The group will use the MERCURY computational resources to run MD simulations of the

proteins in a solvated and neutralized lipid bilayer at room temperature and pressure to simulate the proteins in a realistic cellular environment to determine the stability of protein-drug complexes.

Patricia Soto's research: The **Soto** group focuses on deciphering the pathological folding behavior of prion proteins, the main component of the infectious prion agent responsible for prion disorders,[506] using computational biophysics techniques. The conformational conversion of the cellular form of the prion protein PrP^{C} to the misfolded and aggregated isoform PrP^{Sc} is the key pathological event in prion diseases.[507] MERCURY's facilities are instrumental to examining the hypothesis that prion protein-RNA molecule interactions modulate the protein dimerization mechanism in a protein-sequence-dependent manner. To this goal, they will implement a multi-scale computational protocol that benefits from their demonstrated experience in identifying structural dynamics features of prion protein peptides[508] and prion protein in the bulk.[509]

5 | CONCLUSIONS AND EDUCATIONAL IMPACT

We believe that mentoring students in meaningful research projects is a valuable and integral part of being a research-active chemist at an undergraduate institution, and we choose careers at PUIs with the intention of focusing our energy on undergraduate student involvement. Our objective upon forming the MERCURY consortium was to help our undergraduate research programs to flourish, and this has indeed occurred. To highlight one measure of success, from 2001 to 2019, we have published an average of 1.7 papers/year/faculty, which is 3.4 times more than the usual productivity of a faculty member at a PUI.[46] From 2001 through the summer of 2019, the MERCURY faculty published 361 peer-reviewed products, including 2 in *Chemical Society Reviews*, 1 in *Chemical Reviews*, 1 in *Nature Reviews Chemistry*, 3 in *Science*, 2 in *Nature*, 3 in *Angewandte Chemie International Edition*, 13 in *JACS*, and 3 in *PNAS*. We have demonstrated that the MERCURY consortium provides an ideal environment for providing research experiences for undergraduates. We are a productive and synergistic consortium with a diverse group of students and faculty; two-thirds of our students over the past two decades were female or students of color. Every time we expand our consortium, we further increase the number of high-quality undergraduate research experiences and enhance diversity in the chemical sciences workforce.

When we started in 2001, our goals were twofold: (a) to acquire a supercomputer that would allow us to train undergraduates in computational chemistry, and (b) to achieve excellent research results. Our diverse research interests required a computational system that would allow us to run quantum and MD simulations with a variety of different software. Our students were excited and inspired by participating in cutting-edge research projects, so that many of them matriculated to graduate work, or became citizens with a keener understanding of what research is and how it works. The technical support we hired as part of the first grant was essential for maintaining our shared computer system and ensuring that we split computer time fairly. We had diversity in mind from the very beginning, both with the selection of the initial faculty in the consortium and in the mindset of the faculty. Our idea was to form a northeastern consortium, where we could easily share ideas at an end of summer conference, and learn and network with scientists at research universities, industry, and government laboratories. After our first grant, it dawned on us that we could be national in scope, and as we added resources with subsequent NSF MRI grants, we expanded nationally.

We realized that the conference was the single most brilliant initiative we had started, and we found money to support it after the first grant period. From the very beginning, we opened the meeting to everyone from any institution, with the stipulation that only undergraduates present posters during the poster session. The mentoring, networking, and inspiration that happens at the annual conferences is a must for our faculty, and faculty who stop attending conferences with their students generally realize it is time to step out of MERCURY. Faculty who we invited to join MERCURY are motivated to have active and diverse research groups, and we ask their deans and provosts to make sure they have funding to attend our meeting. As time went on, **Shields** became better at advising speakers on how to structure their talks for the most benefit to the PUI audience. Our undergraduates moved from just listening in the early days, to listening and asking questions in later conferences. A key component of the meetings' success is the undergraduate poster session, where experts are present to talk with students at their posters and with the PUI faculty who attend the meeting, increasing the value of the meeting for everyone in attendance. In addition, the meeting provides a dedicated time for the MERCURY faculty to mentor and advise each other. Students from any one particular research group are always amazed to learn how their own work is put into context and are stimulated by the problems that other groups are trying to solve, as well as their methods for trying to solve them. STEM conferences have historically suffered from a lack of female and minorityfaculty representation, and our efforts to recruit diverse speakers is another key part of the conference as students have visible role models, both from the invited speakers and from the other PUI faculty in attendance. We have had more than 1600 attendees at the 18 MERCURY conferences, with 111 invited speakers, 61 of whom have been female and/or faculty of color. One of the advantages of NSF funding is that the required annual evaluations focus the entire MERCURY faculty on student outcomes and research results. Faculty returning from the conference to their home institutions are motivated as they start the next academic year. Overall, our main goals have not changed and we have been thrilled with our joint success.

The MERCURY consortium has been an outstanding program that has contributed greatly to the development of scientifically trained undergraduates, with a particular focus on diversity and inclusion.[1] Without double-counting female students of color, 75% of our undergraduate research students have been female or students of color. About half of our alumni attend graduate school to obtain advanced degrees in STEM fields, and approximately two-thirds are female and/or students of color. Students mentored by MERCURY faculty have been recognized with

more than 50 national awards, including 1 Rhodes Scholarship, 10 Fulbright Fellowships, 21 Goldwater Fellowships, 2 Gates Cambridge Scholarships, and more than 20 national graduate fellowships (NIH, NASA, NDSEG, NSF). For more information, see https://mercuryconsortium.org.

ACKNOWLEDGEMENTS

This MERCURY consortium has been supported by grants CHE-0116435, CHE-0521063, CHE-0821581, CHE-1229354, and CHE-1626238, 1662030 from the National Science Foundation. GCS acknowledges support from NSF CHE-172151 and CHE-1903871. We thank all the speakers who have given their time to support our conference.

AUTHOR CONTRIBUTIONS

George Shields: Conceptualization; data curation; formal analysis; funding acquisition; investigation; methodology; project administration; resources; validation; writing-original draft; writing-review and editing.

ORCID

George C. Shields https://orcid.org/0000-0003-1287-8585

REFERENCES

[1] G. C. Shields, *Scholarsh. Pract. Undergrad. Res.* **2019**, *2019*, 5.
[2] L. R. Pratt, R. A. LaViolette, M. A. Gomez, M. E. Gentile, *J. Phys. Chem. B* **2001**, *105*, 11662.
[3] P. Grabowski, D. Riccardi, M. A. Gomez, D. Asthagiri, L. R. Pratt, *J. Phys. Chem. A* **2002**, *106*, 9145.
[4] D. Asthagiri, L. R. Pratt, J. D. Kress, M. A. Gomez, *Chem. Phys. Lett.* **2003**, *380*, 530.
[5] D. Asthagiri, L. R. Pratt, J. D. Kress, M. A. Gomez, *Proc. Natl. Acad. Sci. U. S. A.* **2004**, *101*, 7229.
[6] Greathouse, J. A.; Bemis, G.; Palaban, R. T., *Proc. Int. Symp. Water-Rock Interaction*, **2001**, Vol. 1, p. 173.
[7] J. A. Greathouse, R. J. O'Brien, G. Bemis, R. T. Pabalan, *J. Phys. Chem. B* **2002**, *106*, 1646.
[8] J. A. Greathouse, E. W. Storm, *Mol. Simul.* **2002**, *28*, 633.
[9] O. F. Zaidan, J. A. Greathouse, R. T. Pabalan, *Geochim. Cosmochim. Acta* **2002**, *66*, A868.
[10] O. F. Zaidan, J. A. Greathouse, R. T. Pabalan, *Clays Clay Miner.* **2003**, *51*, 372.
[11] J. A. Greathouse, R. T. Cygan, *Phys. Chem. Chem. Phys.* **2005**, *7*, 3580.
[12] J. A. Greathouse, H. R. Stellalevinsohn, M. A. Denecke, A. Bauer, R. T. Pabalan, *Clays Clay Miner.* **2005**, *53*, 278.
[13] C. Parish, R. Lombardi, K. Sinclair, E. Smith, A. Goldberg, M. Rappleye, M. Dure, *J. Mol. Graphics Modell.* **2002**, *21*, 129.
[14] C. A. Parish, M. Zeldin, J. Pratt, *J. Inorg. Organomet. Polym.* **2002**, *12*, 31.
[15] H. Castillo, M. Yarger, M. Rappleye, C. Parish, *THEOCHEM J. Mol. Struct.* **2004**, *710*, 73.
[16] M. Macaluso, C. A. Parish, R. Hoffmann, L. T. Scott, *J. Organomet. Chem.* **2004**, *69*, 8093.
[17] C. A. Parish, M. Yarger, K. Sinclair, M. Dure, A. Goldberg, *J. Med. Chem.* **2004**, *47*, 4838.
[18] S. Feldgus, G. C. Shields, *Chem. Phys. Lett.* **2001**, *347*, 505.
[19] M. D. Liptak, G. C. Shields, *Int. J. Quantum Chem.* **2001**, *85*, 727.
[20] M. D. Liptak, G. C. Shields, *J. Am. Chem. Soc.* **2001**, *123*, 7314.
[21] E. K. Pokon, M. D. Liptak, S. Feldgus, G. C. Shields, *J. Phys. Chem. A* **2001**, *105*, 10483.
[22] E. C. Sherer, S. J. Bono, G. C. Shields, *J. Phys. Chem. B* **2001**, *105*, 8445.
[23] A. M. Toth, M. D. Liptak, D. L. Phillips, G. C. Shields, *J. Chem. Phys.* **2001**, *114*, 4595.
[24] M. D. Liptak, K. C. Gross, P. G. Seybold, S. Feldgus, G. C. Shields, *J. Am. Chem. Soc.* **2002**, *124*, 6421.
[25] M. E. Dunn, E. K. Pokon, G. C. Shields, *Int. J. Quantum Chem.* **2004**, *100*, 1065.
[26] M. E. Dunn, E. K. Pokon, G. C. Shields, *J. Am. Chem. Soc.* **2004**, *126*, 2647.
[27] M. W. Palascak, G. C. Shields, *J. Phys. Chem. A* **2004**, *108*, 3692.
[28] M. B. Day, K. N. Kirschner, G. C. Shields, *Int. J. Quantum Chem.* **2005**, *102*, 565.
[29] F. C. Pickard, E. K. Pokon, M. D. Liptak, G. C. Shields, *J. Chem. Phys.* **2005**, *122*, 024302.
[30] E. Stewart, R. L. Shields, R. S. Taylor, *J. Phys. Chem. B* **2003**, *107*, 2333.
[31] R. S. Taylor, R. L. Shields, *J. Chem. Phys.* **2003**, *119*, 12569.
[32] O. F. Speer, B. C. Wengerter, R. S. Taylor, *J. Chem. Educ.* **2004**, *81*, 1330.
[33] D. L. Cullen, L. V. Desai, J. A. Shelnutt, M. Zimmer, *Struct. Chem.* **2001**, *12*, 127.
[34] M. C. Chen, C. R. Lambert, J. D. Urgitis, M. Zimmer, *Chem. Phys.* **2001**, *270*, 157.
[35] A. Warren, M. Zimmer, *J. Mol. Graphics Modell.* **2001**, *19*, 297.
[36] M. Donnelly, F. Fedeles, M. Wirstam, P. E. Siegbahn, M. Zimmer, *J. Am. Chem. Soc.* **2001**, *123*, 4679.
[37] F. Fedeles, M. Zimmer, *Inorg. Chem.* **2001**, *40*, 1557.
[38] M. Zimmer, *Coord. Chem. Rev.* **2001**, *212*, 133.
[39] T. V. Davis, M. S. Zaveer, M. Zimmer, *J. Chem. Educ.* **2002**, *79*, 1278.
[40] L. N. Todd, M. Zimmer, *Inorg. Chem.* **2002**, *41*, 6831.
[41] M. Zimmer, *Chem. Rev.* **2002**, *102*, 759.
[42] M. S. Zaveer, M. Zimmer, *Bioorg. Med. Chem. Lett.* **2003**, *13*, 3919.
[43] N. Y. A. Baffour-Awuah, M. Zimmer, *Chem. Phys.* **2004**, *303*, 7.
[44] H. De Bari, M. Zimmer, *Inorg. Chem.* **2004**, *43*, 3344.
[45] L. V. Desai, M. Zimmer, *Dalton Trans.* **2004**, *6*, 872.

