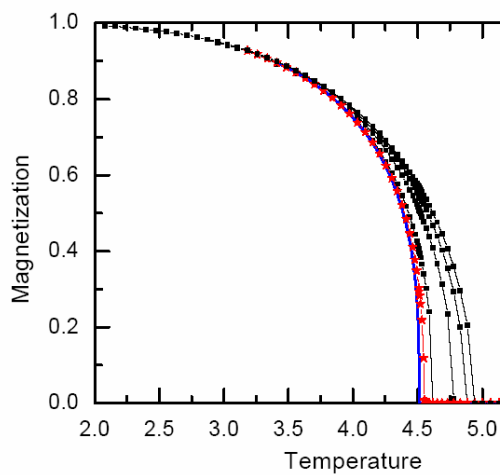
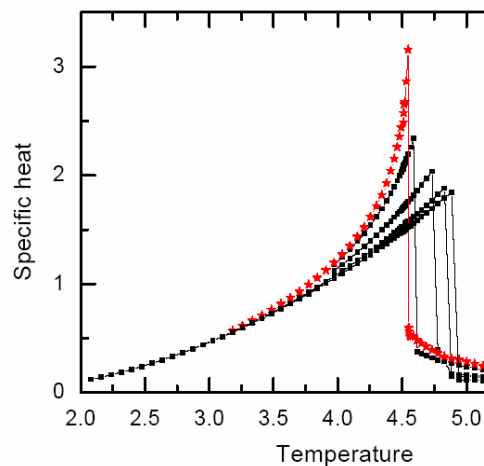


# RESEARCH REPORT

## 2006 – 2007



COLLEGE OF ARTS & SCIENCES

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DEPARTMENT OF PHYSICS

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WESTERN MICHIGAN UNIVERSITY

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Department of Physics

College of Arts and Sciences

Western Michigan University

# Annual Research Report

July 1<sup>st</sup>, 2006 – June 30<sup>th</sup>, 2007

**Edited by T. W. Gorczyca**

# CONTENTS

<b>1</b>	<b>INTRODUCTION</b>	<b>1</b>
<b>2</b>	<b>FROM THE CHAIRPERSON</b>	<b>2</b>
<b>3</b>	<b>ASTRONOMY</b>	<b>3</b>
3.1	Isotopic Observables of the Asymmetry Term of the Nuclear Equation-of-State .....	3
3.2	Astrophysical S-Factors Relevant to p-Process Nuclei.....	7
3.3	Effects of $\beta$ -Decays of Excited State Nuclei on the Astrophysical r-Process.....	9
<b>4</b>	<b>ATOMIC PHYSICS</b>	<b>12</b>
4.1	Size Effects in Angle-Resolved Photoelectron Spectroscopy of Free Rare-Gas Clusters.....	12
4.2	Shape Resonances in K-shell Photodetachment of Small Size-Selected Clusters: Experiment and Theory.....	15
4.3	Photo Double Detachment of CN <sup>-</sup> : Electronic Decay from an Inner-Valence Hole in Molecular Anions.....	17
4.4	X-Ray Absorption in Carbon Ions Near the K-Edge .....	19
4.5	Anomalous Behavior of Auger and Radiative Rates and Fluorescence Yields.....	23
4.6	Modeling of Low-Energy Resonant States in the Photorecombination Spectra of Ti <sup>4+</sup> Ions.....	27
4.7	Shape Resonances in the Absolute K-Shell Photodetachment of B .....	30
4.8	Dielectronic Recombination for Al-Like Sulfur .....	33
4.9	State-Selective Single-Electron Capture in Slow Collisions of Ne <sup>q+</sup> (q = 4 – 6) Ions with Molecules.....	36
4.10	Non-Dissociative Single-Electron Capture in Slow Collisions of O <sub>2</sub> <sup>2+</sup> Ions with O <sub>2</sub> , Ar and Ne .....	38
4.11	Suppression of Primary Electron Interferences in the Ionization of N <sub>2</sub> by 1 – 5 MeV Protons .....	40
4.12	Enhancement of the 1s2s2p <sup>4</sup> P State in Electron Transfer to C <sup>4,5+</sup> Ions .....	43
4.13	Inelastic Guiding of Electrons in Insulating Nanocapillary Foils.....	46
4.14	Interference Effects in Electron Emission from 30 MeV O <sup>8+</sup> + O <sub>2</sub> Collisions .....	49

<b>5</b>	<b><i>NUCLEAR PHYSICS</i></b>	<b>51</b>
5.1	Proton Capture by $^{14}\text{N}$ at Astrophysical Energies.....	51
5.2	The $^2\text{H}(^{12}\text{B},p)^{13}\text{B}$ reaction .....	53
5.3	Carbon Production in Stars and the Triple $\alpha$ Reaction.....	54
5.4	HELIOS: The HELIcal Orbit Spectrometer.....	57
<b>6</b>	<b><i>PHYSICS EDUCATION</i></b>	<b>59</b>
6.1	Promoting Instructional Change in New Faculty: An Evaluation of the Physics and Astronomy New Faculty Workshop .....	59
6.2	Modeling Success: Building Community for Reform .....	63
<b>7</b>	<b><i>PUBLICATIONS</i></b>	<b>66</b>
7.1	Papers Published .....	66
7.2	Papers in Press .....	69
7.3	Papers Submitted.....	70
<b>8</b>	<b><i>DISSERTATIONS</i></b>	<b>71</b>
8.1	Ph.D.....	71
<b>9</b>	<b><i>PRESENTATIONS</i></b>	<b>72</b>
9.1	Research Talks at Professional Meetings and Other Institutions.....	72
	9.1.1 Invited.....	72
	9.1.2 Contributed.....	75
	9.2 Research and Public Lectures at WMU .....	78
<b>10</b>	<b><i>PROPOSALS AND GRANTS</i></b>	<b>81</b>
<b>11</b>	<b><i>SCHOLARLY ACTIVITY</i></b>	<b>85</b>
<b>12</b>	<b><i>PERSONNEL</i></b>	<b>88</b>

# 1 INTRODUCTION

This is the thirty-sixth in a series of annual reports which summarizes the research activities of the members of the Department of Physics at Western Michigan University. The report includes research performed in this department as well as in collaboration with the faculty of other departments at Western, faculty at other institutions, and staff members of national laboratories.

Special thanks are due Ms. Kerry Cochran for her invaluable assistance in the preparation and presentation of this document.

*Thomas W. Gorczyca*  
*Editor*

## **Cover Design:**

Novel many-body method reporting accurate calculation of the spontaneous magnetization and the specific heat of the three dimensional Ising model. The solid line in the top figure is the renormalization group-finite size scaling-Monte Carlo result. The calculated specific heat shows excellent agreement with the experimentally observed specific heat of argon and other liquids through the gas-liquid phase transition.

## 2 FROM THE CHAIRPERSON

This latest issue in our continuing series of Research Reports clearly demonstrates the vigor of Physics research at Western Michigan University. It also provides an opportunity for us to assess our own efforts, somewhat informally. Our faculty and students are managing to produce new knowledge in a variety of fields, in quantity and quality equal to or greater than what we have done in previous years. This despite significant faculty attrition and other stresses, including a general decline in federal funding for basic science. Given the importance of science and technology for the future of our country and the world, we are proud to be making these contributions.

While undergraduate enrollment at WMU has slowed its decline, the anticipated upturn in total headcount has not yet materialized. However, graduate student numbers have increased in the last few years, and Physics has been part of this trend. This has contributed in some measure to our being able to sustain our research efforts during tough times.

Speaking of tough times, one of the biggest issues on our horizon is the imminent retirement of Jerry Hardie from our faculty. Jerry was one of the original users of our tandem Van de Graaff accelerator, and his career in research spanned four decades. Besides doing experiments on the tandem (when nuclear physics was much younger!) he also did a lot of work at Argonne National Lab and the Indiana University Cyclotron Facility, before its demise. We will all miss Jerry very much after this April, but I don't think anyone will miss him more than I will. Thanks for all you have done for WMU Physics, Jerry.

And thanks also to all who have contributed to this report, especially to the editor and the staff who worked with him to put it together. We very much appreciate all of your time and effort.

*Paul V. Pancella*  
*Chair*

## 3 ASTRONOMY

### 3.1 Isotopic Observables of the Asymmetry Term of the Nuclear Equation-of-State

**M. A. Famiano**

Western Michigan University, Kalamazoo, MI 49008-5252

The characterization of dense nuclear matter remains one of the largest unanswered questions in nuclear physics today as reported by the National Academy of Science [1]. The answers to this question will help pave the way to a better understanding of the interior structure of neutron stars. Currently, there is much work to be done concerning the high density behavior of the nuclear equation-of-state

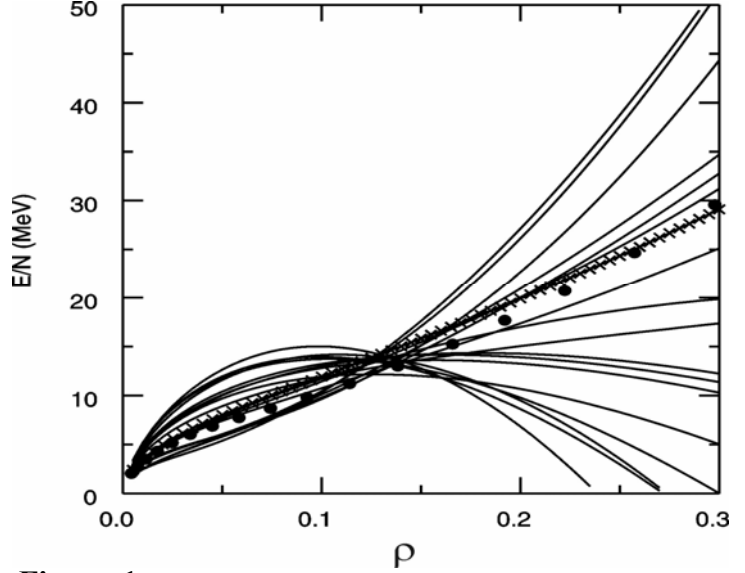
A rudimentary understanding of the nuclear equation-of-state (EOS), the pressure density relationship of nuclear matter, can be attained by examining some of the earlier semi-empirical mass formulae for nuclear binding energies, such as the liquid drop model. This relationship between the nuclear binding energy and the number of protons and neutrons in a system contains bulk and surface terms, a Coulomb term, a pairing term, and the asymmetry term which describes the contribution to the binding energy as a function of the neutron-proton difference,  $E_{\text{sym}}=c(A)(N-Z)^2/A$  where the coefficient  $c(A)$  is a sum of a mass independent volume term and a surface term  $c(A)=c_v+c_sA^{-1/3}$  [1]. Typical values for the coefficients  $c_v$  and  $c_s$  are taken by fitting to known nuclear masses. For the nuclear EOS, the energy per particle can then be written in the parabolic approximation as a function of the density and asymmetry of the system consisting of contributions from a symmetric part, and an asymmetric part:

$$E(\rho, \delta) = E(\rho, \delta = 0) + S(\rho)\delta^2 \quad (1)$$

where the asymmetry energy is given as a product of the density dependent asymmetry energy  $S(\rho)$  and the square of the asymmetry  $\delta=(\rho_n-\rho_p)/(\rho_n+\rho_p)$  [2].

Theoretical descriptions of the asymmetry term in the EOS range from “asy-stiff” terms, in which the pressure increases more sharply as a function of density, and “asy-soft” terms, in which the pressure does not increase as sharply [3]. The density dependent asymmetry energy  $S(\rho)$  can be empirically parameterized as  $S(\rho)=C \cdot F(u)$  where  $u$  is the density relative to normal nuclear density  $\rho_0$ ,  $u=\rho/\rho_0$  so that the asymmetry term is quantified by the function  $F(u)$  [4]. In either case, the potential is attractive for protons and repulsive for neutrons. At densities less than  $\rho_0$ , the difference in proton and neutron potentials is smaller than in the soft case. This fact can be exploited in nuclear collisions as the attractive potential in the asy-soft case exceeds the Coulomb repulsion. Thus, the proton-neutron emission in a nuclear reaction is postulated to be sensitive to the density dependence of the asymmetry term. In this phenomenology, at higher densities, as might occur deeper into the core of a neutron star, the relationship may reverse as indicated in Figure 1, such that the proton potential is stronger for the asy-soft case. However, the high-density behavior of the asymmetry term has yet to be probed experimentally.

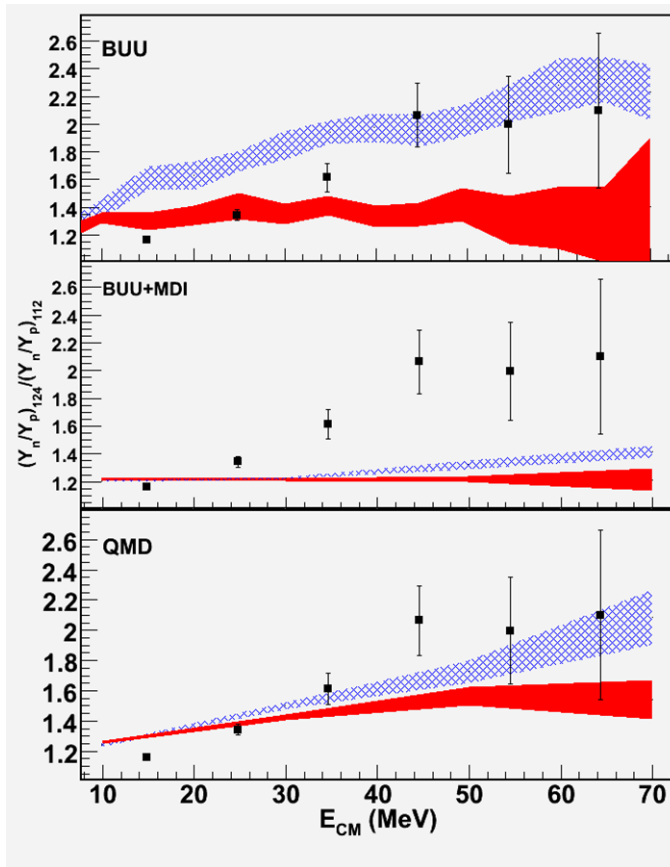
The current difficulty with understanding the asymmetry term of the nuclear EOS is the fact that it is not well constrained. For example, Figure 1 shows the binding energy per nucleon based on several modeled nuclear EOS's differing only by their nuclear asymmetry terms which range from the "asy-stiff" case to the "asy-soft" case [5]. All of the relationships shown in the figure are able to reproduce the nuclear binding energies of all of the stable Sn isotopes. (The dotted line corresponds to the Friedman-Pandirhapande relationship [6], and the cross-hatched region corresponds to results using a Skyrme potential.) It is clear that nuclear binding energy alone is not sufficient to predict the asymmetry term of the nuclear EOS.



**Figure 1** Nuclear energy per nucleon as a function of density for several EOSs which vary only by the asymmetry term [5]. Each line fits the masses of all stable Sn isotopes. The circles correspond to the Friedmann-Pandirhapande relationship [6].

Recent experimentation has explored the isospin asymmetry term via transverse fragment emission in central collisions [7], and deduced neutron-proton emission ratios have been explored using mirror nuclei emission ratios [8]. Transverse emission is studied to prevent screening of fragments by the projectile-like fragment (PLF) in the reaction. In the case of mirror nuclei ratios, the principle of cluster coalescence is invoked as a means of explaining the neutron-proton measurement [9]. In the coalescence model, the probability of cluster production is determined by the overlap of its phase-space density with those of its constituents. However, some studies have indicated light cluster production to be less sensitive to the asymmetry potential for higher energy clusters [10]. Also, some ambiguity remains in this analysis in that fragment decays can contaminate the cluster emission yields [11]. The least ambiguous measurement would be a coalescence-invariant measurement, in which the total nucleon emission spectra are taken as the sum of free nucleons and nucleons bound in clusters,  $Y_n/Y_p = \sum n_i Y_i / \sum z_i Y_i$ . Such a measurement would require a large area neutron detector to measure free neutrons, as well as a high-resolution charged-particle detector for free protons and clusters. Initial measurements of this sort have been conducted by at the National Superconducting Cyclotron Laboratory, and results are compared to calculations in Figure 2 for free nucleons [12]. This particular experiment utilized 50 MeV/A beams of  $^{112}\text{Sn}$  and  $^{124}\text{Sn}$  on identical targets to achieve a wide range of asymmetry. The density of the reaction region is limited by the beam energy. In this case, the effective density studied was  $< 1.2\rho_0$  [13]. Three predictions are indicated in Figure 2 corresponding to three models. The Boltzmann-Uehling-Uhlenbeck (BUU) [14] model is compared to the BUU model with a momentum-dependent interaction (MDI) [15]. Also, shown are results from a recent quantum molecular dynamic (QMD) model [16]. All three models show variations in the relative emission, indicating that more work is necessary in constraining the theory and





**Figure 2** Neutron proton double-ratios for the  $^{112}\text{Sn}+^{112}\text{Sn}$  reaction and the  $^{124}\text{Sn}+^{124}\text{Sn}$  reaction compared to three transport calculations as indicated in each figure [12,14-16]. The cross-hatched regions correspond to predictions assuming an asy-soft EOS while the dark shaded region corresponds to those for an asy-stiff EOS.

experiment. The more recent BUU+MDI and QMD models show significant disagreement. However, this difference may lie in the fact that the BUU models do not take the emission of d, t,  $\alpha$  and heavier clusters explicitly into account and approximate the nucleon effective masses to include momentum dependence, though the reduction in effective masses may differ with system asymmetry and neutron richness.

Currently, understanding the EOS of nuclear matter deep within neutron stars (higher  $\rho$  in nuclear reactions) is limited to extrapolation from current results. Future experimentation will target the high-density behavior of the asymmetry term of the nuclear EOS. This experimentation is planned for late 2007 using  $^{40,48}\text{Ca} + ^{40,48}\text{Ca}$  and  $^{40,48}\text{Ca} + ^{112,124}\text{Sn}$  reactions at projectile energies up to 150 MeV/A. In addition to nucleon emission observables, in-medium nucleon-nucleon (NN) cross sections will be explored to better constrain the results of transport calculations, thus reducing the model-dependence of these results.

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### 3.2 Astrophysical S-Factors Relevant to p-Process Nuclei

**M. A. Famiano, R. S. Kodikara, V. G. Subramanian, B. M. Giacherio, and A. Kayani**

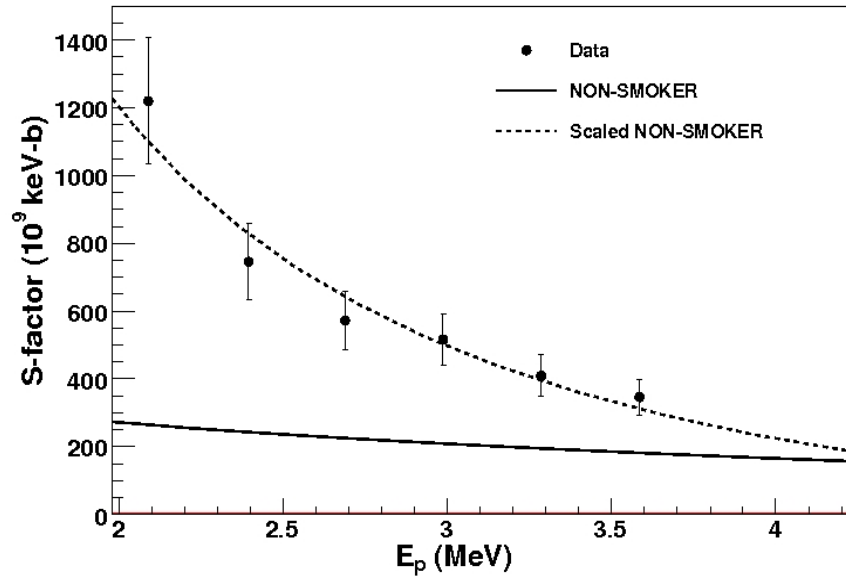
Western Michigan University, Kalamazoo, MI 49008-5252

Nearly all nuclei with masses greater than that of iron have abundances which are not attributed to normal stellar burning processes. In particular, the astrophysical r- and s- processes are thought to be responsible for nearly all of these nuclei [1]. However, significant uncertainty remains on the so-called p-nuclei, nuclei which cannot be produced through  $\beta$ -decay and thus cannot be produced via neutron capture processes. These nuclei are generally some of the least abundant nuclei in the universe, and their presumed production process is not well known.

There are 35 of these nuclei which cannot be produced via a neutron capture process (i.e., the s- and r-processes). Their production is likely due to  $\gamma$ -induced reactions on heavier, stable nuclei in the shock fronts of Type II supernovae [2-4]. Alternate scenarios include the deflagration flame fronts in type I supernovae [5] and the O-Ne burning zones of massive stars [6]. Sites have been simulated in nuclear reaction networks with varying levels of success [3]. Regardless of the true macroscopic nature of the p-process site, results are heavily dependent on nuclear properties [3,7].

This measurement was conducted at the WMU accelerator facility. The procedure and analysis is duplicated from previous measurements to verify and expand the energy region studied for the  $^{116}\text{Sn}(p,\gamma)^{117}\text{Sb}$  reaction and to measure for the first time the cross section of the  $^{114}\text{Sn}(p,\gamma)^{115}\text{Sb}$  reaction. In addition to these two reactions, cross sections have been measured for the  $^{64}\text{Zn}(p,\gamma)^{65}\text{Ga}$  and the  $^{46}\text{Ti}(p,\gamma)^{47}\text{V}$  reactions. While these are not necessarily p-nuclei, their astrophysical relevance may be no less important. The  $^{64}\text{Zn}$  nucleus is the most abundant Zn isotope and its contribution to the solar abundance may be due to contributions from multiple processes; weak p- and s-process contributions have not been ruled out [8]. The radiative proton capture cross section of  $^{64}\text{Zn}$  has been measured over a broader energy range than in previous measurements, allowing for a more accurate scaling of theoretical data used in the calculation of astrophysical S-factors. The  $^{46}\text{Ti}$  nucleus may also be important as a small contributor to the rp-process flux through  $^{47}\text{V}$ [9], contributing to the early burning stages in X-ray bursts, which is important in the initial rise of luminosity of these objects.

The S-factors extracted from the  $^{114}\text{Sn}(p,\gamma)^{115}\text{Sb}$  cross sections are shown in Figure 1 along with the theoretical results from the NON-SMOKER calculation. As in the case of the  $^{116}\text{Sn}$  radiative capture cross-section, the NON-SMOKER calculation underestimates the S-factor. The scaled NON-SMOKER S-factors are also shown in Figure 1. The TRRs for proton capture on  $^{114}\text{Sn}$  based on the scaled NON-SMOKER S-factors can then be estimated using the functional forms for the scaled NON-SMOKER S-factors. It has been seen that both calculations consistently underestimate the TRRs to roughly the same degree.



**Figure 1** Astrophysical S-factors for the  $^{114}\text{Sn}(p,\gamma)^{115}\text{Sb}$  reaction. Also shown are the predictions using the NON-SMOKER calculation along with the scaled NON-SMOKER rates.

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### 3.3 Effects of $\beta$ -Decays of Excited State Nuclei on the Astrophysical r-Process

M. A. Famiano,<sup>1</sup> R. N. Boyd,<sup>2</sup> T. Kajino,<sup>3</sup> K. Otsuki,<sup>4</sup> M. Terasawa,<sup>5</sup> and G. J. Mathews<sup>6</sup>

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The solar system r-process abundances act as the canonical constraint to r-process theories as well as the prime indicator of the success of r-process models. Several r-process sites have been proposed; the hot-bubble region of a type II supernova (SNII) has been modeled fairly successfully. The composition of the environment in which the r-process occurs might be expected to have a profound effect on the final abundance distribution. Observations indicate that the r-process site is primary [1] and further evidence may suggest that the r-process is also unique [2]; it may occur in a single site or event. The uniqueness of the r-process site, however, remains a subject of study [3].

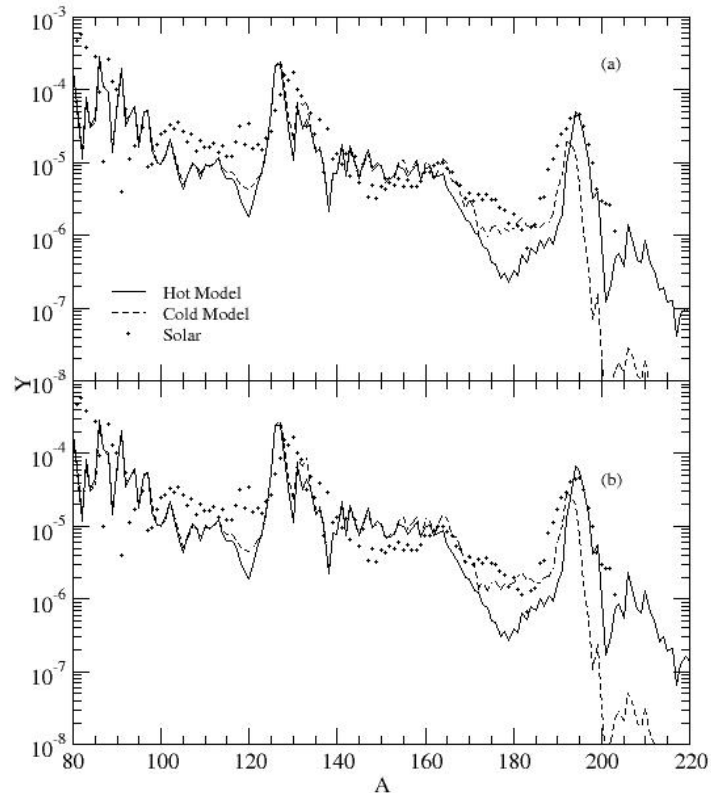
Nuclear properties also constrain the r-process, and the purpose of this work is the examination of one particular characteristic -  $\beta$ -decay - as it relates to the r-process. The  $\beta$ -decay inputs, and other nuclear physics inputs, have been shown [4,5] to have important effects on the success or failure of r-process models. This is somewhat unfortunate, as properties of only a few nuclei on the neutron closed shells closer to stability have been experimentally determined, while data for the rest are relegated to calculation. Of paramount importance is the determination of nuclear masses and  $\beta$ -decay rates. Nuclear mass formulae based on the microscopic properties of nuclei are slowly replacing the empirical droplet models, and these can change resulting reaction rates by factors as large as  $10^8$  [7]. As well, the r-process path is affected by the choice of mass formula, since the path roughly follows a line of constant  $S_n$  [7].

For the purposes of this study, the most recent semi-gross theory of  $\beta$ -decay [8] has been adapted to neutron-rich nuclei relevant to the r-process. The ability of this model to determine decay properties of an extremely wide range of nuclei with reasonable accuracy and speed makes it ideal for this preliminary calculation. In particular, the semi-gross theory has good agreement for very neutron-rich nuclei [9,10]. It has also been used to improve the accuracy of decay rates for astrophysical calculations by incorporating first-forbidden transition strengths [11]. In its original form, the gross theory of  $\beta$ -decay assumed that the energy states of a nucleus consist of a smoothed distribution with transition strengths that peak at or near the energy of the isobaric analog state [12,13]. Subsequent evolutions of the gross theory incorporated strength functions allowing for transitions of higher forbiddenness [14], as well as improvements over the original theory to include odd-odd effects [15], sum rules [16], even-odd mass differences [17], and improvements on the strength functions [18].

The results from several hydrodynamic parameter sets, as well as electron fraction parameter values  $Y_e$ , were examined. For each parameter set, the core mass in solar masses, core radius, neutrino luminosity, initial electron fraction, and whether or not  $\beta$ -delayed neutron emission is included are listed. Using these parameters and the calculations of reference [18] the dynamic timescale and the entropy in the expansion are constrained. Though still in agreement with current predictions, the dynamic timescales in these calculations are shorter than average. However, the entropy is lower, and no artificial increase in the entropy (as is often assumed) was required [3].