[46] *Academic Excellence*: *The Sourcebook*, Research Corporation, **2001**.
[47] D. Gao, P. Svoronos, P. Wong, D. Maddalena, J. Hwang, H. Walker, *Phys. Chem. A* **2005**, *109*, 10776.
[48] W. V. Glassey, *Surf. Sci.* **2006**, *600*, 173.
[49] W. V. Glassey, *J. Chem. Educ.* **2006**, *83*, 327.
[50] M. A. Gomez, M. A. Griffin, S. Jindal, K. D. Rule, V. R. Cooper, *J. Chem. Phys* **2005**, *123*, 094703.
[51] M. A. Gomez, P. Peart, *J. Chem. Phys* **2006**, *125*, 034105.
[52] M. A. Gomez, S. Jindal, K. M. Fletcher, L. S. Foster, N. D. A. Addo, D. Valentin, C. Ghenoiu, A. Hamilton, *J. Chem. Phys* **2007**, *126*, 194701.
[53] M. A. Gomez, L. R. Pratt, J. D. Kress, D. Asthagiri, *Surf. Sci.* **2007**, *601*, 1608.
[54] N. W. Polaske, A. L. Wood, M. R. Campbell, M. C. Nagan, L. M. Pollak, *Starch-Starke* **2005**, *57*, 118.
[55] S. Hati, B. Ziervogel, J. SternJohn, F. C. Wong, M. C. Nagan, A. E. Rosen, P. G. Siliciano, J. W. Chihade, K. Musier-Forsyth, *J. Biol. Chem.* **2006**, *281*, 27862.
[56] N. E. McCrate, M. E. Varner, K. I. Kim, M. C. Nagan, *Nucleic Acids Res.* **2006**, *34*, 5361.
[57] K. N. Kirschner, A. H. Lewin, J. P. Bowen, *J. Comput. Chem.* **2003**, *24*, 111.
[58] S. D. Hillson, E. Smith, M. Zeldin, C. A. Parish, *J. Phys. Chem. A* **2005**, *109*, 8371.
[59] E. M. Brzostowska, R. Hoffmann, C. A. Parish, *J. Am. Chem. Soc.* **2007**, *129*, 4401.
[60] M. B. Day, K. N. Kirschner, G. C. Shields, *J. Phys. Chem. A* **2005**, *109*, 6773.
[61] J. A. Gomez, A. K. Tucker, T. D. Shepherd, W. H. Thompson, *J. Phys. Chem. B* **2005**, *109*, 17479.
[62] M. D. Liptak, G. C. Shields, *Int. J. Quantum Chem.* **2005**, *105*, 580.
[63] F. C. Pickard, M. E. Dunn, G. C. Shields, *J. Phys. Chem. A* **2005**, *109*, 4905.
[64] C. G. Zhan, S. X. Deng, J. G. Skiba, B. A. Hayes, S. M. Tschampel, G. C. Shields, D. W. Landry, *J. Comput. Chem.* **2005**, *26*, 980.
[65] M. A. Allodi, M. E. Dunn, J. Livada, K. N. Kirschner, G. C. Shields, *J. Phys. Chem. A* **2006**, *110*, 13283.
[66] K. S. Alongi, T. S. Dibble, G. C. Shields, K. N. Kirschner, *J. Phys. Chem. A* **2006**, *110*, 3686.
[67] M. E. Dunn, T. M. Evans, K. N. Kirschner, G. C. Shields, *J. Phys. Chem. A* **2006**, *110*, 303.
[68] F. C. Pickard, D. R. Griffith, S. J. Ferrara, M. D. Liptak, K. N. Kirschner, G. C. Shields, *Int. J. Quantum Chem.* **2006**, *106*, 3122.
[69] F. C. Pickard, R. L. Shepherd, A. E. Gillis, M. E. Dunn, S. Feldgus, K. N. Kirschner, G. C. Shields, M. Manoharan, I. V. Alabugin, *J. Phys. Chem. A* **2006**, *110*, 2517.
[70] K. N. Kirschner, G. M. Hartt, T. M. Evans, G. C. Shields, *J. Chem. Phys* **2007**, *126*, 154320.
[71] K. N. Kirschner, K. W. Lexa, A. M. Salisburg, K. A. Alser, L. Joseph, T. T. Andersen, J. A. Bennett, H. I. Jacobson, G. C. Shields, *J. Am. Chem. Soc.* **2007**, *129*, 6263.
[72] K. W. Lexa, K. A. Alser, A. M. Salisburg, D. J. Ellens, L. Hernandez, S. J. Bono, H. C. Michael, J. R. Derby, J. G. Skiba, S. Feldgus, K. N. Kirschner, G. C. Shields, *Int. J. Quantum Chem.* **2007**, *107*, 3001.
[73] N. Y. Baffour-Awuah, F. Fedeles, M. Zimmer, *Chem. Phys.* **2005**, *310*, 25.
[74] N. Y. Baffour-Awuah, S. Maddalo, M. Zimmer, *FEBS J.* **2005**, *272*, 22.
[75] B. R. Branchini, T. L. Southworth, M. H. Murtiashaw, S. R. Wilkinson, N. F. Khattak, J. C. Rosenberg, M. Zimmer, *Biochemistry* **2005**, *44*, 1385.
[76] S. L. Maddalo, M. Zimmer, *Photochem. Photobiol.* **2006**, *82*, 367.
[77] C. Mbofana, M. Zimmer, *Inorg. Chem.* **2006**, *45*, 2598.
[78] B. R. Branchini, D. M. Ablamsky, J. M. Rosenman, L. Uzasci, T. L. Southworth, M. Zimmer, *Biochemistry* **2007**, *46*, 13847.
[79] J. Seckute, J. L. Menke, R. J. Emnett, E. V. Patterson, C. J. Cramer, *J. Organomet. Chem.* **2005**, *70*, 8649.
[80] A. N. Jay, K. A. Daniel, E. V. Patterson, *J. Chem. Theory Comput.* **2007**, *3*, 336.
[81] J. L. Menke, E. V. Patterson, *THEOCHEM J. Mol. Struct.* **2007**, *811*, 281.
[82] A. Szczepanska, J. L. Espartero, A. J. Moreno-Vargas, A. T. Carmona, I. Robina, S. Remmert, C. Parish, *J. Organomet. Chem.* **2007**, *72*, 6776.
[83] M. G. Lauer, J. W. Leslie, A. Mynar, S. A. Stamper, A. D. Martinez, A. J. Bray, S. Negassi, K. McDonald, E. Ferraris, A. Muzny, S. McAvoy, C. P. Miller, K. A. Walters, K. C. Russell, E. Wang, B. Nuez, C. Parish, *J. Organic Chem.* **2008**, *73*, 474.
[84] K. J. Donald, R. Hoffmann, *J. Am. Chem. Soc.* **2006**, *128*, 11236.
[85] G. Merino, K. J. Donald, J. S. D'Acchioli, R. Hoffmann, *J. Am. Chem. Soc.* **2007**, *129*, 15295.
[86] E. B. Wang, C. A. Parish, H. Lischka, *J. Chem. Phys.* **2008**, *129*, 044306.
[87] M. Cafiero, L. Adamowicz, *Int. J. Quantum Chem.* **2007**, *107*, 2679.
[88] L. Hofto, M. Hofto, J. Cross, M. Cafiero, *AIP Conf. Proc.* **2007**, *940*, 127.
[89] M. E. Hofto, J. N. Cross, M. Cafiero, *J. Phys. Chem. B* **2007**, *111*, 9651.
[90] M. E. Hofto, A. Godfrey-Kittle, M. Cafiero, *J. Mol. Struct. THEOCHEM* **2007**, *809*, 125.
[91] K. Van Sickle, L. M. Culberson, J. L. Holzmacher, M. Cafiero, *Int. J. Quantum Chem.* **2007**, *107*, 1523.
[92] M. Pavanello, M. Cafiero, S. Bubin, L. Adamowicz, *Int. J. Quantum Chem.* **2008**, *108*, 2291.
[93] E. Cerpa, F. J. Tenorio, M. Contreras, M. Villanueva, H. I. Beltran, T. Heine, K. J. Donald, G. Merino, *Organometallics* **2008**, *27*, 827.
[94] R. Jambor, B. Kašná, K. N. Kirschner, M. Schürmann, K. Jurkschat, *Angew. Chem. Int. Ed.* **2008**, *47*, 1650.
[95] K. N. Kirschner, A. B. Yongye, S. M. Tschampel, J. González-Outeiriño, C. R. Daniels, B. L. Foley, R. J. Woods, *J. Comput. Chem.* **2008**, *29*, 622.
[96] H. Zhong, K. N. Kirschner, M. Lee, J. P. Bowen, *Bioorg. Med. Chem. Lett.* **2008**, *18*, 542.
[97] N. P. Lemay, A. L. Morgan, E. J. Archer, L. A. Dickson, C. M. Megley, M. Zimmer, *Chem. Phys.* **2008**, *348*, 152.
[98] C. M. Megley, L. A. Dickson, S. L. Maddalo, G. J. Chandler, M. Zimmer, *J. Phys. Chem. B* **2008**, *113*, 302.
[99] M. E. Dunn, G. C. Shields, K. Takahashi, R. T. Skodje, V. Vaida, *J. Phys. Chem. A* **2008**, *112*, 10226.
[100] G. M. Hartt, G. C. Shields, K. N. Kirschner, *J. Phys. Chem. A* **2008**, *112*, 4490.
[101] E. C. Sherer, K. N. Kirschner, F. C. Pickard, C. Rein, S. Feldgus, G. C. Shields, *J. Phys. Chem. B* **2008**, *112*, 16917.
[102] G. C. Shields, K. N. Kirschner, *Synth. React. Inorg. Met. Org. Nano-Met. Chem.* **2008**, *38*, 32.
[103] M. Zimmer, *Coord. Chem. Rev.* **2009**, *253*, 817.
[104] M. Zimmer, *Chem. Soc. Rev.* **2009**, *38*, 2823.
[105] S. Remmert, H. Hollis, C. A. Parish, *Bioorg. Med. Chem.* **2009**, *17*, 1251.

[106] S. Remmert, C. Parish, *J. Comput. Chem.* **2009**, *30*, 992.
[107] L. C. Joseph, J. A. Bennett, K. N. Kirschner, G. C. Shields, J. Hughes, N. Lostritto, H. I. Jacobson, T. T. Andersen, *J. Pept. Sci.* **2009**, *15*, 319.
[108] A. M. Salisburg, A. L. Deline, K. W. Lexa, G. C. Shields, K. N. Kirschner, *J. Comput. Chem.* **2009**, *30*, 910.
[109] G. C. Shields, *Future Med. Chem.* **2009**, *1*, 201.
[110] K. A. Daniel, L. A. Kopff, E. V. Patterson, *J. Phys. Org. Chem.* **2008**, *21*, 321.
[111] B. E. Maki, E. V. Patterson, C. J. Cramer, K. A. Scheidt, *Org. Lett.* **2009**, *11*, 3942.
[112] R. A. Seburg, E. V. Patterson, R. J. McMahon, *J. Am. Chem. Soc.* **2009**, *131*, 9442.
[113] L. R. Hofto, C. E. Lee, M. Cafiero, *J. Comput. Chem.* **2009**, *30*, 1111.
[114] E. A. Kee, M. C. Livengood, E. E. Carter, M. McKenna, M. Cafiero, *J. Phys. Chem. B* **2009**, *113*, 14810.
[115] D. L. Irving, C. W. Padgett, D. W. Brenner, *Modell. Simul. Mater. Sci. Eng.* **2009**, *17*, 015004.
[116] C. Padgett, A. Saad, in *Applications of Soft Computing: From Theory to Praxix*, Vol. 58 (Eds: J. Mehnen, M. Köppen, A. Saad, A. Tiwari), Springer Berlin, Heidelberg, Germany **2009**, p. 181.
[117] C. W. Padgett, K. J. Gutt, T. S. Whiteside, *Comput. Mater. Sci.* **2009**, *46*, 491.
[118] E. Cerpa, A. Krapp, R. Flores-Moreno, K. J. Donald, G. Merino, *Chem. Eur. J.* **2009**, *15*, 1985.
[119] S. Craciun, K. J. Donald, *Inorg. Chem.* **2009**, *48*, 5810.
[120] K. J. Donald, M. Hargittai, R. Hoffmann, *Chem. Eur. J.* **2009**, *15*, 158.
[121] L. A. Michael, J. A. Chenault, B. R. Miller, A. M. Knolhoff, M. C. Nagan, *J. Mol. Biol.* **2009**, *392*, 774.
[122] D. Gao, *J. Chem. Educ.* **2009**, *86*, 864.
[123] A. A. Samma, C. K. Johnson, S. A. Song, S. Alvarez, M. Zimmer, *J. Phys. Chem. B* **2010**, *114*, 15362.
[124] K. J. Donald, B. K. Wittmaack, C. Crigger, *J. Phys. Chem. A* **2010**, *114*, 7213.
[125] K. Ghosh, I. Saha, G. Masanta, E. B. Wang, C. A. Parish, *Tetrahedron Lett.* **2010**, *51*, 343.
[126] M. L. Hamm, A. J. Parker, T. W. E. Steele, J. L. Carman, C. A. Parish, *J. Organomet. Chem.* **2010**, *75*, 5661.
[127] E. B. Wang, C. A. Parish, *J. Organomet. Chem.* **2010**, *75*, 1582.
[128] G. Martinez-Guajardo, K. J. Donald, B. K. Wittmaack, M. A. Vazquez, G. Merino, *Org. Lett.* **2010**, *12*, 4058.
[129] K. S. Alongi, G. C. Shields, in *Annual Reports in Computational Chemistry*, Vol. 6, 6 (Ed: R. A. Wheeler), Elsevier Science Bv, Amsterdam, the Netherlands **2010**, p. 113.
[130] T. E. Morrell, G. C. Shields, *J. Phys. Chem. A* **2010**, *114*, 4266.
[131] R. M. Shields, B. Temelso, K. A. Archer, T. E. Morrell, G. C. Shields, *J. Phys. Chem. A* **2010**, *114*, 11725.
[132] M. A. Gomez, M. Chunduru, L. Chigweshe, K. M. Fletcher, *J. Chem. Phys.* **2010**, *133*, 7.
[133] M. A. Gomez, M. Chunduru, L. Chigweshe, L. Foster, S. J. Fensin, K. M. Fletcher, L. E. Fernandez, *J. Chem. Phys.* **2010**, *132*, 8.
[134] H. Utkov, M. Livengood, M. Cafiero, *Annual Reports in Computational Chemistry*, Vol. 6, Elsevier, Oxford **2010**, p. 97.
[135] K. Van Sickle, M. C. Shroyer, M. Cafiero, *THEOCHEM J. Mol. Struct.* **2010**, *941*, 78.
[136] J. C. Sung, A. W. Van Wynsberghe, R. E. Amaro, W. W. Li, J. A. McCammon, *J. Am. Chem. Soc.* **2010**, *132*, 2883.
[137] A. W. Van Wynsberghe, Q. Cui, *Structure* **2010**, *18*, 281.
[138] J. W. Crill, X. Ji, D. L. Irving, D. W. Brenner, C. W. Padgett, *Modell. Simul. Mater. Sci. Eng.* **2010**, *18*, 034001.
[139] D. A. Nivens, C. W. Padgett, J. M. Chase, K. J. Verges, D. S. Jamieson, *J. Chem. Educ.* **2010**, *87*, 1089.
[140] T. S. Whiteside, M. A. Priest, C. W. Padgett, *Thermochim. Acta* **2010**, *510*, 17.
[141] J. L. Menke, E. V. Patterson, R. J. McMahon, *J. Phys. Chem. A* **2010**, *114*, 6431.
[142] L. M. Tvedte, K. L. Smith, E. V. Patterson, R. G. Baughman, *Acta Crystallogr. Sect. C-Cryst. Struct. Commun.* **2010**, *66*, O101.
[143] B. Temelso, K. A. Archer, G. C. Shields, *J. Phys. Chem. A* **2011**, *115*, 12034.
[144] B. Temelso, G. C. Shields, *J. Chem. Theory Comput.* **2011**, *7*, 2804.
[145] W. J. H. Ong, S. Alvarez, I. E. Leroux, R. S. Shahid, A. A. Samma, P. Peshkepija, A. L. Morgan, S. Mulcahy, M. Zimmer, *Mol. Biosyst.* **2011**, *7*, 984.
[146] H. E. Utkov, A. M. Price, M. Cafiero, *Comput. Theor. Chem.* **2011**, *967*, 171.
[147] W. Sinko, C. de Oliveira, S. Williams, A. Van Wynsberghe, J. D. Durrant, R. Cao, E. Oldfield, J. A. McCammon, *Chem. Biol. Drug Des.* **2011**, *77*, 412.
[148] S. E. Tsutakawa, A. W. Van Wynsberghe, B. D. Freudenthal, C. P. Weinacht, L. Gakhar, M. T. Washington, Z. H. Zhuang, J. A. Tainer, I. Ivanov, *Proc. Natl. Acad. Sci. U. S. A.* **2011**, *108*, 17672.
[149] C. R. Durham, J. M. Chase, D. A. Nivens, W. H. Baird, C. W. Padgett, *J. Chem. Educ.* **2011**, *88*, 819.
[150] M. A. Priest, L. W. Padgett, C. W. Padgett, *J. Chem. Educ.* **2011**, *88*, 983.
[151] K. J. Donald, M. Bober, *Chem.-Eur. J.* **2011**, *17*, 1936.
[152] G. Martinez-Guajardo, K. J. Donald, B. K. Wittmaack, M. A. Vazquez, G. Merino, *Org. Lett.* **2011**, *13*, 172.
[153] N. Perez-Peralta, M. Contreras, W. Tiznado, J. Stewart, K. J. Donald, G. Merino, *Phys. Chem. Chem. Phys.* **2011**, *13*, 12975.
[154] B. K. Wittmaack, C. Crigger, M. Guarino, K. J. Donald, *J. Phys. Chem. A* **2011**, *115*, 8743.
[155] R. M. Mueller, M. A. North, C. Yang, S. Hati, S. Bhattacharyya, *J. Phys. Chem. B* **2011**, *115*, 3632.
[156] X. Song, C. A. Parish, *J. Phys. Chem. A* **2011**, *115*, 14546.
[157] K. Ghosh, T. Sen, A. Patra, J. S. Mancini, J. M. Cook, C. A. Parish, *J. Phys. Chem. B* **2011**, *115*, 8597.
[158] X. L. Song, C. A. Parish, *J. Phys. Chem. A* **2011**, *115*, 2882.
[159] D. E. Husar, B. Temelso, A. L. Ashworth, G. C. Shields, *J. Phys. Chem. A* **2012**, *116*, 5151.
[160] C. Pérez, M. T. Muckle, D. P. Zaleski, N. A. Seifert, B. Temelso, G. C. Shields, Z. Kisiel, B. H. Pate, *Science* **2012**, *336*, 897.
[161] B. Temelso, T. E. Morrell, R. M. Shields, M. A. Allodi, E. K. Wood, K. N. Kirschner, T. C. Castonguay, K. A. Archer, G. C. Shields, *J. Phys. Chem. A* **2012**, *116*, 2209.
[162] B. Temelso, T. N. Phan, G. C. Shields, *J. Phys. Chem. A* **2012**, *116*, 9745.
[163] J. S. Klimavicz, J. F. Mike, A. Bhuwalka, A. L. Tomlinson, M. Jeffries-El, *Pure Appl. Chem.* **2012**, *84*, 991.
[164] B. M. Kobilka, A. V. Dubrovskiy, M. D. Ewan, A. L. Tomlinson, R. C. Larock, S. Chaudhary, M. Jeffries-El, *Chem. Commun.* **2012**, *48*, 8919.
[165] J. Baltrusaitis, E. V. Patterson, C. Hatch, *J. Phys. Chem. A* **2012**, *116*, 9331.
[166] T. D. Shepherd, M. A. Koc, V. Molinero, *J. Phys. Chem. C* **2012**, *116*, 12172.