Each simulation is run until several seconds beyond freezeout. While this time is sufficient to gauge the gross features of the r-process abundance distribution, a longer simulation may have resulted in more post-processing, allowing for smoother abundance distributions. One notes some residual even-odd effects in the calculated distribution as the effects of smoothing may not be complete, though the gross features of the distribution are noted.

Results from two representative models are displayed in Figure 1 for both the hot (i.e., including excited-state decays, solid line) and cold (i.e., not including excited state decays, dotted line) models [45]. The  $A \sim 195$  peak is most profoundly affected, along with the nuclei just below this mass region. From the relationship between the decay rates and temperature, it can be seen that decay rates of the nuclei in the region just below the  $A \sim 195$  peak (and - to a lesser extent - the region just below the  $A \sim 130$  peak) are quite sensitive to changes in temperature even at low temperatures. This is expected due to the high level densities of these nuclei (lying just below the  $N=126$  and  $N=82$  closed shells). Shell quenching has not been included in this calculation, though the effect is noted, and no conclusions can be drawn from this study to evaluate the effects of quenched closed shells far from stability. Other rates, however, are not as sensitive to temperature changes at low temperatures and, as the r-process progresses, these rates would drop to their ground-state values before those of the nuclei in the regions below the abundance peaks. The decay rates of nuclei in this region would increase relative to those of nuclei in other regions of the path, selectively depleting the abundances of nuclei in this region.



**Figure 1** Comparison of r-process freezeout abundance distributions for two models (a) and (b) [45]. The dots correspond to the solar abundance distribution. The dashed line corresponds to a freezeout distribution assuming excited-state  $\beta$ -decays, and the solid line corresponds to a model using only ground-state decays.

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## 4 ATOMIC PHYSICS

### 4.1 Size Effects in Angle-Resolved Photoelectron Spectroscopy of Free Rare-Gas Clusters

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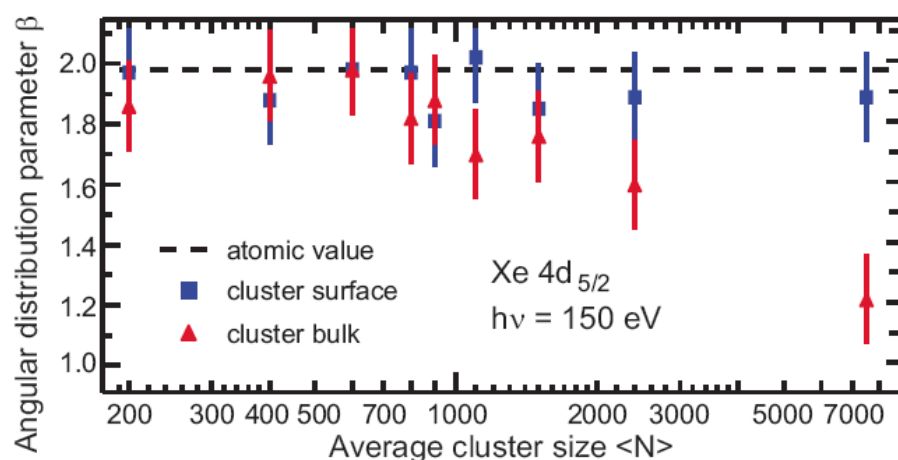
Several decades after its beginnings, cluster research continues to be an exciting area of science as most cluster properties remain much less known than those of their constituent atoms and molecules. Moreover, the scalability of clusters allows interpolation between the individual atom, the surface, and the bulk, bridging the gap between single atoms or molecules and condensed matter systems. This makes clusters unique targets to advance both the fundamental understanding of the many-body problem as well as nanotechnological applications [1]. Of particular interest are phenomena exhibiting cluster size dependence that underline the transition from individual atoms and molecules to large cluster systems with typical solid-state behavior, such as changes in cluster geometry and electronic structure. As each atom in the cluster is surrounded by an increasing number of neighbors, its electronic structure is altered by the resulting changes in the cluster potential and the atomic orbitals evolve into the band structure of the solid state. Cluster-size-dependent electronic properties can be probed directly using angle-resolved photoelectron spectroscopy, a well established technique for the study of the electronic structure of atoms, molecules, as well as condensed matter [2]. However, while photoelectron spectroscopy of clusters, and in particular rare-gas clusters, has been a growing field since the late 1980s [3,4], there is a paucity of angle-resolved measurements, mainly due to low target densities in the cluster beam and the resulting low signal intensities in angle-resolved measurements. To date, measurements of the photoelectron angular distribution parameter are only available for small metal clusters [5]. For rare-gas clusters, recent qualitative studies by Öhrwall et al. [6] have shown substantial differences in the angular dependence of the photoelectron intensity from Xe clusters compared to free Xe atoms, but their experiment did not provide absolute measurements of the angular distribution parameter.

We have carried out the first quantitative measurement of the photoelectron angular distribution parameter as a function of photon energy and cluster size for any rare-gas cluster system. Our experimental results are supported by multiple scattering calculations, which elucidate the effect of elastic electron scattering. The measurements were carried out with linearly polarized synchrotron radiation from the undulator beamlines 8.0.1, 9.0.2, and 10.0.1 of the ALS to cover a broad photon energy range. A beam of rare-gas van der Waals clusters was produced by an adiabatic expansion cluster source and crossed with a beam of tunable synchrotron radiation bandwidth (100–150 meV). For the present experiment, xenon gas was expanded in order to produce clusters with average sizes  $\langle N \rangle$  between 60 and 8000 atoms [7]. Photoelectrons were detected simultaneously in two electron TOF analyzers situated in the plane perpendicular to the light propagation direction at the “magic angle” (54.7°) and at 0° with respect to the light



polarization. Simultaneous measurement at both angles is crucial for a quantitative determination of the photoelectron angular distribution parameter as it is independent of temperature and density fluctuations of the cluster beam.

The cluster size dependence of the angular distribution parameter for Xe 4d surface and bulk photoelectrons, measured at a photon energy  $h\nu=150$  eV, where the angular anisotropy  $\beta$  is highest, is presented in Fig. 1. A significant decrease of the angular distribution parameter of the bulk component is observed for average cluster sizes larger than  $\langle N \rangle=1000$ , while the angular distribution of the surface component is only slightly smaller than the atomic value and stays constant within the range of the experimental error. These observations are consistent with the qualitative findings by Öhrwall *et al.* [6], who reported a more isotropic angular distribution of photoelectrons from clusters with



**Figure 1** Xe 4d photoelectron angular distribution parameter at  $h\nu = 150$  eV as a function of cluster size.

average sizes  $\langle N \rangle=1000-4000$  compared to photoelectrons from free atoms. This effect is attributed to elastic scattering of the photoelectrons by neighboring atoms in the cluster, leading to more isotropic angular distributions for electrons from the interior of the cluster than for those from the surface or a free atom. In order to investigate the role of electron scattering in more detail, we have performed multiple scattering (MS) model calculations [8] and compare them to our experimental data. Our model calculations reproduced the experimentally observed trends [8] and confirm that the increased isotropy of the cluster photoelectrons can be attributed to elastic scattering of the ejected electrons by the neighboring atoms in the cluster.

Graduate student Ms. Huaizhen Zhang is presently analyzing similar data in the case of Kr and Ar clusters in order to find out if there is a trend in size effects, in other  $Z$  rare gas clusters probed using angle-resolved photoelectron spectroscopy. This work will be part of her PhD dissertation.

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## 4.2 Shape Resonances in K-shell Photodetachment of Small Size-Selected Clusters: Experiment and Theory

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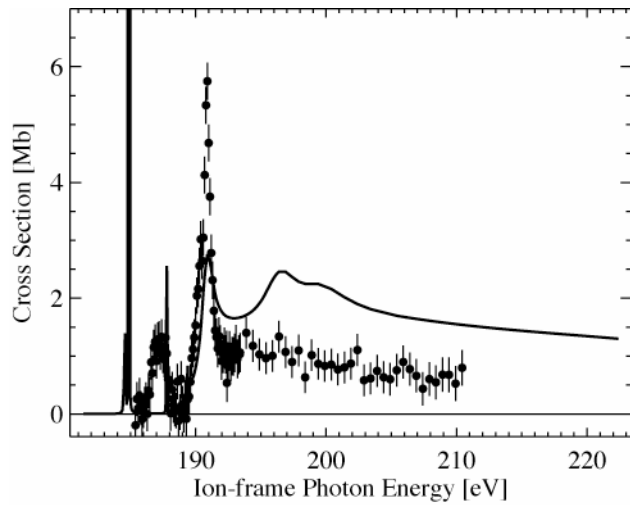
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Inner-shell photoexcitation/photodetachment offers the unique opportunity to study clusters and molecules with site specificity. While the interaction between photons and molecules or clusters is more intricate than the atomic case (due to the more complicated electronic structure and coupling to nuclear motion in the polyatomic system), the site specificity of inner-shell excitation can make the complex reaction dynamics tractable as was found in this work.

K-shell absolute photodetachment cross sections of size-selected  $B_2^-$  and  $B_3^-$  cluster anions has been measured and calculated for the first time. They display two mechanisms, ionization and dissociation leading to many possible decay pathways. The  $B_2^-$  case consists of three possible decay pathway:(a)  $B_2^- + h\nu \rightarrow B_2^+ + 2e^-$ ; (b)  $B_2^- + h\nu \rightarrow B^+ + B + 2e^-$ ; (c)  $B_2^- + h\nu \rightarrow B^+ + B^- + e^-$ . These processes lead to the loss of two electrons due to direct double ionization or most probably due to single ionization followed by Auger decay. Our experimental technique allowed for only the measurement of cationic products, i.e.  $B_2^+$  and  $B^+$ , but not of neutral B. In addition we attempted to detect  $B^-$ , but none was observed. The experimental absolute photodetachment cross sections exhibit bound resonances below threshold and two shape resonances above the K-shell threshold. Similar results were obtained for all of the cationic products observed,  $B^+$  and  $B_2^+$  from  $B_2^-$ , as well as  $B^+$ ,  $B_2^+$  and  $B_3^+$  from  $B_3^-$ .

These findings are similar to the recent measurement and calculation results in the photodetachment of the monomer  $B^-$  resulting in  $B^+$  [1]. The resonances below threshold are likely arising from sequential double Auger decay of the resonant states. Moreover, photodetachment scattering dynamics calculations of  $B_2^-$  have been carried out using the multichannel Schwinger variational method. It is capable of accounting for both initial and final-state correlation effects through a configuration-interaction (CI) treatment of anionic and final (neutral) target state, and of the interchannel coupling, through a limited-size close-coupling (CC) expansion of the stationary scattering wave function.

The overall agreement between measured and calculated photodetachment cross sections is very good as shown in Figure 1. However, the theoretical study yielded additional bound resonances below threshold not observed in the experimental data [2].



**Figure 1** Comparison between the measured two-electron detachment ( $B^+ + B_2^+$ ) yields from  $B_2^-$  (filled circles) and theoretical 5C-MCCI results for  $B_2^-$  single electron photodetachment (solid line).

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### 4.3 Photo Double Detachment of $\text{CN}^-$ : Electronic Decay from an Inner-Valence Hole in Molecular Anions

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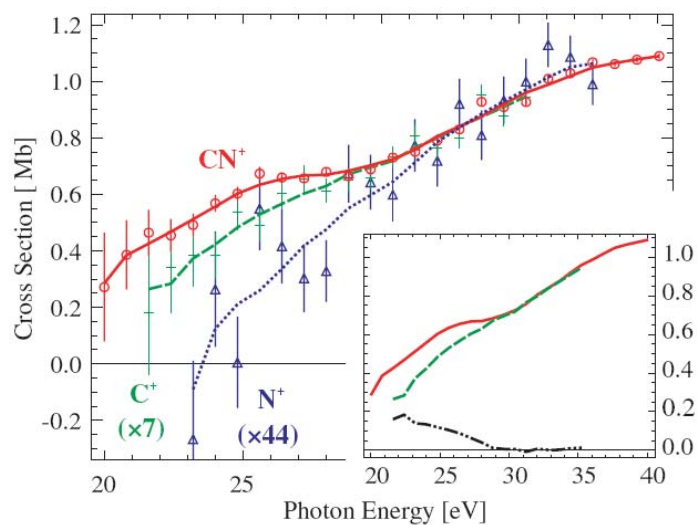
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The first experimental and theoretical inner-valence photodetachment studies from a molecular negative ion,  $\text{CN}^-$ , have been carried out around the 2-electron threshold (25–90 eV). The work is motivated by a phenomenon predicted recently by Santra et al. [1] to occur in molecular anions, but not generally in neutral or cationic targets. Specifically, theoretical work [1] predicted that the removal of one inner-valence electron from  $\text{CN}^-$ , giving rise to inner valence excited  $\text{CN}$ , can result in the formation of vibrationally bound  $\text{CN}^+$  through a relaxation mechanism that occurs via electron emission, effectively leading to double detachment. In the case of  $\text{CN}^-$ , the majority of the singly detached  $3\sigma$  states is located above the  $\text{CN}^+$  continuum threshold, and can thus decay by electron emission. This mechanism is usually ruled out for small neutral molecules because insufficient internal energy is available for electron emission, but is predicted to be generally accessible for molecular anions.  $\text{CN}^+$  is produced by the removal of two electrons either simultaneously or sequentially through an inner-valence mediated process, while the weaker  $\text{C}^+$  and  $\text{N}^+$  signals are produced by dissociation of the excited molecule. The cross sections for all the products exhibit a similar shape as described in detail in Ref. [2]. In order to have detailed information about the onset of the photo-double-detachment process, we measured with improved statistics the molecular photodetachment and dissociation channels near the  $\text{CN}^-$  double-detachment threshold. The three products curves are shown in Figure 1 scaled to coincide around 34 eV. The ‘knee’ shown in Figure 1 is consistent with the theoretical predictions [1]. This work demonstrates the inner-valence mediated production of  $\text{CN}^+$ , as predicted [1]. The present result is the first experimental demonstration of this effect in anions. This electron emission relaxation mechanism is forbidden in isoelectronic neutral molecules ( $\text{CO}$  and  $\text{N}_2$ ) because their inner valence regions lie below the double ionization channels.