[167] M. A. Gomez, D. Shepardson, L. T. Nguyen, T. Kehinde, *Solid State Ionics* **2012**, *213*, 8.
[168] S. Q. Fisher, M. Weck, J. E. Landers, J. Emrich, S. A. Middleton, J. Cox, L. Gentile, C. A. Parish, *J. Struct. Biol.* **2012**, *177*, 602.
[169] A. J. Parker, J. Stewart, K. J. Donald, C. A. Parish, *J. Am. Chem. Soc.* **2012**, *134*, 5165.
[170] X. Song, M. G. Fanelli, J. M. Cook, F. Bai, C. A. Parish, *J. Phys. Chem. A* **2012**, *116*, 4934.
[171] A. C. Castro, G. Martinez-Guajardo, T. Johnson, J. M. Ugalde, Y.-B. Wu, J. M. Mercero, T. Heine, K. J. Donald, G. Merino, *Phys. Chem. Chem. Phys.* **2012**, *14*, 14764.
[172] C. Crigger, B. K. Wittmaack, M. Tawfik, G. Merino, K. J. Donald, *Phys. Chem. Chem. Phys.* **2012**, *14*, 14775.
[173] E. Osorio, V. Villalobos, J. C. Santos, K. J. Donald, G. Merino, W. Tiznado, *Chem. Phys. Lett.* **2012**, *522*, 67.
[174] B. Sanford, B. Cao, J. M. Johnson, K. Zimmerman, A. M. Strom, R. M. Mueller, S. Bhattacharyya, K. Musier-Forsyth, S. Hati, *Biochemistry* **2012**, *51*, 2146.
[175] B. Li, R. Shahid, P. Peshkepija, M. Zimmer, *Chem. Phys.* **2012**, *392*, 143.
[176] M. Zimmer, *What Does it Take to Improve Existing Fluorescent Proteins for in vivo Imaging Applications? Methods in Molecular Biology*, Vol. 872 Springer, Clifton, NJ **2012**, p. 235.
[177] R. R. Knauf, H. M. Helminiak, J. P. Wrass, T. M. Gallert, J. A. Phillips, *J. Phys. Org. Chem.* **2012**, *25*, 493.
[178] C. Pérez, S. Lobsiger, N. A. Seifert, D. P. Zaleski, B. Temelso, G. C. Shields, Z. Kisiel, B. H. Pate, *Chem. Phys. Lett.* **2013**, *571*, 1.
[179] G. C. Shields, P. G. Seybold, *Computational Approaches for the Prediction of pK_a Values*, CRC Press, Boca Raton **2013**.
[180] B. Temelso, T. Koddermann, K. N. Kirschner, K. Klein, G. C. Shields, *Comput. Theor. Chem.* **2013**, *1021*, 240.
[181] A. R. Buchberger, S. J. Danforth, K. M. Bloomgren, J. A. Rohde, E. L. Smith, C. C. A. Gardener, J. A. Phillips, *J. Phys. Chem. B* **2013**, *117*, 11687.
[182] G. Murdachaew, M. E. Varner, L. F. Phillips, B. J. Finlayson-Pitts, R. B. Gerber, *Phys. Chem. Chem. Phys.* **2013**, *15*, 204.
[183] H. H. Hu, T. D. Shepherd, *ACM Trans. Comput. Educ.* **2013**, *13*(3), 1.
[184] S. Qu, E. P. Kolodziej, S. A. Long, J. B. Gloer, E. V. Patterson, J. Baltrusaitis, G. D. Jones, P. V. Benchetler, E. A. Cole, K. C. Kimbrough, M. D. Tarnoff, D. M. Cwiertny, *Science* **2013**, *342*, 347.
[185] R. N. Witts, E. C. Hopson, D. E. Koballa, T. A. Van Boening, N. H. Hopkins, E. V. Patterson, M. C. Nagan, *J. Phys. Chem. B* **2013**, *117*, 7489.
[186] R. B. Kinnel, A. W. Van Wynsberghe, I. J. Rosenstein, K. S. Brewer, M. Cotten, G. C. Shields, C. J. Borton, S. Z. Senior, G. S. Rahn, T. E. Elgren, *Developing and Maintaining a Successful Undergraduate Research Program*, Vol. 1156, American Chemical Society, Washington, DC **2013**, p. 5.
[187] M. A. Gomez, F.-J. Liu, *Solid State Ionics* **2013**, *252*, 40.
[188] M. Contreras, E. Osorio, F. Ferraro, G. Puga, K. J. Donald, J. G. Harrison, G. Merino, W. Tiznado, *Chem.-Eur. J.* **2013**, *19*, 2305.
[189] K. J. Donald, J. Kovac, *Sci. Eng. Ethics* **2013**, *19*, 1229.
[190] K. J. Donald, M. Tawfik, *J. Phys. Chem. A* **2013**, *117*, 14176.
[191] E. Osorio, A. Vasquez, E. Florez, F. Mondragon, K. J. Donald, W. Tiznado, *Phys. Chem. Chem. Phys.* **2013**, *15*, 2222.
[192] B. C. Tlach, A. L. Tomlinson, A. G. Ryno, D. D. Knoble, D. L. Drochner, K. J. Krager, M. Jeffries-El, *J. Organomet. Chem.* **2013**, *78*, 6570.
[193] B. L. Eggimann, V. V. Vostrikov, G. Veglia, J. I. Siepmann, *Theor. Chem. Acc.* **2013**, *132*, 1388.
[194] R. K. Lindsey, J. L. Rafferty, B. L. Eggimann, J. I. Siepmann, M. R. Schure, *J. Chromatogr. A* **2013**, *1287*, 60.
[195] J. M. Johnson, B. L. Sanford, A. M. Strom, S. N. Tadayon, B. P. Lehman, A. M. Zirbes, S. Bhattacharyya, K. Musier-Forsyth, S. Hati, *Biochemistry* **2013**, *52*, 4399.
[196] K. L. Copeland, S. J. Pellock, J. R. Cox, M. L. Cafiero, G. S. Tschumper, *J. Phys. Chem. B* **2013**, *117*, 14001.
[197] K. M. DiGiovanni, A. K. Hatstat, J. Rote, M. Cafiero, *Comput. Theor. Chem.* **2013**, *1007*, 41.
[198] D. J. Bustos, B. Temelso, G. C. Shields, *J. Phys. Chem. A* **2014**, *118*, 7430.
[199] C. Pérez, D. P. Zaleski, N. A. Seifert, B. Temelso, G. C. Shields, Z. Kisiel, B. H. Pate, *Angew. Chem., Int. Ed. Engl.* **2014**, *53*, 14368.
[200] B. Temelso, K. A. Alser, A. Gauthier, A. K. Palmer, G. C. Shields, *J. Phys. Chem. B* **2014**, *118*, 4514.
[201] S. Wenzel, H. Nemec, K. E. Anderson, J. I. Siepmann, *Langmuir* **2014**, *30*, 3086.
[202] P. H. Nguyen, H. West, B. D. Feske, C. W. Padgett, *Int. Sch. Res. Notices* **2014**, *2014*, 12428.
[203] T. S. Whiteside, M. A. Priest, C. W. Padgett, *Int. J. Comput. Mater. Sci. Eng.* **2014**, *3*, 1450014.
[204] T. G. Bartholow, B. L. Sanford, B. Cao, H. L. Schmit, J. M. Johnson, J. Meitzner, S. Bhattacharyya, K. Musier-Forsyth, S. Hati, *Biochemistry* **2014**, *53*, 1059.
[205] A. M. Strom, S. C. Fehling, S. Bhattacharyya, S. Hati, *J. Mol. Model.* **2014**, *20*, 2245.
[206] D. Gao, D. Lang, T. Robinson, *Theor. Chem. Acc.* **2014**, *133*, 1577.
[207] B. C. Tlach, A. L. Tomlinson, K. D. Morgan, C. R. Collins, M. D. Zenner, M. Jeffries-El, *Aust. J. Chem.* **2014**, *67*, 711.
[208] F. Cervantes-Navarro, G. Martinez-Guajardo, E. Osorio, D. Moreno, W. Tiznado, R. Islas, K. J. Donald, G. Merino, *Chem. Commun.* **2014**, *50*, 10680.
[209] R. P. F. Kanters, K. J. Donald, *J. Chem. Theory Comput.* **2014**, *10*, 5729.
[210] M. Tawfik, K. J. Donald, *J. Phys. Chem. A* **2014**, *118*, 10090.
[211] H. M. Helminiak, R. R. Knauf, S. J. Danforth, J. A. Phillips, *J. Phys. Chem. A* **2014**, *118*, 4266.
[212] G. Murdachaew, M. E. Varner, W. E. van der Veer, R. B. Gerber, L. F. Phillips, *J. Chem. Phys* **2014**, *140*, 184702.
[213] J. P. Wrass, D. Sadowsky, K. M. Bloomgren, C. J. Cramer, J. A. Phillips, *Phys. Chem. Chem. Phys.* **2014**, *16*, 16480.
[214] D. Kohrt, J. Crary, M. Zimmer, A. N. Patrick, H. L. Ford, P. W. Hinds, M. J. Grossel, *Cell Cycle* **2014**, *13*, 62.
[215] M. H. Zimmer, B. Li, R. Shahid, P. Peshkepija, M. Zimmer, *Chem. Phys.* **2014**, *429*, 5.
[216] B. L. Eggimann, A. J. Sunnarborg, H. D. Stern, A. P. Bliss, J. I. Siepmann, *Mol. Simul.* **2014**, *40*, 101.
[217] B. R. Miller III., C. A. Parish, E. Y. Wu, *PLoS Comput. Biol.* **2014**, *10*, e1003961.
[218] B. R. Miller III., L. S. Beese, C. A. Parish, E. Y. Wu, *Structure* **2015**, *23*, 1609.
[219] J. T. Muya, A. Ceulemans, G. Gopakumar, C. A. Parish, *J. Phys. Chem. A* **2015**, *119*, 4237.
[220] E. Y. Wu, A. R. Walsh, E. C. Materne, E. P. Hiltner, B. Zielinski, B. R. Miller III., L. Mawby, E. Modeste, C. A. Parish, W. M. Barnes, M. B. Kermekchiev, *Biochemistry* **2015**, *54*, 881.
[221] P. G. Seybold, G. C. Shields, *Wiley Interdiscip. Rev. Comput. Mol. Sci.* **2015**, *5*, 290.
[222] J. S. Swan, P. M. Findeis, S. Hilton, K. M. Lebold, B. Temelso, G. C. Shields, *Int. J. Mass Spectrom.* **2015**, *381*, 25.
[223] B. Temelso, C. R. Renner, G. C. Shields, *J. Chem. Theory Comput.* **2015**, *11*, 1439.

[224] W. E. Lynch, C. W. Padgett, B. Quillian, J. Haddock, *Acta Crystallographica Section C-Structural Chemistry* **2015**, *71*, 298.
[225] W. H. Baird, C. W. Padgett, J. A. Secrest, *Phys. Educ.* **2015**, *50*, 224.
[226] D. Ghosh, S. Rhodes, K. Hawkins, D. Winder, A. Atkinson, W. Ming, C. Padgett, J. Orvis, K. Aiken, S. Landge, *New J. Chem.* **2015**, *39*, 295.
[227] B. Quillian, J. Hendricks, M. Trivitayakhun, C. W. Padgett, *Acta Crystallogr. Sect. E Crystallogr. Commun.* **2015**, *71*, 606.
[228] D. J. Bigler, L. W. Peterson, M. Cafiero, *Comput. Theor. Chem.* **2015**, *1068*, 63.
[229] D. J. Bigler, L. W. Peterson, M. Cafiero, *Comput. Theor. Chem.* **2015**, *1051*, 79.
[230] C. G. Bresnahan, C. R. Reinhardt, T. G. Bartholow, J. P. Rumpel, M. North, S. Bhattacharyya, *J. Phys. Chem. A* **2015**, *119*, 172.
[231] K. J. Donald, W. J. Kretz, O. Omorodion, *Chem.-Eur. J.* **2015**, *21*, 16848.
[232] K. J. Donald, J. Stewart, M. Guarino, *Struct. Chem.* **2015**, *26*, 1179.
[233] K. J. Donald, M. Tawfik, B. Buncher, *J. Phys. Chem. A* **2015**, *119*, 3780.
[234] Y. Shao, Z. Gan, E. Epifanovsky, A. T. B. Gilbert, M. Wormit, J. Kussmann, A. W. Lange, A. Behn, J. Deng, X. Feng, D. Ghosh, M. Goldey, P. R. Horn, L. D. Jacobson, I. Kaliman, R. Z. Khaliullin, T. Kus, A. Landau, J. Liu, E. I. Proynov, Y. M. Rhee, R. M. Richard, M. A. Rohrdanz, R. P. Steele, E. J. Sundstrom, H. L. Woodcock III., P. M. Zimmerman, D. Zuev, B. Albrecht, E. Alguire, B. Austin, G. J. O. Beran, Y. A. Bernard, E. Berquist, K. Brandhorst, K. B. Bravaya, S. T. Brown, D. Casanova, C.-M. Chang, Y. Chen, S. H. Chien, K. D. Closser, D. L. Crittenden, M. Diedenhofen, R. A. DiStasio Jr., H. Do, A. D. Dutoi, R. G. Edgar, S. Fatehi, L. Fusti-Molnar, A. Ghysels, A. Golubeva-Zadorozhnaya, J. Gomes, M. W. D. Hanson-Heine, P. H. P. Harbach, A. W. Hauser, E. G. Hohenstein, Z. C. Holden, T.-C. Jagau, H. Ji, B. Kaduk, K. Khistyaev, J. Kim, J. Kim, R. A. King, P. Klunzinger, D. Kosenkov, T. Kowalczyk, C. M. Krauter, K. U. Lao, A. D. Laurent, K. V. Lawler, S. V. Levchenko, C. Y. Lin, F. Liu, E. Livshits, R. C. Lochan, A. Luenser, P. Manohar, S. F. Manzer, S.-P. Mao, N. Mardirossian, A. V. Marenich, S. A. Maurer, N. J. Mayhall, E. Neuscamman, C. M. Oana, R. Olivares-Amaya, D. P. O'Neill, J. A. Parkhill, T. M. Perrine, R. Peverati, A. Prociuk, D. R. Rehn, E. Rosta, N. J. Russ, S. M. Sharada, S. Sharma, D. W. Small, A. Sodt, T. Stein, D. Stueck, Y.-C. Su, A. J. W. Thom, T. Tsuchimochi, V. Vanovschi, L. Vogt, O. Vydrov, T. Wang, M. A. Watson, J. Wenzel, A. White, C. F. Williams, J. Yang, S. Yeganeh, S. R. Yost, Z.-Q. You, I. Y. Zhang, X. Zhang, Y. Zhao, B. R. Brooks, G. K. L. Chan, D. M. Chipman, C. J. Cramer, W. A. Goddard III., M. S. Gordon, W. J. Hehre, A. Klamt, H. F. Schaefer III., M. W. Schmidt, C. D. Sherrill, D. G. Truhlar, A. Warshel, X. Xu, A. Aspuru-Guzik, R. Baer, A. T. Bell, N. A. Besley, J.-D. Chai, A. Dreuw, B. D. Dunietz, T. R. Furlani, S. R. Gwaltney, C.-P. Hsu, Y. Jung, J. Kong, D. S. Lambrecht, W. Liang, C. Ochsenfeld, V. A. Rassolov, L. V. Slipchenko, J. E. Subotnik, T. Van Voorhis, J. M. Herbert, A. I. Krylov, P. M. W. Gill, M. Head-Gordon, *Mol. Phys.* **2015**, *113*, 184.
[235] S. D. P. Flores, G. C. Martin-Noble, R. L. Phillips, J. Schrier, *J. Phys. Chem. C* **2015**, *119*, 21800.
[236] R. A. Krueger, F. G. Haibach, D. L. Fry, M. A. Gomez, *J. Chem. Phys* **2015**, *142*, 154110.
[237] A. H. Nguyen, M. A. Koc, T. D. Shepherd, V. Molinero, *J. Phys. Chem. C* **2015**, *119*, 4104.
[238] J. Schrier, *Introduction to Computational Physical Chemistry*, University Science Books, Mill Valley, CA **2017**.
[239] G. C. Shields, P. G. Seybold, *Computational approaches for the prediction of pKa values*, CRC Press, Boca Raton, FL **2017**.
[240] J. G. Navea, V. H. Grassian, in *Encyclopedia of Interfacial Chemistry: Surface Science and Electrochemistry* (Eds: K. Wandelt, K. Kolasinski), Elsevier, Amsterdam, the Netherlands **2017**.
[241] G. C. Shields, D. A. Gajdosik-Nivens, T. Ness, in *Educational and Outreach Projects from the Cottrell Scholars Collaborative: Undergraduate and Graduate Education*, Vol. 1, 1248 (Eds: R. Waterman, A. Feig American Chemical Society, Washington, DC) **2017**, p. 107.
[242] D. Rovnyak, G. C. Shields, in *Credit Where Credit Is Due: Respecting Authorship and Intellectual Property*, Vol. 1291 (Eds: P. A. Mabrouk, J. N. Currano American Chemical Society, Washington, DC) **2018**, p. 105.
[243] S. Hati, S. Bhattacharyya, *Best Practices for Supporting and Expanding Undergraduate Research in Chemistry*, Vol. 1275, American Chemical Society, Washington, DC **2018**, p. 119.
[244] L. C. Carter, K. M. Foss, D. L. Mohler, D. L. Wilson, I. Sumner, *Building and Maintaining Award-Winning ACS Student Member Chapters Volume 3*, Vol. 1278, American Chemical Society, Washington, DC **2018**, p. 27.
[245] C. D. Bruce, *Using Computational Methods To Teach Chemical Principles*, Vol. 1312, American Chemical Society, Washington, DC **2019**, p. 11.
[246] J. A. Phillips, *Using Computational Methods To Teach Chemical Principles*, Vol. 1312, American Chemical Society, Washington, DC **2019**, p. 33.
[247] A. R. McDonald, J. P. Hagen, *Using Computational Methods To Teach Chemical Principles*, Vol. 1312, American Chemical Society, Washington, DC **2019**, p. 195.
[248] Y. Kholod, D. Kosenkov, *Using Computational Methods To Teach Chemical Principles*, Vol. 1312, American Chemical Society, Washington, DC **2019**, p. 227.
[249] P. D. F. Adler, R. J. Xu, J. H. Olshansky, M. D. Smith, K. C. Elbert, Y. Yang, G. M. Ferrence, M. Zeller, J. Schrier, A. J. Norquist, *Polyhedron* **2016**, *114*, 184.
[250] J. L. Baker, H. Jafri, *J. Mol. Graphics Modell.* **2016**, *70*, 100.
[251] K. A. Ball, J. R. Johnson, M. K. Lewinski, J. Guatelli, E. Verschueren, N. J. Krogan, M. P. Jacobson, *PLoS Comput. Biol.* **2016**, *12*, e1004898.
[252] J. Baltrusaitis, E. V. Patterson, M. O'Connor, S. Qu, E. P. Kolodziej, D. M. Cwiertny, *Environ. Sci. Technol.* **2016**, *50*, 6753.
[253] J. Borgatta, A. Paskavitz, D. Kim, J. G. Navea, *Environ. Chem.* **2016**, *13*, 902.
[254] I. Chavez, Ramiro, M. Cai, B. Tlach, D. L. Wheeler, R. Kaudal, A. Tsyrenova, A. L. Tomlinson, R. Shinar, J. Shinar, M. Jeffries-EL, *J. Mater. Chem. C* **2016**, *4*, 3765.
[255] H. Chen, M. E. Varner, R. B. Gerber, B. J. Finlayson-Pitts, *J. Phys. Chem. B* **2016**, *120*, 1526.
[256] K. E. Du Pont, A. M. McKenzie, O. Kokhan, I. Sumner, C. E. Berndsen, *Biochemistry* **2016**, *55*, 940.
[257] N. Famularo, Y. Kholod, D. Kosenkov, *J. Chem. Educ.* **2016**, *93*, 175.
[258] M. A. Gomez, D. L. Fry, M. E. Sweet, *J. Korean Ceram. Soc.* **2016**, *53*, 521.
[259] P. K. Gurunathan, A. Acharya, D. Ghosh, D. Kosenkov, I. Kaliman, Y. Shao, A. I. Krylov, L. V. Slipchenko, *J. Phys. Chem. B* **2016**, *120*, 6562.
[260] A. K. Hatstat, M. Morris, L. W. Peterson, M. Cafiero, *Comput. Theor. Chem.* **2016**, *1078*, 146.
[261] G. M. Hocky, J. L. Baker, M. J. Bradley, A. V. Sinitskiy, E. M. De La Cruz, G. A. Voth, *J. Phys. Chem. B* **2016**, *120*, 4558.
[262] Z. Homayoon, S. Pratihar, E. Dratz, R. Snider, R. Spezia, G. L. Barnes, V. Macaluso, A. Martin Somer, W. L. Hase, *J. Phys. Chem. A* **2016**, *120*, 8211.
[263] S. Jalife, L. Liu, S. Pan, J. L. Cabellos, E. Osorio, C. Lu, T. Heine, K. J. Donald, G. Merino, *Nanoscale* **2016**, *8*, 17639.
[264] D. Kosenkov, *J. Comput. Chem.* **2016**, *37*, 1847.
[265] D. Kosenkov, J. Shaw, J. Zuczek, Y. Kholod, *J. Chem. Educ.* **2016**, *93*, 1299.

[266] A. Nourmahnad, M. B. Wenny, M. Zeller, J. Schrier, A. J. Norquist, *J. Solid State Chem.* **2016**, *236*, 215.
[267] O. Omorodion, M. Bober, K. J. Donald, *J. Phys. Chem. A* **2016**, *120*, 8896.
[268] J. A. Phillips, *Theor. Chem. Acc.* **2016**, *136*, 16.
[269] S. Pratihar, G. L. Barnes, W. L. Hase, *Chem. Soc. Rev.* **2016**, *45*, 3595.
[270] S. Pratihar, G. L. Barnes, J. Laskin, W. L. Hase, *J. Phys. Chem. Lett.* **2016**, *7*, 3142.
[271] P. Raccuglia, K. C. Elbert, P. D. F. Adler, C. Falk, M. B. Wenny, A. Mollo, M. Zeller, S. A. Friedler, J. Schrier, A. J. Norquist, *Nature* **2016**, *533*, 73.
[272] J. O. Richardson, C. Perez, S. Lobsiger, A. A. Reid, B. Temelso, G. C. Shields, Z. Kisiel, D. J. Wales, B. H. Pate, S. C. Althorpe, *Science* **2016**, *351*, 1310.
[273] N. M. Weiss, A. W. Waller, J. A. Phillips, *J. Mol. Struct.* **2016**, *1105*, 341.
[274] A. Beane, B. R. Miller, C. A. Parish, *J. Mol. Graphics Modell.* **2017**, *74*, 251.
[275] G. L. Barnes, A. Podczerwinski, *J. Phys. Chem. C* **2017**, *121*, 14628.
[276] H. Bunn, R. M. Soliday, I. Sumner, P. L. Raston, *Astrophys. J.* **2017**, *847*, 67.
[277] S. Chaudhuri, S. Hedstrom, D. D. Mendez-Hernandez, H. P. Hendrickson, K. A. Jung, J. M. Ho, V. S. Batista, *J. Chem. Theory Comput.* **2017**, *13*, 6000.
[278] K. J. Donald, E. Befekadu, S. Prasad, *J. Phys. Chem. A* **2017**, *121*, 8982.
[279] M. A. Gomez, G. Kwan, W. Zhu, M. Chelliah, X. Zuo, A. Eshun, V. Blackmer, T. Huynh, M. Huynh, *Solid State Ionics* **2017**, *304*, 126.
[280] Y. Guo, H. P. Hendrickson, P. E. Videla, Y.-N. Chen, J. Ho, S. Sekharan, V. S. Batista, J. C. Tully, E. C. Y. Yan, *J. Chem. Phys.* **2017**, *146*, 215104.
[281] A. J. Heyert, S. L. Knox, G. E. Lindberg, J. L. Baker, *J. Mol. Liq.* **2017**, *227*, 66.
[282] M. Jafari, A. R. Welden, K. L. Williams, B. Winograd, E. Mulvihill, H. P. Hendrickson, M. Lenard, A. Gottfried, E. Geva, *J. Chem. Educ.* **2017**, *94*, 1896.
[283] B. Kacar, V. Hanson-Smith, Z. R. Adam, N. Boekelheide, *Geobiology* **2017**, *15*, 628.
[284] J. M. Lipchock, H. P. Hendrickson, B. B. Douglas, K. E. Bird, P. S. Ginther, I. Rivalta, N. S. Ten, V. S. Batista, J. P. Loria, *Biochemistry* **2017**, *56*, 96.
[285] S. N. Malkowski, C. F. Dishuck, G. G. Lamanilao, C. P. Embry, C. S. Grubb, M. Cafiero, L. W. Peterson, *Molecules* **2017**, *22*, 1682.
[286] J. G. Navea, E. Richmond, T. Stortini, J. Greenspan, *Langmuir* **2017**, *33*, 10161.
[287] C. Perez, A. L. Steber, A. M. Rijs, B. Temelso, G. C. Shields, J. C. Lopez, Z. Kisiel, M. Schnell, *Phys. Chem. Chem. Phys.* **2017**, *19*, 14214.
[288] J. A. Phillips, S. J. Danforth, N. J. Hora, J. R. Lanska, A. W. Waller, *J. Phys. Chem. A* **2017**, *121*, 9252.
[289] S. Pratihar, X. Ma, Z. Homayoon, G. L. Barnes, W. L. Hase, *J. Am. Chem. Soc.* **2017**, *139*, 3570.
[290] J. Carro, M. Martinez-Julvez, M. Medina, A. T. Martinez, P. Ferreira, *Phys. Chem. Chem. Phys.* **2017**, *19*, 28666.
[291] I. Saha, E. B. Wang, C. A. Parish, K. Ghosh, *ChemistrySelect* **2017**, *2*, 4794.
[292] S. Sarkar, H. P. Hendrickson, D. Lee, F. DeVine, J. Jung, E. Geva, J. Kim, B. D. Dunietz, *J. Phys. Chem. C* **2017**, *121*, 3771.
[293] A. L. Steber, C. Perez, B. Temelso, G. C. Shields, A. M. Rijs, B. H. Pate, Z. Kisiel, M. Schnell, *J. Phys. Chem. Lett.* **2017**, *8*, 5744.
[294] C. A. Taylor, B. R. Miller, C. A. Parish, *J. Mol. Graphics Modell.* **2017**, *75*, 71.
[295] C. A. Taylor, B. R. Miller III., S. S. Shah, C. A. Parish, *Proteins Struct. Funct. Bioinf.* **2017**, *85*, 221.
[296] B. Temelso, J. M. Mabey, T. Kubota, N. Appiah-Padi, G. C. Shields, *J. Chem. Inf. Model.* **2017**, *57*, 1045.
[297] A. K. Vasiliou, H. Hu, T. W. Cowell, J. C. Whitman, J. Porterfield, C. A. Parish, *J. Phys. Chem. A* **2017**, *121*, 7655.
[298] A. W. Waller, N. M. Weiss, D. A. Decato, J. A. Phillips, *J. Mol. Struct.* **2017**, *1130*, 984.
[299] W. Wang, C. Taylor, H. Hu, K. L. Humphries, A. Jaini, M. Kitimet, T. Scott, Z. Stewart, K. J. Ulep, S. Houck, A. Luxon, B. Zhang, B. Miller, C. A. Parish, A. E. Pomerantz, O. C. Mullins, R. N. Zare, *Energy Fuels* **2017**, *31*, 9140.
[300] D. L. Wheeler, L. E. Rainwater, A. R. Green, A. L. Tomlinson, *Phys. Chem. Chem. Phys.* **2017**, *19*, 20251.
[301] R. H. Wilson, S. Zamfir, I. Sumner, *J. Mol. Graphics Modell.* **2017**, *76*, 403.
[302] B. Yao, S. Mandrà, J. O. Curry, S. Shaikhutdinov, H.-J. Freund, J. Schrier, *ACS Appl. Mater. Interfaces* **2017**, *9*, 43061.
[303] A. V. Yeager, J. M. Swails, B. R. Miller, *J. Chem. Theory Comput.* **2017**, *13*, 4624.
[304] D. T. Christiansen, D. L. Wheeler, A. L. Tomlinson, J. R. Reynolds, *Polym. Chem.* **2018**, *9*, 3055.
[305] J. C. Dewar, A. S. Thakur, W. W. Brennessel, M. Cafiero, L. W. Peterson, W. T. Eckenhoff, *Inorg. Chim. Acta* **2018**, *473*, 15.
[306] J. J. Dong, S. Klumpp, *Soft Matter* **2018**, *14*, 1908.
[307] M. H. Esseffar, C. A. Parish, R. Jalal, A. M. Lamsabhi, *J. Phys. Chem. A* **2018**, *122*, 3076.
[308] R. Evans, L. Peterson, M. Cafiero, *Comput. Theor. Chem.* **2018**, *1140*, 145.
[309] D. Frederickson, M. McDonough, G. L. Barnes, *J. Phys. Chem. B* **2018**, *122*, 9549.
[310] N. J. Hora, B. M. Wahl, C. Soares, S. A. Lara, J. R. Lanska, J. A. Phillips, *J. Mol. Struct.* **2018**, *1157*, 679.
[311] H. Hu, B. Zhang, A. Luxon, T. Scott, B. Wang, C. A. Parish, *J. Phys. Chem. A* **2018**, *122*, 3688.
[312] N. H. Hunter, B. C. Bakula, C. D. Bruce, *J. Biomol. Struct. Dyn.* **2018**, *36*, 1893.
[313] Y. Kholod, E. Hoag, K. Muratore, D. Kosenkov, *J. Chem. Educ.* **2018**, *95*, 882.
[314] Y. Kholod, M. DeFilippo, B. Reed, D. Valdez, G. Gillan, D. Kosenkov, *J. Comput. Chem.* **2018**, *39*, 438.
[315] A. Kumar, A. H. Nguyen, R. Okumu, T. D. Shepherd, V. Molinero, *J. Am. Chem. Soc.* **2018**, *140*, 16071.
[316] A. R. Luxon, N. Orms, R. Kanters, A. I. Krylov, C. A. Parish, *J. Phys. Chem. A* **2018**, *122*, 420.
[317] B. Mellis, P. Soto, C. D. Bruce, G. Lacueva, A. M. Wilson, R. Jayasekare, *PLoS One* **2018**, *13*, e0196338.
[318] C. F. A. Negre, U. N. Morzan, H. P. Hendrickson, R. Pal, G. P. Lisi, J. P. Loria, I. Rivalta, J. M. Ho, V. S. Batista, *Proc. Natl. Acad. Sci. U. S. A.* **2018**, *115*, E12201.
[319] M. L. Newkirk, K. J. Rubenstein, J. Y. Kim, C. L. Labrecque, J. Airas, C. A. Taylor, H. D. Evans, Q. McKoy, C. A. Parish, J. A. Pollock, *Biochemistry* **2018**, *57*, 5169.
[320] C. J. Ostaszewski, N. M. Stuart, D. M. B. Lesko, D. Kim, M. J. Lueckheide, J. G. Navea, *J. Phys. Chem. A* **2018**, *122*, 6360.
[321] A. L. Paskavitz, J. Quintana, D. Cangussu, C. Tavera-Montañez, Y. Xiao, S. Ortiz-Miranda, J. G. Navea, T. Padilla-Benavides, *J. Trace Elem. Med. Biol.* **2018**, *49*, 27.
[322] S. Prasad, B. K. Wittmaack, K. J. Donald, *J. Phys. Chem. A* **2018**, *122*, 9065.
[323] C. R. Reinhardt, Q. H. Hu, C. G. Bresnahan, S. Hati, S. Bhattacharyya, *ACS Catal.* **2018**, *8*, 12015.
[324] A. Rodríguez, R. Rodríguez-Fernández, A. Vázquez S, L. Barnes G, J. P. Stewart J, E. Martínez-Núñez, *J. Comput. Chem.* **2018**, *39*, 1922.
[325] J. D. Shaprio, J. C. Sonberg, B. C. Schafer, C. C. Williams, H. R. Ferris, E. W. Reinheimer, A. W. Van Wynsberghe, C. E. Kriley, M. M. Majireck, *Molecules* **2018**, *23*, 413.