**Figure 1** Measured  $\text{CN}^+$  ( $\circ$ ),  $\text{C}^+$  ( $+$ ), and  $\text{N}^+$  ( $\Delta$ ) production following photodetachment of an inner-valence electron just above the 2-electron threshold. Scale factors of 7 ( $\text{C}^+$ ) and 44 ( $\text{N}^+$ ) have been applied so that the magnitude of the curves are comparable in the region around 34 eV

To more clearly show the ‘knee’, the same smoothed curves for  $\text{CN}^+$  and  $\text{C}^+$  are plotted in the inset with the difference between these curves plotted as the dash-dot-dot curve.

### Acknowledgement:

All of the research work reported here is supported by the DoE, Office of Science, Basic Energy Sciences, Division of Chemical, Geosciences and Biological Science. D. Rolles is indebted to the Alexander von Humboldt Foundation for a Feodor Lynen Fellowship.

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## 4.4 X-Ray Absorption in Carbon Ions Near the K-Edge

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K-shell photoabsorption calculations are important for determining the elemental abundances of the interstellar medium (ISM) from observed X-ray absorption spectra.

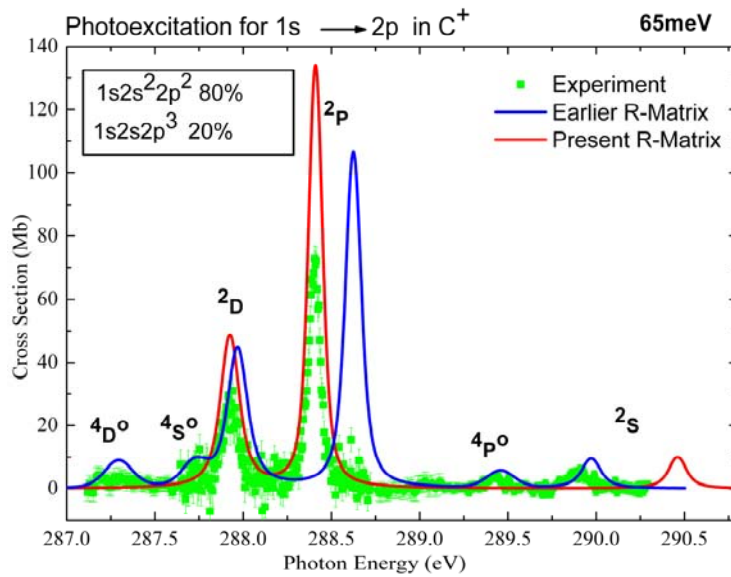
Our interest in inner-shell photoabsorption began through collaborations with experimental researchers at synchrotron radiation facilities, including the Advanced Light Source (ALS). In order to provide theoretical support in the interpretation of high-resolution photoabsorption measurements, it was found that, within our R-matrix approach, it is necessary to include spectator Auger broadening using an optical potential [1] and relaxation effects by using additional pseudoorbitals with the necessary pseudoresonance removal [2]. Use of this R-matrix optical potential method gave excellent agreement with inner-shell synchrotron measurements for O, Ne, and Ar [3,4,1].

Furthermore, astronomers analyze the spectrum of X-rays from distant emitters to study the contents of the ISM. In the X-ray energy region, the inner-shell excitation and ionization features of the elements in the ISM can be easily detected in the spectrum. The advent of new satellites with high-resolution features has opened a new window to study the ISM. For instance, photoabsorption features found in carbon to iron ions fall into the spectral range of data obtained from the Chandra (<http://chandra.harvard.edu/>) and XMM-Newton (<http://xmm.vilspa.esa.es/>) missions. Therefore, astrophysicists need reliable photoabsorption data to study the high-resolution X-ray spectra transmitted through the ISM.

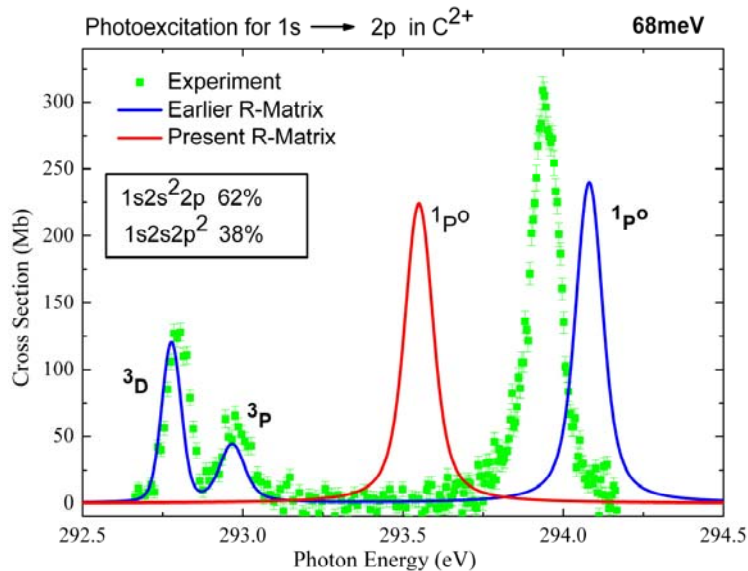
Recently, K-shell photoabsorption cross sections of O [3,5] and Ne [4,6] ions were computed. Those results were used with high-resolution spectroscopy of the ISM [7,6] to determine the ISM abundances of oxygen and neon ions in various observations of X-ray-emitting cosmic sources.

Previously, we performed reliable K-shell photoabsorption calculations for oxygen [3,5,7] and neon [4,7] ions. Here, we have executed detailed R-matrix calculations for carbon ions, where we have included both Auger broadening and relaxation effects by using an optical potential [1] and pseudoorbitals with the necessary pseudoresonance elimination [2] respectively.

We have compared our latest  $1s \rightarrow 2p$  absorption results for  $C^+$  and  $C^{2+}$  with available earlier experimental and theoretical R-matrix results [8, 9] (see Figures 1 and 2).



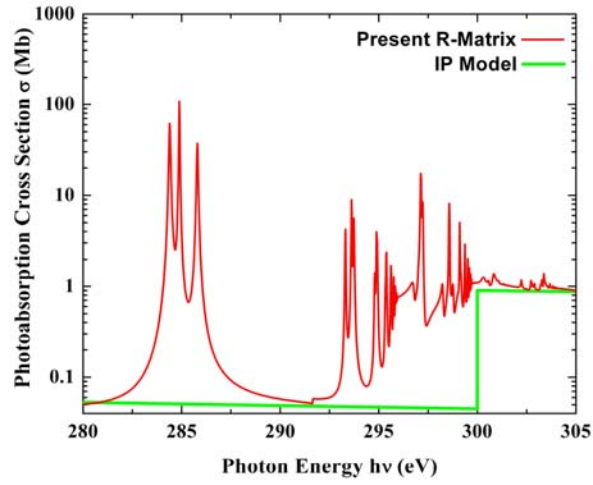
**Figure 1** Comparison among earlier R-matrix and experimental [8] results and present optical potential R-matrix results. The agreement between present R-matrix and experimental results is good in energy scale comparing to earlier R-matrix and experimental results, but there is a poor agreement in line strength.



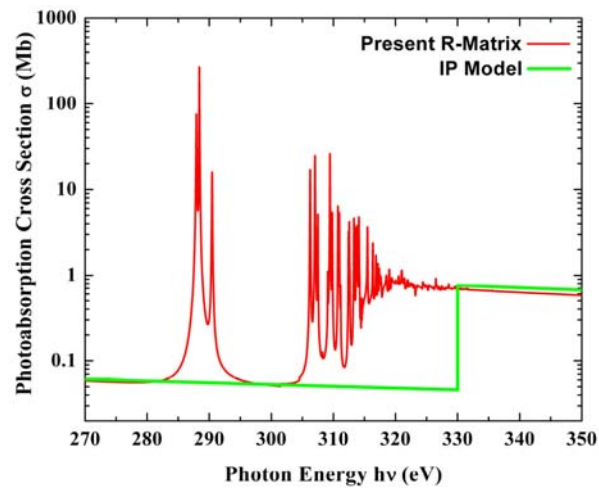
**Figure 2** Comparison among earlier R-matrix and experimental [9] results and present optical potential R-matrix results. The agreement between present R-matrix and experimental results is good in energy scale comparing to earlier R-matrix and experimental results, but there is a poor agreement in line strength.

Also, we have compared our photoabsorption cross sections (see Figures 3-5) with that obtained using an independent particle model (Reilman and Manson 1979). As is clearly seen, our background cross section is in agreement with the IP results. Note that all previously-reported work only includes the strong  $1s \rightarrow 2p$  absorption features, but our results also include the important  $1s \rightarrow np$  absorption features that are necessary for understanding abundances in the ISM.

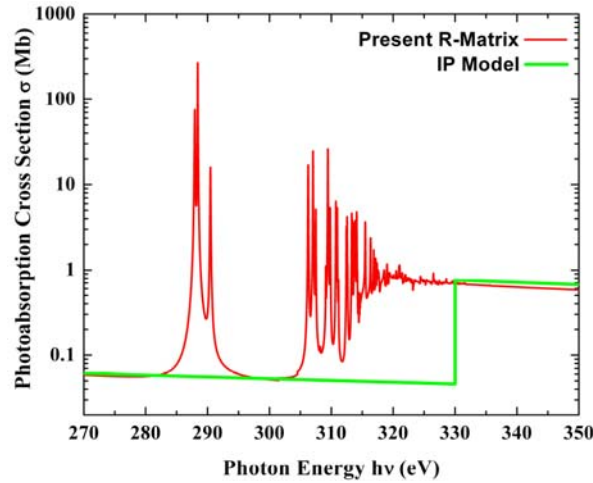




**Figure 3** K-shell photoabsorption cross section of C at the K-edge. Logarithmic plot showing the natural-width resonance features and the oft-used, resonance-less IP model results [10].



**Figure 4** K-shell photoabsorption cross section of C<sup>+</sup> at the K-edge. Logarithmic plot showing the natural-width resonance features and the oft-used, resonance-less IP model results [10].



**Figure 5** K-shell photoabsorption cross section of C<sup>2+</sup> at the K-edge. Logarithmic plot showing the natural-width resonance features and the oft-used, resonance-less IP model results [10].

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## 4.5 Anomalous Behavior of Auger and Radiative Rates and Fluorescence Yields

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The fluorescence yield is an indicator of the response of a system to the vacancy created by the excitation or ionization of an inner-shell electron. Specifically, the fluorescence yield is the measure of the fraction of these inner-shell vacancies that relax via emission of a photon (typically an X-ray), as opposed to relaxation via nonradiative Auger decay. Defining the radiative decay rate as  $A_r$  and the Auger decay rate as  $A_a$ , then the (K-shell, for our purposes) fluorescence yield,  $\omega_K$ , is defined as

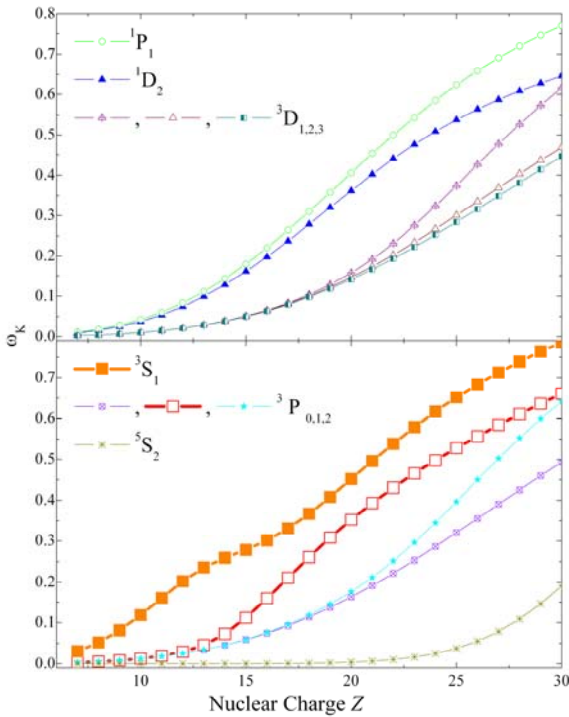
$$\omega_K = \frac{A_r}{A_a + A_r}.$$

Thus, the fluorescence yield provides general information as to how the inner-shell vacancy relaxes. The fluorescence yields resulting from excitation or ionization of inner-shell electrons from neutral atoms has been the subject of numerous studies, experimental and theoretical [1-2]. For multicharged positive ions, there is effectively no experiment. But there does exist a body of theoretical work [3-4], stimulated largely by the needs of x-ray astrophysics and plasma research, where a quantitative understanding of the creation and decay of inner-shell vacancies of atomic ions is of great importance. In particular, these data are used in various state-of-the-art astrophysical modeling codes [5-7]. Of significance here is that much of the fluorescence yield data employed has resulted from interpolation and extrapolation techniques [8]. In this work it is shown that such procedures could produce rather inaccurate results. Specifically, our present work explores the fluorescence yields of the  $^3S_1$  and  $^3P_1$  states of the six-electron  $1s2s^22p^3$  inner-shell-vacancy isoelectronic sequence, along with the associated radiative and Auger decay rates (see Figures 1 and 2).