[326] B. Temelso, K. L. Klein, J. W. Mabey, C. Perez, B. H. Pate, Z. Kisiel, G. C. Shields, *J. Chem. Theory Comput.* **2018**, *14*, 1141.
[327] B. Temelso, E. F. Morrison, D. L. Speer, B. C. Cao, N. Appiah-Padi, G. Kim, G. C. Shields, *J. Phys. Chem. A* **2018**, *122*, 1612.
[328] V. Vassilev-Galindo, S. Pan, K. J. Donald, G. Merino, *Nat. Rev. Chem.* **2018**, *2*, UNSP 0114
[329] J. Wang, A. S. Jeevarathinam, K. Humphries, A. Jhunjhunwala, F. Chen, A. Hariri, B. R. Miller, J. V. Jokerst, *Bioconjugate Chem.* **2018**, *29*, 3768.
[330] R. J. Xu, J. H. Olshansky, P. D. F. Adler, Y. Huang, M. D. Smith, M. Zeller, J. Schrier, A. J. Norquist, *Mol. Systems Design Eng.* **2018**, *3*, 473.
[331] A. Yeager, K. Humphries, E. Farmer, G. Cline, B. R. Miller, *J. Chem. Inf. Model.* **2018**, *58*, 338.
[332] L. M. Adams, R. J. Andrews, Q. H. Hu, H. L. Schmit, S. Hati, S. Bhattacharyya, *Biophys. J.* **2019**, *117*, 1269.
[333] K. A. Ball, L. M. Chan, D. J. Stanley, E. Tierney, S. Thapa, H. M. Ta, L. Burton, J. M. Binning, M. P. Jacobson, J. D. Gross, *Biophys. J.* **2019**, *116*, 1432.
[334] E. E. Carter, A. J. Heyert, M. De Souza, J. L. Baker, G. E. Lindberg, *Phys. Chem. Chem. Phys.* **2019**, *21*, 17950.
[335] R. Chavez, L. Diodati, D. L. Wheeler, J. Shaw, A. L. Tomlinson, M. Jeffries-El, *J. Phys. Chem. A* **2019**, *123*, 1343.
[336] D. T. Christiansen, A. L. Tomlinson, J. R. Reynolds, *J. Am. Chem. Soc.* **2019**, *141*, 3859.
[337] D. T. Christiansen, S. Ohtani, Y. Chujo, A. L. Tomlinson, J. R. Reynolds, *Chem. Mater.* **2019**, *31*, 6841.
[338] K. J. Donald, S. Gillespie, Z. Shafi, *Tetrahedron* **2019**, *75*, 335.
[339] D. N. Grace, J. R. Sharp, R. E. Holappa, E. N. Lugos, M. B. Sebold, D. R. Griffith, H. P. Hendrickson, M. M. Galloway, *ACS Earth Space Chem.* **2019**, *3*, 2472.
[340] J. R. Greene, K. L. Merrett, A. J. Heyert, L. F. Simmons, C. M. Migliori, K. C. Vogt, R. S. Castro, P. D. Phillips, J. L. Baker, G. E. Lindberg, D. T. Fox, R. E. Del Sesto, A. T. Koppisch, *PLoS One* **2019**, *14*, e0222211.
[341] K. Hull, R. M. Soliday, I. Sumner, P. L. Raston, *J. Chem. Phys.* **2019**, *150*, 057101.
[342] A. K. A. Jaini, L. B. Hughes, M. M. Kitimet, K. J. Ulep, M. C. Leopold, C. A. Parish, *ACS Sensors* **2019**, *4*, 389.
[343] X. Jia, J. L. Dixon, M. Zeller, J. Schrier, A. J. Norquist, *J. Solid State Chem.* **2019**, *273*, 158.
[344] X. Jia, A. Lynch, Y. Huang, M. Danielson, I. Lang'at, A. Milder, A. E. Ruby, H. Wang, S. A. Friedler, A. J. Norquist, J. Schrier, *Nature* **2019**, *573*, 251.
[345] W. M. Jones, A. G. Davis, R. H. Wilson, K. L. Elliott, I. Sumner, *J. Comput. Chem.* **2019**, *40*, 1969.
[346] G. Linden, L. Zhang, F. Pieck, U. Linne, D. Kosenkov, R. Tonner, O. Vázquez, *Angew. Chem., Int. Ed.* **2019**, *58*, 12868.
[347] R. K. Lindsey, B. L. Eggimann, D. R. Stoll, P. W. Carr, M. R. Schure, J. I. Siepmann, *J. Chromatogr. A* **2019**, *1589*, 47.
[348] C. Londergan, J. Schrier, *J. Phys. Chem. A* **2019**, *123*, 3239.
[349] J. C. Lopez, C. Perez, S. Blanco, V. A. Shubert, B. Temelso, G. C. Shields, M. Schnell, *Phys. Chem. Chem. Phys.* **2019**, *21*, 2875.
[350] G. Palermo, K. A. Armacost, M. C. Nagan, *J. Chem. Inf. Model.* **2019**, *59*, 4061.
[351] A. D. Matthews, S. Prasad, N. D. Schley, K. J. Donald, M. W. Johnson, *Inorg. Chem.* **2019**, *58*, 15983.
[352] E. Modeste, L. Mawby, B. Miller, E. Wu, C. A. Parish, *J. Chem. Inf. Model.* **2019**, *59*, 2423.
[353] I. M. Pendleton, G. Cattabriga, Z. Li, M. A. Najeeb, S. A. Friedler, A. J. Norquist, E. M. Chan, J. Schrier, *MRS Commun.* **2019**, *9*, 846.
[354] M. C. Perchik, L. W. Peterson, M. Cafiero, *Comput. Theor. Chem.* **2019**, *1153*, 19.
[355] N. C. Pflug, E. V. Patterson, D. Martinović-Weigelt, E. P. Kolodziej, J. B. Gloer, K. McNeill, D. M. Cwiertny, K. H. Wammer, *J. Organic Chem.* **2019**, *84*, 11366.
[356] K. R. Sabsay, R. T. Lee, L. M. Ravatt, J. P. Oza, A. R. McDonald, *J. Chem. Inf. Model.* **2019**, *59*, 2383.
[357] D. J. Schmucker, S. R. Dunbar, T. D. Shepherd, M. A. Bertucci, *J. Phys. Chem. A* **2019**, *123*, 2537.
[358] T. Scott, R. Nieman, A. Luxon, B. Zhang, H. Lischka, L. Gagliardi, C. A. Parish, *J. Phys. Chem. A* **2019**, *123*, 2049.
[359] S. J. V. Gordon, Y. Xiao, A. L. Paskavitz, N. Navarro-Tito, J. G. Navea, T. Padilla-Benavides, *JoVE* **2019**, *147*, e59519.
[360] R. M. Soliday, H. Bunn, I. Sumner, P. L. Raston, *J. Phys. Chem. A* **2019**, *123*, 1208.
[361] C. Tavera-Montañez, S. J. Hainer, D. Cangussu, S. J. V. Gordon, Y. Xiao, P. Reyes-Gutierrez, A. N. Imbalzano, J. G. Navea, T. G. Fazzio, T. Padilla-Benavides, *FASEB J.* **2019**, *33*, 14556.
[362] E. Uwimana, B. Cagle, C. Yeung, X. Li, E. V. Patterson, J. A. Doorn, H.-J. Lehmler, *Toxicol. Sci.* **2019**, *171*, 406.
[363] A. C. Vilchis-Nestor, L. M. Roldán, A. Leonardi, J. G. Navea, T. Padilla-Benavides, L. Shoshani, *Int. J. Mol. Sci.* **2019**, *20*, 2111.
[364] D. S. Rovnyak, G. C. Shields, *How Undergraduate Research Drives Science Forward*, Inside Higher Ed, Washington, DC **2017**.
[365] K. K. Karukstis, *Scholarsh. Pract. Undergrad. Res.* **2019**, *3*, 46.
[366] K. J. Theobald, M. J. Hill, E. Tran, S. Agrawal, E. N. Arroyo, S. Behling, N. Chambwe, D. L. Cintron, J. D. Cooper, G. Dunster, J. A. Grummer, K. Hennessey, J. Hsiao, N. Iranon, L. Jones, H. Jordt, M. Keller, M. E. Lacey, C. E. Littlefield, A. Lowe, S. Newman, V. Okolo, S. Olroyd, B. R. Peecook, S. B. Pickett, D. L. Slager, I. W. Caviedes-Solis, K. E. Stanchak, V. Sundaravardan, C. Valebenito, C. R. Williams, K. Zinsli, S. Freeman, *Proc. Natl. Acad. Sci.* **2020**, *117*, 6476.
[367] M. Crowe, D. Brakke, *Scholarsh. Pract. Undergrad. Res.* **2019**, *3*, 21.
[368] J. Foertsch, *Scholarsh. Pract. Undergrad. Res.* **2019**, *3*, 31.
[369] M. D. Sorcinelli, J. Yun, *Change Mag. Higher Learn.* **2007**, *39*, 58.
[370] G. C. Shields, G. J. Hewitt, L. North, *CUR Q.* **2010**, *31*, 43.
[371] G. C. Shields, *CUR Q.* **2010**, *30*, 18.
[372] I. Oikawa, H. Takamura, *Chem. Mater.* **2015**, *27*, 6660.
[373] A. F. Voter, *Phys. Rev. B* **1998**, *57*, 13985.
[374] M. R. Sorensen, A. F. Voter, *J. Chem. Phys.* **2000**, *112*, 9599.
[375] S. C. Schultz, G. C. Shields, T. A. Steitz, *Science* **1991**, *253*, 1001.
[376] E. C. Sherer, G. Yang, G. M. Turner, G. C. Shields, D. W. Landry, *J. Phys. Chem. A* **1997**, *101*, 8526.
[377] G. C. Shields, C. A. Laughton, M. Orozco, *J. Am. Chem. Soc.* **1997**, *119*, 7463.
[378] G. C. Shields, C. A. Laughton, M. Orozco, *J. Am. Chem. Soc.* **1998**, *120*, 5895.
[379] M. W. Jurema, G. C. Shields, *J. Comput. Chem.* **1993**, *14*, 89.
[380] M. W. Jurema, K. N. Kirschner, G. C. Shields, *J. Comput. Chem.* **1993**, *14*, 1326.
[381] K. N. Kirschner, G. C. Shields, *Int. J. Quantum Chem.* **1994**, *52*, 349.
[382] J. H. Lu, H. T. Li, M. C. Liu, J. P. Zhang, M. Li, X. M. An, W. R. Chang, *Biochem. Biophys. Res. Commun.* **2005**, *335*, 417.
[383] J. C. Rote, S. N. Malkowski, C. S. Cochrane, G. E. Bailey, N. S. Brown, M. Cafiero, L. W. Peterson, *Synth. Commun.* **2017**, *47*, 435.

[384] R. J. Roldan, A. O. Pajarillo, J. D. Greenberg, J. E. Karlinsey, M. Cafiero, E. R. Frawley, L. W. Peterson, *Bioorg. Med. Chem. Lett.* **2020**, *30*, 126875.
[385] S. Prasad, N. Walker, M. Henry, K. J. Donald, *Organometallics* **2020**, *39*, 34.
[386] R. Báez-Grez, D. Inostroza, V. García, A. Vásquez-Espinal, K. J. Donald, W. Tiznado, *Phys. Chem. Chem. Phys.* **2020**, *22*, 1826.
[387] V. Molinero, E. B. Moore, *J. Phys. Chem. B* **2009**, *113*, 4008.
[388] R. C. DeMille, V. Molinero, *J. Chem. Phys* **2009**, *131*, 034107.
[389] L. C. Jacobson, W. Hujo, V. Molinero, *J. Phys. Chem. B* **2010**, *114*, 13796.
[390] Z. D. Nagel, J. P. Klinman, *Chem. Rev.* **2010**, *110*, PR41.
[391] J. Vina-Gonzalez, D. Jimenez-Lalana, F. Sancho, A. Serrano, A. T. Martinez, V. Guallar, M. Alcalde, *Adv. Synth. Catal.* **2019**, *361*, 2514.
[392] A. A. Eigner, J. A. Rohde, C. C. Knutson, J. A. Phillips, *J. Phys. Chem. B* **2007**, *111*, 1402.
[393] J. A. Phillips, C. J. Cramer, *J. Phys. Chem. B* **2007**, *111*, 1408.
[394] K. R. Leopold, M. Canagaratna, J. A. Phillips, *Acc. Chem. Res.* **1997**, *30*, 57.
[395] J. A. Phillips, J. A. Halfen, J. P. Wrass, C. C. Knutson, C. J. Cramer, *Inorg. Chem.* **2006**, *45*, 722.
[396] J. F. Mike, K. Nalwa, A. J. Makowski, D. Putnam, A. L. Tomlinson, S. Chaudhary, M. Jeffries-El, *Phys. Chem. Chem. Phys.* **2011**, *13*, 1338.
[397] B. C. Tlach, A. L. Tomlinson, A. Bhuwalka, M. Jeffries-El, *J. Organomet. Chem.* **2011**, *76*, 8670.
[398] K. Boutilier, M. Ross, A. V. Podtelejnikov, C. Orsi, R. Taylor, P. Taylor, D. Figeys, *Anal. Chim. Acta* **2005**, *534*, 11.
[399] S. A. Miller, D. E. Riederer, R. G. Cooks, W. R. Cho, H. W. Lee, H. Kang, *J. Phys. Chem.* **1994**, *98*, 245.
[400] A. L. McCormack, A. Somogyi, A. R. Dongre, V. H. Wysocki, *Anal. Chem.* **1993**, *65*, 2859.
[401] J. Laskin, E. Denisov, J. Futrell, *J. Am. Chem. Soc.* **2000**, *122*, 9703.
[402] P. Wang, O. Hadjar, P. L. Gassman, J. Laskin, *Phys. Chem. Chem. Phys.* **2008**, *10*, 1512.
[403] J. Laskin, E. Denisov, J. Futrell, *J. Phys. Chem. B* **2001**, *105*, 1895.
[404] D. J. Douglas, *J. Am. Soc. Mass Spectrom.* **1998**, *9*, 101.
[405] A. R. Dongre, J. L. Jones, A. Somogyi, V. H. Wysocki, *J. Am. Chem. Soc.* **1996**, *118*, 8365.
[406] B. Paizs, S. Suhai, *Mass Spectrom. Rev.* **2005**, *24*, 508.
[407] L. Morrison, A. Somogyi, V. H. Wysocki, *Int. J. Mass Spectrom.* **2012**, *325*, 139.
[408] W. Ijaz, Z. Gregg, G. L. Barnes, *J. Phys. Chem. Lett.* **2013**, *4*, 3935.
[409] Z. Gregg, W. Ijaz, S. Jannetti, G. L. Barnes, *J. Phys. Chem. C* **2014**, *118*, 22149.
[410] K. Shaikh, J. Blackwood, G. L. Barnes, *Chem. Phys. Lett.* **2015**, *637*, 83.
[411] A. Geragotelis, G. L. Barnes, *J. Phys. Chem. C* **2013**, *117*, 13087.
[412] L. Levi, Z. Wang, M. K. Doud, S. L. Hazen, N. Noy, *Nat. Commun.* **2015**, *6*, 8794.
[413] Y. K. Kosenkov, D. Kosenkov, *J. Chem. Phys.* **2019**, *151*, 144101.
[414] D. Ghosh, D. Kosenkov, V. Vanovschi, C. F. Williams, J. M. Herbert, M. S. Gordon, M. W. Schmidt, L. V. Slipchenko, A. I. Krylov, *J. Phys. Chem. A* **2010**, *114*, 12739.
[415] W. H. James III., E. G. Buchanan, C. W. Mueller, J. C. Dean, D. Kosenkov, L. V. Slipchenko, L. Guo, A. G. Reidenbach, S. H. Gellman, T. S. Zwier, *J. Phys. Chem. A* **2011**, *115*, 13783.
[416] G. Prato, S. Silvent, S. Saka, M. Lamberto, D. Kosenkov, *J. Phys. Chem. B* **2015**, *119*, 3335.
[417] D. Ghosh, D. Kosenkov, V. Vanovschi, J. Flick, I. Kaliman, Y. Shao, A. T. B. Gilbert, A. I. Krylov, L. V. Slipchenko, *J. Comput. Chem.* **2013**, *34*, 1060.
[418] J. C. Flick, D. Kosenkov, E. G. Hohenstein, C. D. Sherrill, L. V. Slipchenko, *J. Chem. Theory Comput.* **2012**, *8*, 2835.
[419] D. Kosenkov, L. V. Slipchenko, *J. Phys. Chem. A* **2011**, *115*, 392.
[420] J. H. Seinfeld, S. N. Pandis, *Atmospheric Chemistry and Physics: From Air Pollution to Climate Change*, 2nd ed., John Wiley & Sons, Inc, New York, NY **2006**, p. 1.
[421] K. A. Prather, C. D. Hatch, V. H. Grassian, *Annual Rev. Anal. Chem.* **2008**, *1*, 485.
[422] B. J. Finlayson-Pitts, *Phys. Chem. Chem. Phys.* **2009**, *11*, 7760.
[423] H. Chen, J. G. Navea, M. A. Young, V. H. Grassian, *J. Phys. Chem. A* **2011**, *115*, 490.
[424] C. R. Usher, A. E. Michel, V. H. Grassian, *Chem. Rev.* **2003**, *103*, 4883.
[425] C. Linke, O. Moehler, A. Veres, A. Mohacsi, Z. Bozoki, G. Szabo, M. Schnaiter, *Atmos. Chem. Phys.* **2006**, *6*, 3315.
[426] F. Hanisch, J. N. Crowley, *Atmos. Chem. Phys.* **2003**, *3*, 119.
[427] D. M. B. Lesko, E. M. Coddens, H. D. Swomley, R. M. Welch, J. Borgatta, J. G. Navea, *Phys. Chem. Chem. Phys.* **2015**, *17*, 20775.
[428] J. Baltrusaitis, J. Schuttlefield, J. H. Jensen, V. H. Grassian, *Phys. Chem. Chem. Phys.* **2007**, *9*, 4970.
[429] P. Galhotra, J. G. Navea, S. C. Larsen, V. H. Grassian, *Energy Environ. Sci.* **2009**, *2*, 401.
[430] K. K. Irikura, R. D. Johnson, R. N. Kacker, *J. Phys. Chem. A* **2005**, *109*, 8430.
[431] D. M. Wenzel, K. E. Stoll, R. E. Klevit, *Biochem. J.* **2011**, *433*, 31.
[432] L. Bedford, J. Lowe, L. R. Dick, R. J. Mayer, J. E. Brownell, *Nat. Rev. Drug Discov.* **2011**, *10*, 29.
[433] P. Y. Wu, M. Hanlon, M. Eddins, C. Tsui, R. S. Rogers, J. P. Jensen, M. J. Matunis, A. M. Weissman, C. P. Wolberger, C. M. Pickart, *EMBO J.* **2003**, *22*, 5241.
[434] K. G. Tanner, R. C. Trievel, M. H. Kuo, R. M. Howard, S. L. Berger, C. D. Allis, R. Marmorstein, J. M. Denu, *J. Biol. Chem.* **1999**, *274*, 18157.
[435] C. E. Berndsen, R. Wiener, I. W. Yu, A. E. Ringel, C. Wolberger, *Nat. Chem. Biol.* **2013**, *9*, 154.
[436] H. Chen, M. J. Ezell, K. D. Arquero, M. E. Varner, M. L. Dawson, R. B. Gerber, B. J. Finlayson-Pitts, *Phys. Chem. Chem. Phys.* **2015**, *17*, 13699.
[437] R. B. Gerber, M. E. Varner, A. D. Hammerich, S. Riikonen, G. Murdachaew, D. Shemesh, B. J. Finlayson-Pitts, *Acc. Chem. Res.* **2015**, *48*, 399.
[438] G. S. Tschumper, T. L. Ellington, S. N. Johnson, in *Annual Reports in Computational Chemistry*, Vol. 13 (Ed: D. A. Dixon Elsevier, Oxford) **2017**, p. 93.
[439] S. N. Johnson, C. R. Hutchison, C. M. Williams, H. L. Hus, G. S. Tschumper, N. I. Hammer, *J. Phys. Chem. C* **2018**, *122*, 27673.
[440] S. N. Johnson, G. S. Tschumper, *J. Comput. Chem.* **2018**, *39*, 839.
[441] S. N. Johnson, T. L. Ellington, D. T. Ngo, J. L. Nevarez, N. Sparks, A. L. Rheingold, D. L. Watkins, G. S. Tschumper, *CrystEngComm* **2019**, *21*, 3151.
[442] N. Biais, D. L. Higashi, J. Brujić, M. So, M. P. Sheetz, *Proc. Natl. Acad. Sci.* **2010**, *107*, 11358.
[443] J. L. Baker, N. Biais, F. Tama, *PLoS Comput. Biol.* **2013**, *9*, e1003032.
[444] J. L. Baker, J. Furbish, G. E. Lindberg, *J. Mol. Graphics Modell.* **2015**, *62*, 202.