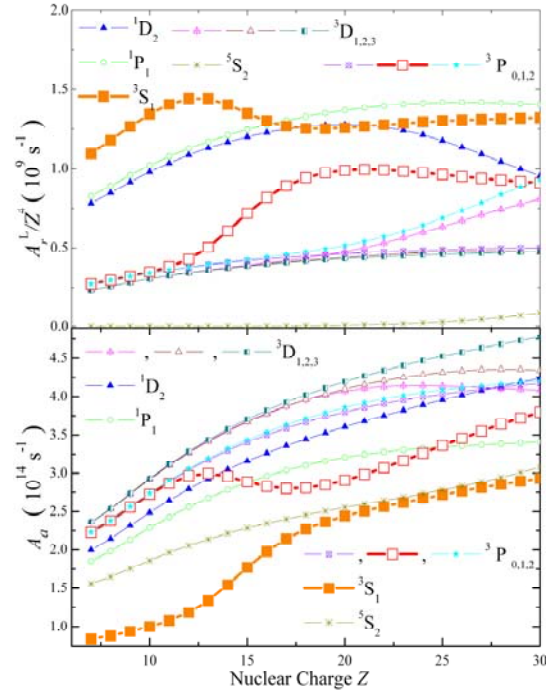
We have employed the atomic structure and collision code AUTOSTRUCTURE [10] to calculate *ab initio* matrix elements contributing to the various energy levels and rates  $A_r$  and  $A_a$ . We have also recomputed earlier results [4] using a multiconfiguration Dirac-Fock (MCDF) method that has been amended to treat the lower- $Z$  region better. As this approach is based on the Dirac equation, it implicitly includes all relativistic effects. We have found that these two approaches are usually in quite good agreement for fluorescence yield calculations [12-13]. Of particular interest is the anomalous behavior of these rates, as a function of  $Z$ , which translates to anomalous behavior of the fluorescence yields; this phenomenology is described and explained [14].

The anomalous behavior seen in the quantities  $A_r$ ,  $A_a$ , and, accordingly,  $\omega_K$ , can be explained by consideration of configuration interaction (CI) and semi-relativistic interactions between the three (single-configuration (SC), nonrelativistic) eigenstates  $|\psi_1\rangle = |1s2s^22p^3(^3P_1)\rangle$ ,  $|\psi_2\rangle = |1s2p^5(^3P_1)\rangle$ , and  $|\psi_3\rangle = |1s2s^22p^3(^3S_1)\rangle$ , leading to a “mixed” state for what we label as, for example, “ $1s2s^22p^3(^3P_1)$ ”:  $|\psi\rangle = c_1|\psi_1\rangle + c_2|\psi_2\rangle + c_3|\psi_3\rangle$ . In going from a non-relativistic (LS), single-configuration approximation (Fig. 3a) to a full LSCI calculation (Fig. 3b), the energies of states 1 and 3 now cross at  $Z \approx 20$ . The (relatively small) spin-orbit interaction at low-to intermediate- $Z$  nevertheless enhances mixing between these same states due to the well known Von Neuman-Wigner [15] avoided crossing phenomena due to small energy eigenvalue differences (see Figures 3b,c, and d).

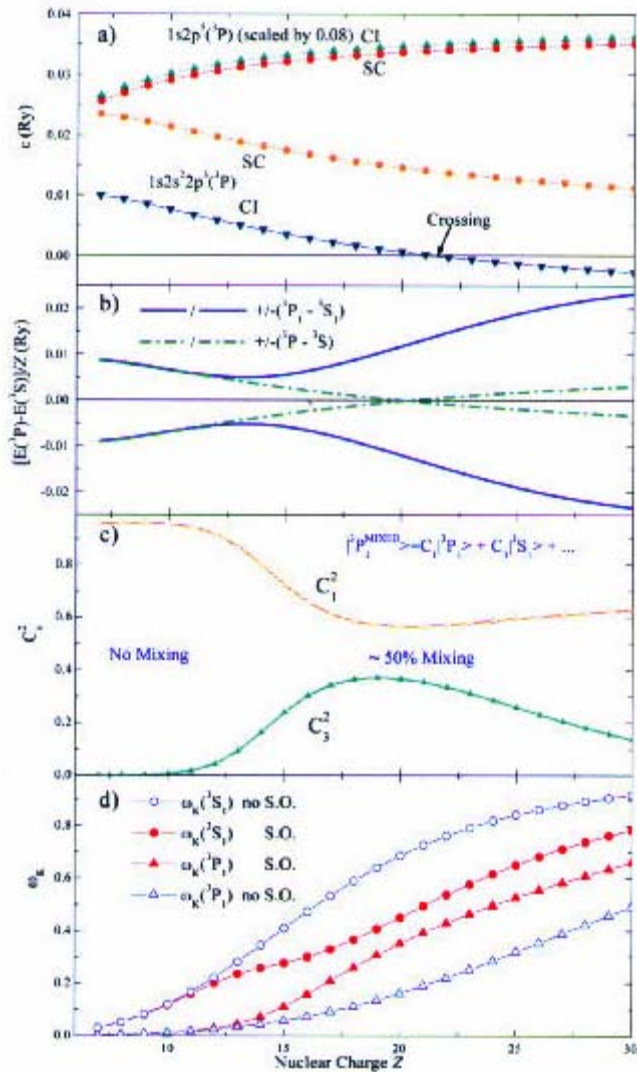
In conclusion, we have demonstrated that higher order CI, spin-orbit, and energy crossing effects, all considered together, can result in anomalous behavior of the calculated radiative and Auger rates and fluorescence yields. This can be understood by considering the well known Von Neuman-Wigner avoided crossings phenomena; an accidental degeneracy, or crossing, of the  $1s2s^22p^3(^3P_1)$  and  $1s2s^22p^3(^3S_1)$  non-relativistic energies at  $Z \approx 20$  results in significant spin-orbit mixing (nearly 50% of each). This in turn leads to final radiative and Auger rates of mixed character and unpredictable behavior as a function of  $Z$ . Consequently, we have demonstrated that, in general, even interpolation of rates and yields along an isoelectronic sequence is unsafe and for one more reason, explicit calculations for each member of a sequence is necessary.



**Figure 1** Calculated fluorescence yields  $\omega_K$  for K-shell vacancy C-like  $1s2s22p3(2S+1LJ)$ .



**Figure 2** Calculated radiative Ar (top) and Auger Aa (bottom) rates for the 10 K-shell vacancy levels  $1s2s22p3(2S+1LJ)$  of the C-like isoelectronic sequence. Note that Ar is scaled by  $1/Z^4$  to factor out the strong  $Z^4$  dependence.



**Figure 3** (a,b) Scaled energies  $(E_i - E_3^{SC})/Z$  of the three states considered at various levels of approximation, showing in (b) an energy crossing ( $E_1^{CI} - E_3^{CI}$  goes through zero) at  $Z \approx 20$ . In (a), the CI between states 1 and 2 causes a constant shift downward (upward) in  $E_1(E_2)$  by a term linear in  $Z$ , as can be shown by studying a typical 2-state system with interactions based on hydrogenic scaling. In (c), the mixing coefficients  $c_1^2$  and  $c_3^2 \approx 1 - c_1^2$  show the relative weightings between the two closely-interacting  $1s2s^2 2p^3$  ( $J=1$ ) levels due to spin-orbit effects. In (d), the fluorescence yields excluding and including spin-orbit effects for the  $1s2s^2 2p^3(^3P_1)$  and  $1s2s^2 2p^3(^3S_1)$  states. The anomalous fluorescence yield behavior of the resultant “states” is seen to occur once there is appreciable spin-orbit mixing  $c_3^2 \leq c_1^2$ .

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## 4.6 Modeling of Low-Energy Resonant States in the Photorecombination Spectra of $\text{Ti}^{4+}$ Ions

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Atomic structure of low-charged Ar-like ions, particularly inner-shell excitation followed by autoionization, revealed that contributions to the total photorecombination (PR) cross sections coming from low-energy resonant states can be significant [1-3]. This work is based on benchmark calculations for ions with partially filled M shells [4, 5], and represents continuation of our efforts to accurately address electron-ion recombination of  $\text{Ti}^{4+}$  ions [6]. Using an iterative deconvolution procedure [7] we are able to extract the experimental dielectronic recombination (DR) cross section from storage ring data [3]. As a result, we can investigate subtle features of interference between DR and radiative recombination (RR) channels, which are manifested most clearly in the asymmetry of the broad  $3p^5 3d^2 \ ^2F$  autoionizing state [1]. Furthermore, we demonstrate that nearby  $3p^5 3d 4s \ ^2P$  resonances play a crucial role in describing the shape of the  $3p^5 3d^2 \ ^2F$  resonance.

The cross section for PR of a free electron, at energy  $\epsilon = E_c - E_{ion}$  above the ground state  $E_{ion}$  of the target ion, into a bound state  $b$  of the recombined ion, is given by [1, 8]:

$$\sigma_{c \rightarrow b}^{\text{PR}} = \frac{8\pi}{3} \frac{g_b}{2g_{ion}} \frac{\alpha^3 \omega_{c \rightarrow b}^3}{k\epsilon} |M_{b \rightarrow c}|^2, \quad (1)$$

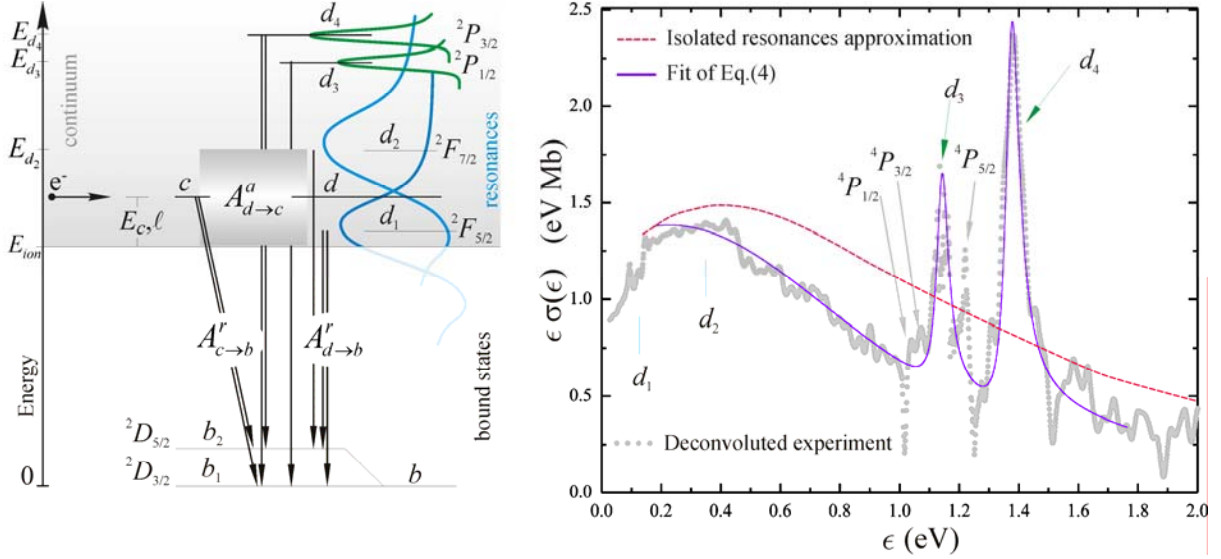
where  $\omega_{c \rightarrow b}$  is the frequency of radiation field,  $\alpha$  is the fine-structure constant,  $k$  is the linear momentum of the continuum electron,  $g_b$  and  $g_{ion}$  are the statistic weights of the bound state  $b$  in the recombined ion and the ground state of the target ion, and  $M_{b \rightarrow c}$  is the complex photoionization (PI) matrix element of the corresponding transition and may be expressed as:

$$M_{b \rightarrow c} = \langle c | \mathbb{R} | b \rangle \left( 1 + \sum_d \frac{Q_{b \rightarrow c}^d - \imath B_{d \rightarrow c}^a}{\epsilon_d + \imath} \right). \quad (2)$$

In Eq. (2),  $\mathbb{R}$  represents the electric-dipole moment of the recombined ion (in atomic units),  $|b\rangle$  is the bound state in recombined ion and  $|c\rangle$  is the ground state of the target ion plus continuum electron, the reduced center-of-mass collision energy is  $\epsilon_d = (E_d - E_c)/(\bar{\Gamma}_d/2)$  in the vicinity of the doubly-excited state  $|d\rangle$  with total width  $\bar{\Gamma}_d$  and branching ratio  $B_{d \rightarrow c}^a = A_{d \rightarrow c}^a/\bar{\Gamma}_d$  for autoionization. In most cases that we study, a short-lived resonant state  $|d\rangle$  will Auger decay without completing the PR, meaning its total width is dominated by its autoionization rate  $A_{d \rightarrow c}^a$  and consequently  $B_{d \rightarrow c}^a \approx 1$ . The partial PR cross section involving a doubly-excited resonant state  $|d\rangle$  can be described by a Fano profile [9, 10] with an asymmetry parameter  $Q_{b \rightarrow c}^d$  given by:

$$Q_{b \rightarrow c}^d = \frac{\langle c | \mathbb{V} | d \rangle \langle d | \mathbb{R} | b \rangle}{(\Gamma_d / 2) \langle c | \mathbb{R} | b \rangle}. \quad (3)$$

In Eq. (3),  $\mathbb{V}$  represents the electron-electron interaction (in atomic units) between the captured electron and all target electrons, which is responsible for the autoionizing nature of the resonant state  $|d\rangle$ .



**Figure 1** Modeling of the resonant low-energy part of the experimental DR spectra of  $Ti^{4+}$ . (left) Schematic diagram of the most relevant electron-ion recombination paths involving two asymmetric  $3p^5 3d^2 2F_{5/2,7/2}$  resonances straddling the first ionization limit  $E_{ion}$ . Zero energy is assigned to the  $2D_{3/2}$  ground state of  $Ti^{3+}$ . (right) Comparison of the deconvoluted experimental DR spectra, its best fit using Eq.(4) and the effect of the isolated resonances approximation on the shape and the strength of the  $3p^5 3d^2 2F_{5/2,7/2}$  autoionizing states.