[445] A. Kojima, K. Teshima, Y. Shirai, T. Miyasaka, *J. Am. Chem. Soc.* **2009**, *131*, 6050.
[446] M. S. Wrighton, A. B. Ellis, P. T. Wolczanski, D. L. Morse, H. B. Abrahamson, D. S. Ginley, *J. Am. Chem. Soc.* **1976**, *98*, 2774.
[447] J. G. Mavroides, J. A. Kafalas, D. F. Kolesar, *Appl. Phys. Lett.* **1976**, *28*, 241.
[448] C. A. Daly, E. J. Berquist, T. Brinzer, S. Garrett-Roe, D. S. Lambrecht, S. A. Corcelli, *J. Phys. Chem. B* **2016**, *120*, 12633.
[449] E. J. Berquist, C. A. Daly, T. Brinzer, K. K. Bullard, Z. M. Campbell, S. A. Corcelli, S. Garrett-Roe, D. S. Lambrecht, *J. Phys. Chem. B* **2017**, *121*, 208.
[450] C. A. Daly, L. M. Streacker, Y. C. Sun, S. R. Pattenaude, A. A. Hassanali, P. B. Petersen, S. A. Corcelli, D. Ben-Arnotz, *J. Phys. Chem. Lett.* **2017**, *8*, 5246.
[451] T. Brinzer, C. A. Daly, C. Allison, S. Garrett-Roe, S. A. Corcelli, *J. Phys. Chem. B* **2018**, *122*, 8931.
[452] C. A. Daly, T. Brinzer, C. Allison, S. Garrett-Roe, S. A. Corcelli, *J. Phys. Chem. Lett.* **2018**, *9*, 1393.
[453] C. A. Daly, C. Allison, S. A. Corcelli, *J. Phys. Chem. B* **2019**, *123*, 3797.
[454] C. I. Drexler, T. C. Miller, B. A. Rogers, Y. G. C. Li, C. A. Daly, T. L. Yang, S. A. Corcelli, P. S. Cremer, *J. Am. Chem. Soc.* **2019**, *141*, 6930.
[455] W. D. Derricotte, *J. Phys. Chem. A* **2019**, *123*, 7881.
[456] N. Zhang, C. Han, Y.-J. Xu, J. J. Foley Iv, D. Zhang, J. Codrington, S. K. Gray, Y. Sun, *Nat. Photonics* **2016**, *10*, 473.
[457] J. Codrington, N. Eldabagh, K. Fernando, J. J. Foley, *ACS Photonics* **2017**, *4*, 552.
[458] N. Eldabagh, M. Micek, A. E. DePrince, J. J. Foley, *J. Phys. Chem. C* **2018**, *122*, 18256.
[459] J. F. Varner, N. Eldabagh, D. Volta, N. Eldabagh, J. J. Foley IV., *J. Open Res. Softw.* **2019**, *7*, 1
[460] J. F. Varner, D. Wert, A. Matari, R. Nofal, J. J. Foley, *Phys. Rev. Research* **2020**, *2*, 013018
[461] K. D. He, W. D. Allen, *J. Chem. Theory Comput.* **2016**, *12*, 3571.
[462] R. J. Xu, B. Blasiak, M. Cho, J. P. Layfield, C. H. Londergan, *J. Phys. Chem. Lett.* **2018**, *9*, 2560.
[463] J. S. Perkyns, G. C. Lynch, J. J. Howard, B. M. Pettitt, *J. Chem. Phys.* **2010**, *132*, 064106.
[464] T. Luchko, S. Gusarov, D. R. Roe, C. Simmerling, D. A. Case, J. Tuszynski, A. Kovalenko, *J. Chem. Theory Comput.* **2010**, *6*, 607.
[465] J. Johnson, D. A. Case, T. Yamazaki, S. Gusarov, A. Kovalenko, T. Luchko, *J. Phys. Condens. Matter* **2016**, *28*, 344002.
[466] T. Luchko, N. Blinov, G. C. Limon, K. P. Joyce, A. Kovalenko, *J. Comput.-Aided Mol. Des.* **2016**, *30*, 1115.
[467] S. Genheden, T. Luchko, S. Gusarov, A. Kovalenko, U. Ryde, *J. Phys. Chem. B* **2010**, *114*, 8505.
[468] G. M. Giambasu, T. Luchko, D. Herschlag, D. M. York, D. A. Case, *Biophys. J.* **2014**, *106*, 883.
[469] G. M. Giambasu, M. K. Gebala, M. T. Panteva, T. Luchko, D. A. Case, D. M. York, *Nucleic Acids Res.* **2015**, *43*, 8405.
[470] C. Nguyen, T. Yamazaki, A. Kovalenko, D. A. Case, M. K. Gilson, T. Kurtzman, T. Luchko, *PLoS One* **2019**, *14*, e0219473.
[471] T. Tsednee, T. Luchko, *Phys. Rev. E* **2019**, *99*, 032130
[472] S. L. Miller, *Science* **1969**, *165*, 489.
[473] D. Archer, B. Buffett, V. Brovkin, *Proc. Natl. Acad. Sci. U. S. A.* **2009**, *106*, 20596.
[474] K. A. Kvenvolden, *Global Biogeochem. Cycles* **1988**, *2*, 221.
[475] E. D. Sloan, *Nature* **2003**, *426*, 353.
[476] I. Chatti, A. Delahaye, L. Fournaison, J. P. Petitet, *Energy Convers. Manage.* **2005**, *46*, 1333.
[477] J. Ghosh, R. R. J. Methikkalam, R. G. Bhuin, G. Ragupathy, N. Choudhary, R. Kumar, T. Pradeep, *Proc. Natl. Acad. Sci. U. S. A.* **2019**, *116*, 1526.
[478] A. Desmedt, L. Martin-Gondre, T. T. Nguyen, C. Petuya, L. Barandiaran, O. Babot, T. Toupance, R. G. Grim, A. K. Sum, *J. Phys. Chem. C* **2015**, *119*, 8904.
[479] T. Ikeda, S. Mae, T. Uchida, *J. Chem. Phys.* **1998**, *108*, 1352.
[480] J. H. Jia, Y. F. Liang, T. Tsuji, S. Murata, T. Matsuoka, *Sci. Rep.* **2017**, *7*, 1
[481] H. Nada, *J. Phys. Chem. B* **2006**, *110*, 16526.
[482] X. X. Cao, Y. Su, J. J. Zhao, *J. Phys. Chem. A* **2015**, *119*, 7063.
[483] H. K. Srivastava, G. N. Sastry, *J. Phys. Chem. A* **2011**, *115*, 7633.
[484] C. Qu, J. M. Bowman, *J. Phys. Chem. C* **2016**, *120*, 3167.
[485] Q. N. Lu, X. He, W. X. Hu, X. J. Chen, J. F. Liu, *J. Phys. Chem. C* **2019**, *123*, 12052.
[486] M. R. Tinsley, S. Nkomo, K. Showalter, *Nat. Phys.* **2012**, *8*, 662.
[487] S. Nkomo, M. R. Tinsley, K. Showalter, *Phys. Rev. Lett.* **2013**, *110*, 244102
[488] S. Nkomo, M. R. Tinsley, K. Showalter, *Chaos* **2016**, *26*, 094826.
[489] E. Sanganyado, S. Nkomo, *Educ. Sci.* **2018**, *8*, 39
[490] A. S. Gzyl, A. O. Oliynyk, L. A. Adutwum, A. Mar, *Inorg. Chem.* **2019**, *58*, 9280.
[491] M. A. Matlinska, M. Ha, B. Hughton, A. O. Oliynyk, A. K. Iyer, G. M. Bernard, G. Lambkin, M. C. Lawrence, M. J. Katz, A. Mar, V. K. Michaelis, *ACS Appl. Mater. Interfaces* **2019**, *11*, 32739.
[492] A. O. Oliynyk, J. M. Buriak, *Chem. Mater.* **2019**, *31*, 8243.
[493] A. M. Tehrani, A. O. Oliynyk, Z. Rizvi, S. Lotfi, M. Parry, T. D. Sparks, J. Brgoch, *Chem. Mater.* **2019**, *31*, 7696.
[494] G. Viswanathan, A. O. Oliynyk, E. Antono, J. Ling, B. Meredig, J. Brgoch, *Inorg. Chem.* **2019**, *58*, 9004.
[495] Y. Q. Zhou, A. K. Iyer, A. O. Oliynyk, M. Heyberger, Y. X. Lin, Y. Qiu, A. Mar, *J. Solid State Chem.* **2019**, *278*, UNSP 120914.
[496] C. E. Scott, D. A. Kendall, in *Cannabinoids and Their Receptors*, Vol. 593 (Ed: P. H. Reggio Elsevier, San Diego) **2017**, p. 317.
[497] L. M. Ogawa, N. T. Burford, Y. H. Liao, C. E. Scott, A. M. Hine, C. Dowling, J. Chin, M. Power, E. J. Hunnicutt, V. L. Emerick, M. Banks, L. T. Zhang, S. W. Gerritz, A. Alt, D. A. Kendall, *Slas Discov.* **2018**, *23*, 375.
[498] B. D. Stewart, C. E. Scott, T. P. McCoy, G. Yin, F. Despa, S. Despa, P. M. Kekenes-Huskey, *Cell Calcium* **2018**, *71*, 65.
[499] P. M. Kekenes-Huskey, C. E. Scott, S. Atalay, *J. Phys. Chem. B* **2016**, *120*, 8696.
[500] A. N. Kucharski, C. E. Scott, J. P. Davis, P. M. Kekenes-Huskey, *J. Phys. Chem. B* **2016**, *120*, 8617.
[501] C. E. Scott, K. H. Ahn, S. T. Graf, W. A. Goddard, D. A. Kendall, R. Abrol, *J. Chem. Inf. Model.* **2016**, *56*, 201.
[502] K. H. Ahn, C. E. Scott, R. Abrol, W. A. Goddard, D. A. Kendall, *Proteins Struct. Function Bioinform.* **2013**, *81*, 1304.
[503] C. E. Scott, R. Abrol, K. H. Ahn, D. A. Kendall, W. A. Goddard, *Protein Sci.* **2013**, *22*, 101.
[504] J. K. Bray, R. Abrol, W. A. Goddard, B. Trzaskowski, C. E. Scott, *Proc. Natl. Acad. Sci. U. S. A.* **2014**, *111*, E72.
[505] A. S. Hauser, S. Chavali, I. Masuho, L. J. Jahn, K. A. Martemyanov, D. E. Gloriam, M. M. Babu, *Cell* **2018**, *172*, 41.

[506] C. J. Sigurdson, J. C. Bartz, M. Glatzel, in *Annual Review of Pathology: Mechanisms of Disease*, Vol. 14 (Eds: A. K. Abbas, J. C. Aster, M. B. Feany Annual Reviews, Palo Alto) **2019**, p. 497.
[507] N. R. Deleault, B. T. Harris, J. R. Rees, S. Supattapone, *Proc. Natl. Acad. Sci. U. S. A.* **2007**, *104*, 9741.
[508] M. Grabenauer, C. Wu, P. Soto, J. E. Shea, M. T. Bowers, *J. Am. Chem. Soc.* **2010**, *132*, 532.
[509] P. Soto, I. A. Claflin, A. L. Bursott, A. D. Schwab-McCoy, J. C. Bartz, *J. Biomol. Struct. Dyn.* **2020**, *118*, 509A.

How to cite this article: Shields GC. Twenty years of exceptional success: The molecular education and research consortium in undergraduate computational chemistry (MERCURY). *Int J Quantum Chem*. 2020;e26274. https://doi.org/10.1002/qua.26274