In principle, the sum in Eq. (2) goes over all doubly-excited states  $|d\rangle$  that are accessible by the free electron and the total PR cross section is obtained by summing Eq. (1) over all recombined bound states  $|b\rangle$  open for radiative decay of  $|d\rangle$ . Modeling of the total PR cross section of  $Ti^{4+}$  ions has been done for collision energies  $\epsilon$  below 2 eV (see Fig.1). This low-energy part of the photorecombination spectrum contains seven resonant states, two of which are  $3p^5 3d^2 2F_{5/2,7/2}$  that are broad, asymmetric, and straddling the first ionization limit  $E_{ion}$ . The other five resonant states belong to the  $3p^5 3d 4s$  configuration. Three remaining states  $3p^5 3d 4s 4P_{1/2,3/2,5/2}$  are much weaker and presently are excluded from further consideration. The hyperfine structure of the ground state in the recombined  $Ti^{3+}$  ion consists of the  $3p^6 3d 2D_{3/2,5/2}$  levels, denoted in Fig.1 as  $|b_1\rangle$  and  $|b_2\rangle$  respectively. Radiative decay of all four resonances considered here is predominantly to those two bound states, leading to an approximate form of the total PR collision strength:

$$\epsilon \sigma^{PR}(\epsilon) \approx \frac{8\pi}{3} \sum_{b=b_1}^{b_2} \frac{g_b}{2g_{ion}} \frac{\alpha^3 \omega_{c \rightarrow b}^3}{k} |\langle c | \mathbb{R} | b \rangle|^2 \left| 1 + \sum_{d=d_1}^{d_4} \frac{Q_{b \rightarrow c}^d - \nu}{\epsilon_d + \nu} \right|^2 \quad (4)$$

Even in its approximate form, Eq.(4) involves tedious algebraic manipulation mainly due to the complex nature of the PI matrix, and in order to use it for modelling purposes, all fitting parameters had to be renormalized to parameters belonging to the broad and asymmetric



resonances  $3p^5 3d^2 \ ^2F_{5/2,7/2}$ . In this way, we fit only the resonance position  $E_{d_1}$ , its width  $\Gamma \equiv \bar{\Gamma}_{d_1} = \bar{\Gamma}_{d_2}$ , asymmetry parameter  $q \equiv Q_{b_1 \rightarrow c}^{d_1} = Q_{b_2 \rightarrow c}^{d_2}$ , and integrated strength  $S \equiv S_{d_1 \rightarrow b_1}$ . The fitting parameters of all other resonances considered here are conveniently expressed through former ones and assigned an initial value obtained in the present calculations using AUTOSTRUCTURE and R-matrix methods combined with Smith's time delay matrix [11]. Converged values for the fitting parameters are summarized in Table 1 and compared with data found in the literature.

**Table 1** Positions, integrated strengths, widths, and asymmetry parameters for the two lowest resonant states above the first ionization limit of  $Ti^{3+}$  investigated in this work. Numbers in parentheses are experimental uncertainties.

resonant state:	position: $E_d - E_{ion}$ (eV)	integrated strength: $S$ (eV Mb)	width: $\Gamma$ (eV)	asymmetry: $q$
$(d_1) \ 3p^5 3d^2 \ ^2F_{5/2}$	0.1293 <sup>a</sup> , 0.129(1) <sup>†,‡</sup> 0.1295 <sup>c</sup> , 0.19(8) <sup>c</sup>	1.564(5) <sup>†</sup> , 1.34(1) <sup>‡</sup>	1.665 <sup>a</sup> , 1.65(1) <sup>†</sup> 1.5(1) <sup>c</sup> , 1.2(1) <sup>d</sup>	6.16 <sup>a</sup> , 5.9(1) <sup>†</sup> ; 3.1(8) <sup>c</sup>
$(d_2) \ 3p^5 3d^2 \ ^2F_{7/2}$	0.3558 <sup>a</sup> , 0.355(1) <sup>†,‡</sup> 0.3585 <sup>b</sup> , 0.3282 <sup>c</sup> , 0.45(4) <sup>d</sup>	1.642(5) <sup>†</sup> , 0.36(1) <sup>‡</sup>	0.93(4) <sup>b</sup> , 0.77(1) <sup>‡</sup>	3.03(1) <sup>‡</sup>

<sup>a</sup>) Present calculations; <sup>†</sup>) Parameters obtained by fit to Eq(4); <sup>‡</sup>) Fit to Eq(4) without  $3p^5 3d4s$  resonances and neglecting  $d_1 - b_2$  contribution [6];  
<sup>b</sup>) Vacuum spark emission spectroscopy (unresolved resonances) [12]; <sup>c</sup>) Theory [13]; <sup>d</sup>) PR experiment (fit of unresolved resonances) [3a]; <sup>e</sup>) PI experiment (fit of unresolved resonances) [3b].

We conclude that the calculated and fitted values for resonance positions are in excellent agreement, as long as the modelled PR cross section accounts for the dominant part of the resonance interaction. Furthermore, any attempt to reproduce experimental spectra within the isolated resonances approximation will give more asymmetric, narrower and weaker  $3p^5 3d^2 \ ^2F_{5/2,7/2}$  profiles than what computational results suggest. This becomes more evident as the main findings of [6] are reinstated simply by retaining only  $|d_1\rangle$  and  $|d_2\rangle$  resonances in Eq.(4) and by ignoring  $d_1 \rightarrow b_2$  contributions.

### Acknowledgments:

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## 4.7 Shape Resonances in the Absolute K-Shell Photodetachment of $B^-$

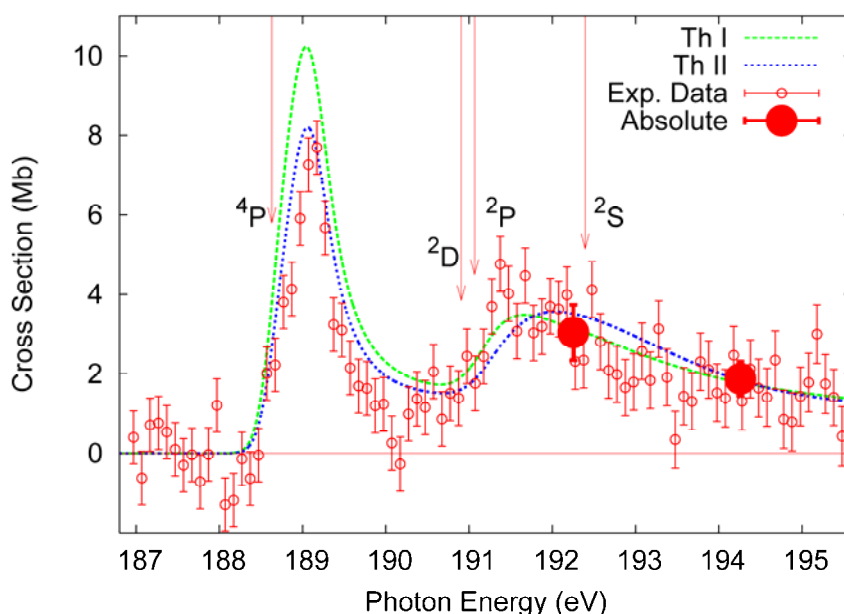
N. Berrah,<sup>1</sup> R. C. Bilodeau,<sup>1,2</sup> I. Dumitriu,<sup>1</sup> J. D. Bozek,<sup>2</sup> N. D. Gibson,<sup>3</sup> C. W. Walters,<sup>3</sup> G. D. Ackerman,<sup>2</sup> O. Zatsarinny,<sup>1</sup> and T. W. Gorczyca<sup>1</sup>

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<sup>2</sup>Lawrence Berkeley National Laboratory, Advanced Light Source, Berkeley, CA 94720

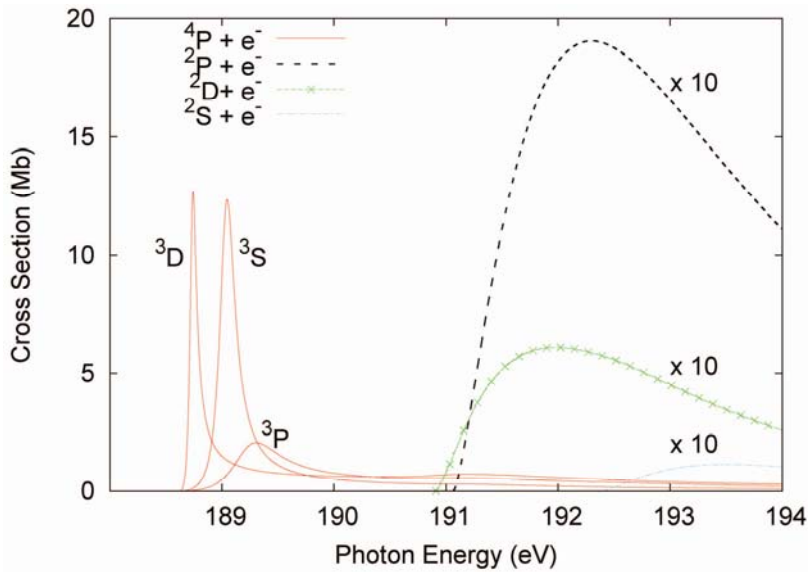
<sup>3</sup>Denison University, Granville, OH 43023

The present work has explored experimentally and theoretically the K-shell photodetachment of a light negative ion,  $B^-$ . The experiment was able to provide absolute cross sections that could then be compared directly to two separate, somewhat different R-matrix calculations (see Figure 1).



**Figure 1** Lower-resolution (390 meV) detection of  $B^+$  ions following K-shell photodetachment of  $B^-$  over a broad photon energy range. The open red circles are the experimental data while the two solid red circles are absolute cross section measurements used to calibrate the spectrum. The ThI (non-orthogonal basis, B-spline R-matrix results; long-dashed green curve) and ThII (orthogonal basis R-matrix results; short-dashed blue curve) convoluted (390 meV) results are also shown. The four vertical arrows show the positions of the four  $B^+ 1s2s^2 2p^2$  ( $^4P, ^2D, ^2P, ^2S$ ) thresholds from the ThII calculations (both ThI and ThII results have been aligned such that the  $^4P$  threshold energy is 188.63 eV).

A detailed analysis of the spectrum reveals three near-threshold shape resonances (see Figure 2) that are each accurately described by a combination of Wigner-threshold and Breit-Wigner Lorentzian resonance profiles.

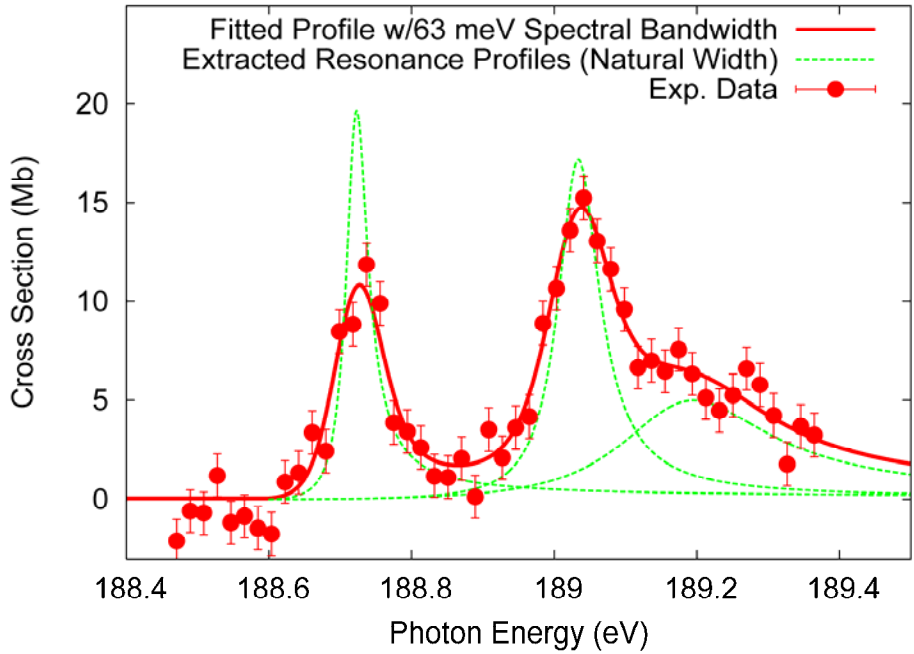


**Figure 2** A partitioning, within the ThII calculations, of the photodetachment cross section into the  $^4P$  (solid red),  $^2P$  (dashed black),  $^2D$  (green crosses), and  $^2S$  (dash-dot cyan) channel contributions. The  $^2D$ ,  $^2P$ , and  $^2S$  channels have been magnified by a factor of 10 for clarity whereas the dominant  $^4P$  channel has been further broken into the incoherent contributions from each of the three final  $^3D$ ,  $^3P$ , and  $^3S$  symmetries, indicating a separate shape resonance within each partial wave.

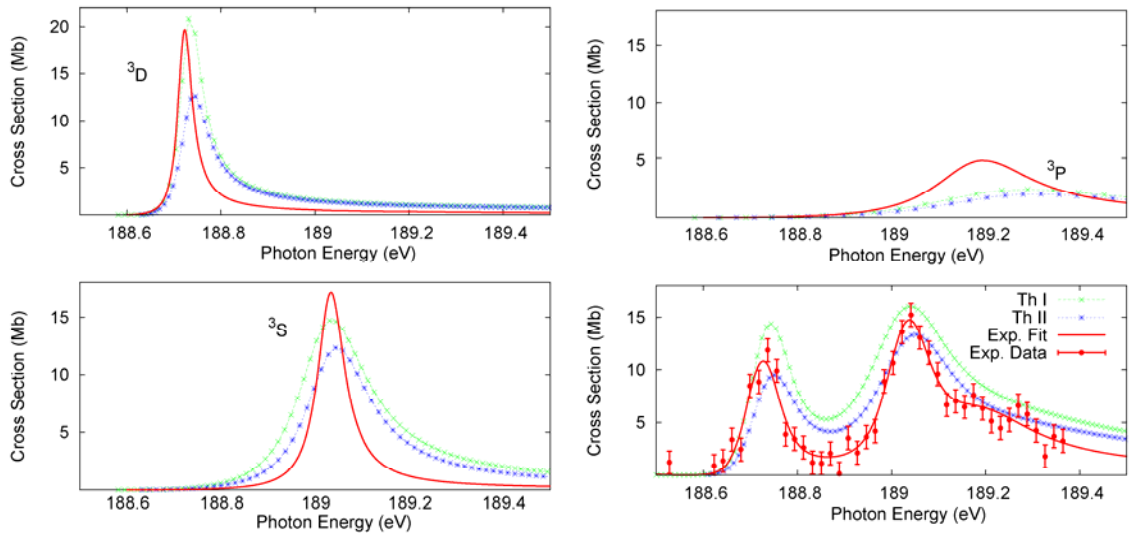
The main difference between our two R-matrix approaches is that the ThI method is tailored to use a sufficiently-large, separate basis of orbitals for *each* of the initial  $B^-$ , intermediate  $B^{*-}$ , and residual  $B$  and  $B^*$  (plus a free electron) states - a so-called non-orthogonal basis approach. The ThI results are in very good agreement with the experimentally-observed spectrum (see Figures 3 and 4) except for a disturbing, unresolved discrepancy, by several standard deviations between the theoretically-predicted and measured widths for the  $1s2s^22p^3(^3S)$  shape resonance and by as much as a factor of two in the energy-integrated resonance cross sections.

The ThII method, being limited to the use of the *same* orthogonal basis to describe each of the initial, intermediate, and final states, is clearly a less accurate description of the photodetachment process in question, yielding resonance energy positions, in particular, that are unphysical. Further convergence of the ThII calculations would require additional consideration of  $4l$  and  $5l$  orbitals and the accompanying single- and double-promotional configuration-interaction expansions, which leads to a tremendously more complicated computation. And since the overall qualitative agreement between ThII and either ThI or experiment, for the most part, seems sufficient, we choose not to pursue further ThII convergence.

Our measurements provide the total cross section which do not allow direct, detailed understanding of the measured features. Nevertheless, we have ruled out the possibility of post-collision photoelectron recapture, which otherwise would require a modification of the computed cross sections to reproduce the actual near-threshold  $B^+$  positive ion yield. In the future, more intense photon sources and higher resolution photoelectron spectroscopy experiments that measure the partial cross sections will allow better quantitative comparisons between theory and experiment.



**Figure 3** Experimental cross sections for K-shell photodetachment of  $B^-$  leading to  $B^+$  over the photon energy range of the first structure shown in Figure. 1. Here, the three structures observed and fitted are the  $1s2s^22p^3(^3D, ^3S, ^3P)$  shape resonances.



**Figure 4** Partial and total cross sections for photodetachment of  $B^-$  leading to  $B^+$  The experimentally-inferred resonance profiles (solid red lines) and theoretical results (green crosses for ThI results, blue squares for ThII results) are shown for (top to bottom) the,  $^3D$ ,  $^3S$ , and  $^3P$  symmetries followed by the summed, convoluted (with 63 meV Gaussians) cross sections.

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## 4.8 Dielectronic Recombination for Al-Like Sulfur

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Dielectronic recombination (DR) is the dominant electron-ion recombination process in both photoionized and electron-collisional plasmas. While earlier DR work has been sufficiently summarized [1-4] our more recent work [5] has involved extensive DR calculations for first and second row isoelectronic sequences [6-14]. Extended work for more complicated, third row isoelectronic sequences has been started [15-18]. These data, along with the radiative recombination (RR) data, have been used to provide new ionization balance determinations for photoionized (low-T) and collisionally-ionized (higher-T) plasmas of astrophysical and/or fusion-related interest. Also, these data are benchmarked against experiment for lower and higher-Z elements [19-23].

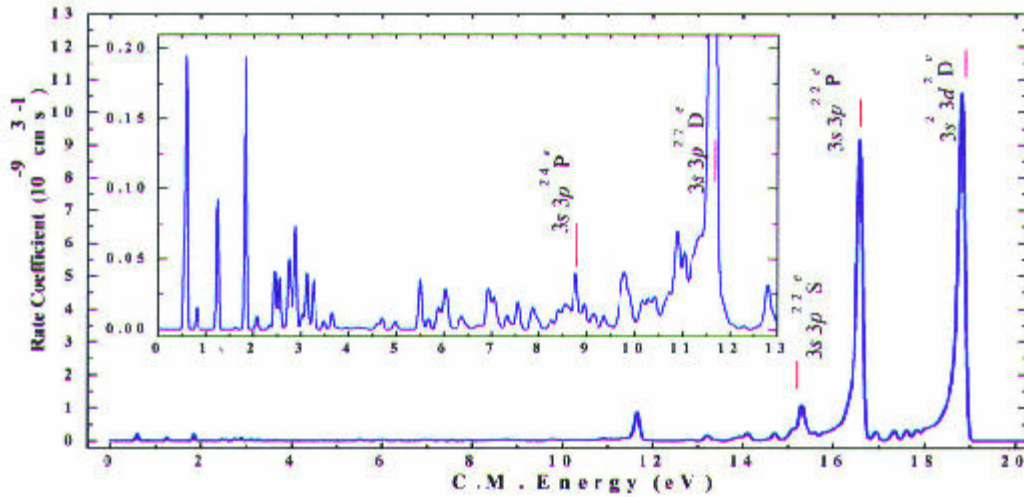
In the independent processes, isolated resonances distorted wave (IPIRDW) approximation, the DR is a two step process. In the first step, the incident electron with energy  $E_i$  is captured by the target ion  $A^{q+}$  forming a doubly excited state  $A^{(q-1)**+}$ .

This unstable doubly excited state can stabilize either by autoionization or by radiation. When the second case takes place, the DR process is completed:

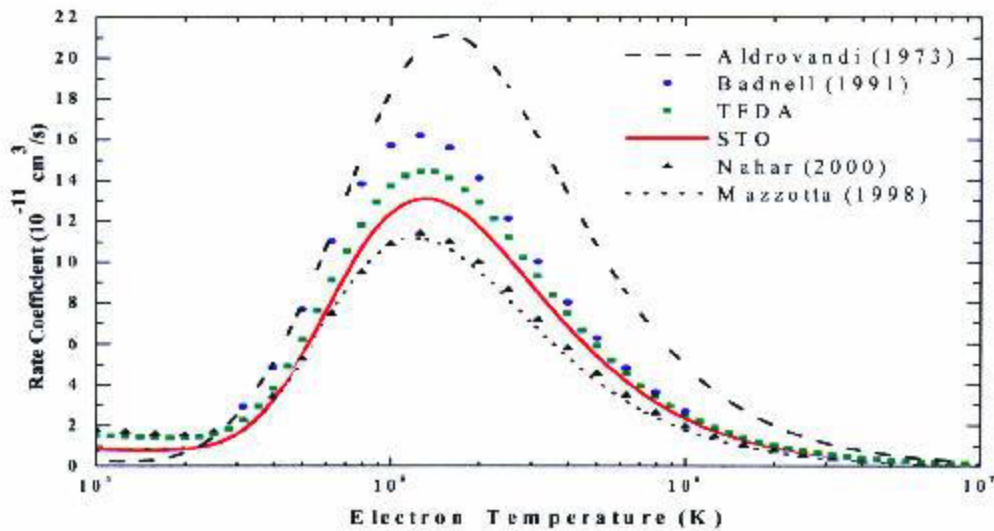


Recently, we have focused our work on the complex third-row M-shell isoelectronic sequences. Al-like  $Fe^{13+}$  DR calculations have been completed and tested against Heidelberg Heavy-Ion Test Storage Ring facility measurements [17]. Also, recombination cross sections and rate coefficients are calculated for M-shell argon atomic ions using a configuration-average distorted-wave method [18], where good agreement is found with previous level-resolved distorted-wave calculations for  $Ar^{6+}$  and  $Ar^{7+}$ .

We extend our efforts for Al-like systems to  $S^{3+}$ . Although previous calculations on  $S^{3+}$  exist [24-27], they were performed only within a non-relativistic LS-coupling approximation. Fig. 1 represents the DR rate coefficients for Al-like  $S^{3+}$  using the level-resolved, multi-configuration, distorted-wave AUTOSTRUCTURE package. We have carried out two different types of calculations for the DR rate coefficients for  $S^{3+}$  by using a Thomas-Fermi-Dirac approximation (TFDA) and a Slater-Type-Orbital (STO) approach. Comparisons between our recent calculations and others are seen in Fig. 2. Calculations for intermediate coupling and other Sulfur ions are underway.



**Figure 1** Calculated non-relativistic (LS) dielectronic recombination rate coefficient for  $S^{3+}$ . Upper inset enlarges the spectra of Rydberg series converging to the two lowest thresholds  $3s3p^2$  ( $^4P^{\circ}$ ) and  $3s3p^2$  ( $^2D^{\circ}$ ). The presented rate coefficient is obtained using a flattened Maxwellian electron velocity distribution often found in heavy-ion storage rings equipped with electron coolers, with parameters  $kT_{\parallel}=0.8$  meV and  $kT_{\perp}=10$  meV.



**Figure 2** Maxwellian rate coefficient (LS) for  $S^{3+}$ : dashed black curve, currently recommended DR+RR by Aldrovandi [1]; Blue circle curve, earlier AUTOSTRUCTURE results by Badnell [25]; green square curve, our results with a TFDA generating potential; red solid curve, our results with a STO generating potential; triangle curve, total DR+ RR by Nahar [27]; black dotted curve, total DR + RR by Mazzotta et al. [4] based on the results of Nahar [27].

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## 4.9 State-Selective Single-Electron Capture in Slow Collisions of $\text{Ne}^{q+}$ ( $q = 4 - 6$ ) Ions with Molecules

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State-selective single-electron capture process for slow collisions of  $\text{Ne}^{q+}$  ( $q = 4 - 6$ ) ions, produced in a recoil-ion source, with atmospheric and cometary gases have been studied experimentally at laboratory impact energies between 15 and 500 qeV (where  $q$  is the projectile charge state) and scattering angles between  $0^\circ$  and  $5^\circ$  by means of a differential energy-gain spectrometer [1].

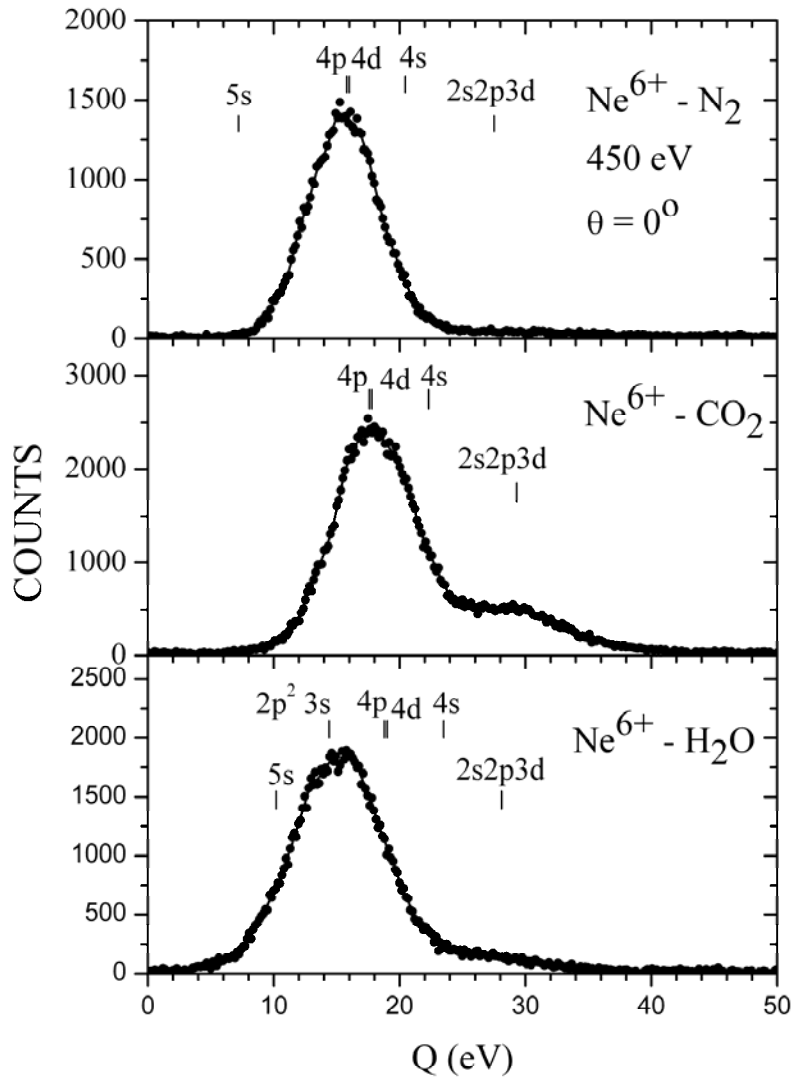
The study of electron capture processes by multiply charged ions from molecular targets has recently received considerable attention. These processes are of interest as they are most likely to have impact on the fields such as low- and high-temperature laboratory plasmas, astrophysics, atmospheric sciences and even material science [2,3].

Figure 1 shows the translational energy-gain spectra for single-electron capture by  $\text{Ne}^{6+}$  ions from  $\text{N}_2$ ,  $\text{CO}_2$  and  $\text{H}_2\text{O}$  at a laboratory impact energy of 450 eV and  $0^\circ$  scattering angle. In  $\text{Ne}^{6+} - \text{N}_2$  and  $\text{CO}_2$  collisions, the dominant peak correlates with non-dissociative single-electron capture into 4p and 4d states of  $\text{Ne}^{5+}$  ions with production of the molecular product ions in the ground state. There is also some contribution from capture into the 4s state of  $\text{Ne}^{5+}$ .

In the  $\text{Ne}^{6+} - \text{CO}_2$  collisions, the unresolved structure at about 29 eV probably arises from core-varying capture into the 3s 3p ( $^3\text{P}$ ) 3d state of  $\text{Ne}^{5+}$ . In  $\text{Ne}^{6+} - \text{H}_2\text{O}$  collisions, capture into  $2p^2 3s$  of  $\text{Ne}^{5+}$  is observed to be the dominant reaction channel. There are smaller contributions due to capture into 5s, 4p, 4d, 4s, and 2s2p3d states. There is probably also some contribution due to transfer excitation into 4p and 4d states of  $\text{Ne}^{5+}$  accompanied by excitation of the target product in the excited states of  $\text{H}_2\text{O}^+$ .

Additional measurements of double-differential cross sections and absolute total cross sections compared to cross-sections calculated using Landau-Zener model are in progress.





**Figure 1** Translational energy-gain Spectra for single-electron capture by 450 eV  $\text{Ne}^{6+}$  ions from  $\text{N}_2$ ,  $\text{CO}_2$  and  $\text{H}_2\text{O}$  targets at  $0^\circ$  scattering angle.

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## 4.10 Non-Dissociative Single-Electron Capture in Slow Collisions of $O_2^{2+}$ Ions with $O_2$ , Ar and Ne

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Experimental and theoretical investigations of dissociative and non-dissociative electron capture processes occurring in collisions between doubly charged molecular ions and atomic or molecular targets have recently received considerable attention. Molecular oxygen ions are of particular interest due to their potential influence on the properties of the ionosphere and their involvement in many atmospheric and astrophysical phenomena.

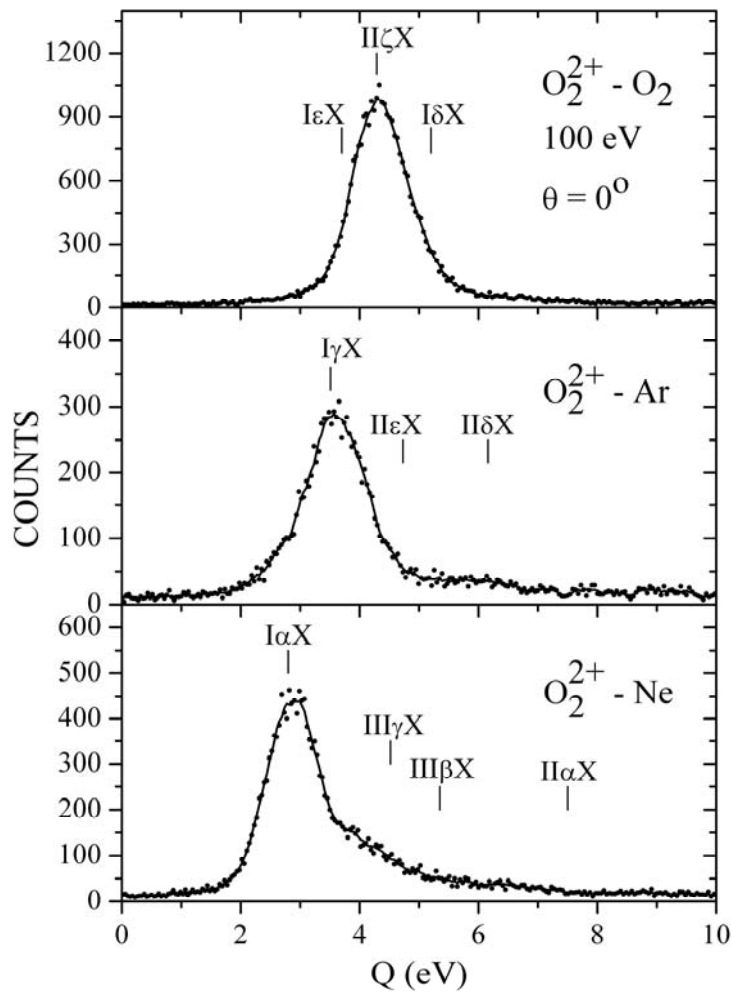
Single-electron capture by  $O_2^{2+}$  ions from atomic targets has been studied previously in the keV region [1]. However, in the case of molecular targets, there have been no previous experimental measurements at low-energy collisions to our knowledge.

In the present work, non-dissociative single-electron capture from He, Ne, Ar,  $O_2$ ,  $N_2$ , and  $H_2O$  by  $O_2^{2+}$  ions produced in a recoil ion source have been studied experimentally at laboratory impact energy of 100 eV and scattering angles between  $0^\circ$  and  $5^\circ$  by means of the translational energy-gain spectroscopy technique [2].

Figure 1 shows the translational energy-gain spectra for single-electron capture by  $O_2^{2+}$  ions from  $O_2$ , Ar, and Ne at a laboratory impact energy of 100 eV and  $0^\circ$  scattering angle. The energy scale in Fig. 1 was calibrated by using the energy-gain spectrum for 100 eV  $N_2^{2+}$  - Ne system that had previously been observed in the same apparatus [2].

In  $O_2^{2+}$  - Ar and Ne collisions, the dominant peak correlates with single-electron capture from ground state ( $^1\Sigma_g^+$ ) of  $O_2^{2+}$  ions into A  $^2\Pi_u$  (peak I $\gamma$ X) and X  $^2\Pi_g$  (peak I $\alpha$ X) states of  $O_2^+$ , respectively. In  $O_2^{2+}$  -  $O_2$  system, the observed spectrum shows that the dominant exit channel (peak II $\zeta$ X) is due to capture by low-lying metastable incident ions into the (c  $^4\Sigma_u$ ) state of  $O_2^+$ .

In all the collision systems studied here, contributions from processes commencing with a long-lived metastable states in the incident  $O_2^{2+}$  ion beam are detected. Additional measurements of differential cross sections are in progress.



**Figure 1** Translational energy-gain spectra for single-electron capture by 100 eV  $O_2^{2+}$  ions from  $O_2$ , Ar, and Ne at  $0^\circ$  scattering angle. The designations I, II, and III represent, respectively, the ground, first, and second electronically excited states of  $O_2^{2+}$ ;  $\alpha$ ,  $\beta$ , and  $\gamma$  represent the ground and subsequent electronically excited states of  $O_2^+$  ion; X represents the ground state of the target product.

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## 4.11 Suppression of Primary Electron Interferences in the Ionization of N<sub>2</sub> by 1 – 5 MeV Protons

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Studies with H<sub>2</sub> have revealed interference structures when an electron is ejected from this two-center system by fast ion impact [1]. The phenomenon of interference associated with electron ejection from homonuclear diatomic molecules is analogous to Young's two-slit experiment with the atomic centers acting as "slits". This atomic Young-type electron interference, previously investigated for Kr<sup>33,34+</sup> ( $v/c \sim 0.3$ ) [1,2,3] and H<sup>+</sup> ( $v/c \sim 0.1$ ) [4] ions interacting with H<sub>2</sub>, is designated the *primary interference* and is in general agreement with theoretical calculations for H<sub>2</sub> [5,6,7]. Fast moving electrons ( $v/c \sim 0.1$ ) interacting with D<sub>2</sub> have also been investigated [8] and found to exhibit similar Young-type interferences. These results have prompted new studies for H<sub>2</sub> by other investigators [9,10,11,12]. Additionally, for Kr<sup>33+</sup> + H<sub>2</sub> [3] and H<sup>+</sup> + H<sub>2</sub> [4] *secondary interference* structures were found to be superimposed on the primary interference pattern with amplitudes 4-5 times smaller than the primary amplitudes. These secondary interferences have been attributed to scattering of the primary ionization wave from the adjacent nucleus causing subsequent interference with the original wave. This latter mechanism was suggested by Kronig [13] in reference to the photoionization of K-shell electrons ejected from one nucleus in a heteronuclear diatomic molecule followed by scattering from the other nucleus.

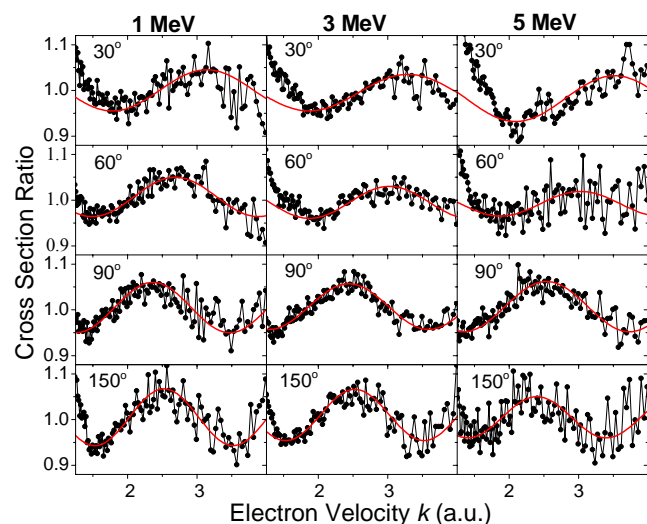
Primary interference structures have been found to depend strongly on the electron observation angle [2,4] and to a lesser extent on the collision velocity [4]. For an observation angle of 90° the primary interferences showed relatively little structure [1,2,3,4], also in agreement with theory [5,6,7]. In contrast, the secondary interference structures, with approximately double the oscillation frequencies, showed little variation with either the emission angle or the collision velocity [3,4], and notably showed equally strong oscillatory structures at 90° as for other angles.

To date, electron interferences in diatomic molecules more complicated than H<sub>2</sub> or D<sub>2</sub> have only been studied for the ejection of particular valence electrons by photons from N<sub>2</sub> and O<sub>2</sub> [14,15] and for the ejection of K-shell electrons in N<sub>2</sub> [16]. In the present work, electron interferences are investigated for the more complicated N<sub>2</sub> molecule (compared to H<sub>2</sub>) impacted by 1 – 5 MeV H<sup>+</sup> ions. Electron emission spectra are measured for ejection energies ranging from 5-410 eV and for observation angles 30° – 150°. The measurements were conducted at Western Michigan University using the 6-MV tandem Van de Graaff accelerator.

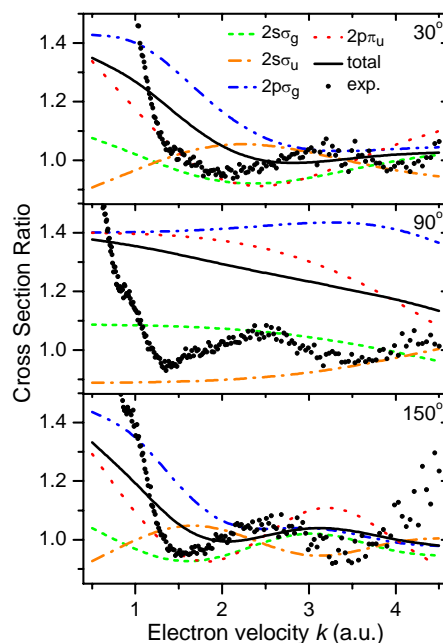
The experimental molecular N<sub>2</sub> cross sections were divided by the theoretical atomic N cross sections, giving ratios as shown in Fig. 1. The cross section ratios, normalized to about unity for convenience, show clear evidence of oscillatory behavior. The striking feature of the ratios shown in Figure 1 is that the oscillatory structures show no significant dependence on the electron observation angle or the collision velocity. Furthermore, the structures for 90° are as prominent as for the other angles. These results are contrary to earlier results for H<sup>+</sup> [4] and Kr<sup>33+</sup> [1,2]+ H<sub>2</sub> for

which there was a strong dependence of the primary interference structures on the observation angle, with no oscillatory structure for  $90^\circ$ , and a smaller but definite dependence on the collision velocity. Qualitatively, these features suggest that the oscillatory structures observed for  $N_2$  are not due to primary interferences, but instead are due to secondary interferences resulting from intramolecular scattering.

In order to provide support for this tentative conclusion, we have performed theoretical calculations for the ionization of  $N_2$  obtaining molecular to atomic cross section ratios. The model takes into account only the first-order interference effects caused by the two-center character of the initial wavefunction and is similar to the formalism developed for  $H_2$  [5]. The results of these first-order calculations for the cross section ratios are presented in Figure 2 along with the experimental data. It is clear from the calculations for the individual molecular orbitals that the different symmetries of the orbitals cause a significant part of the first-order oscillations in the total cross section ratios to cancel and consequently the interference structures are suppressed causing the second-order interferences to dominate. Thus, it seems there is a fundamental difference between  $H_2$  and  $N_2$  targets in giving rise to interferences in electron emission that is not completely understood nor predicted by theory.



**Figure 1** Ratios obtained by dividing the measured molecular  $N_2$  cross sections by atomic N cross sections. Results shown are for 1, 3 and 5 MeV  $H^+$  ions at the indicated observation angles.



**Figure 2** Theoretical first-order ionization cross-section ratios for 3 MeV  $H^+$  impact on  $N_2$  for electron ejection angles of  $30^\circ$ ,  $90^\circ$ , and  $150^\circ$  as a function of ejected electron velocity in comparison to the experimental data.

### Acknowledgement:

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## 4.12 Enhancement of the $1s2s2p\ ^4P$ State in Electron Transfer to $C^{4,5+}$ Ions

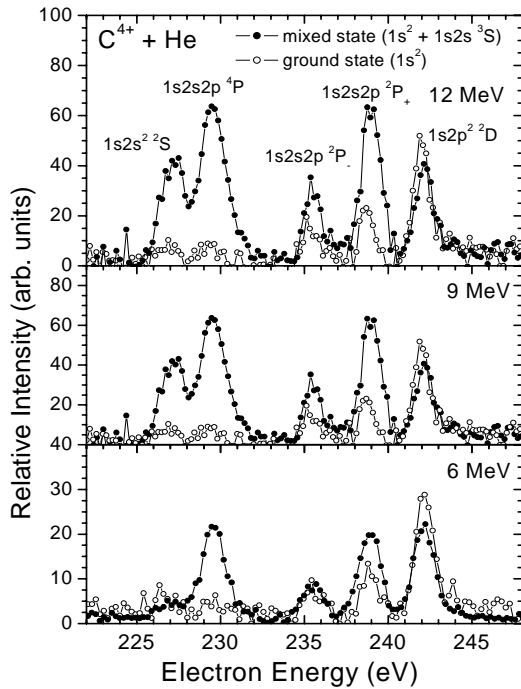
Diane Strohschein-Lovett, J. Baran, and J. A. Tanis

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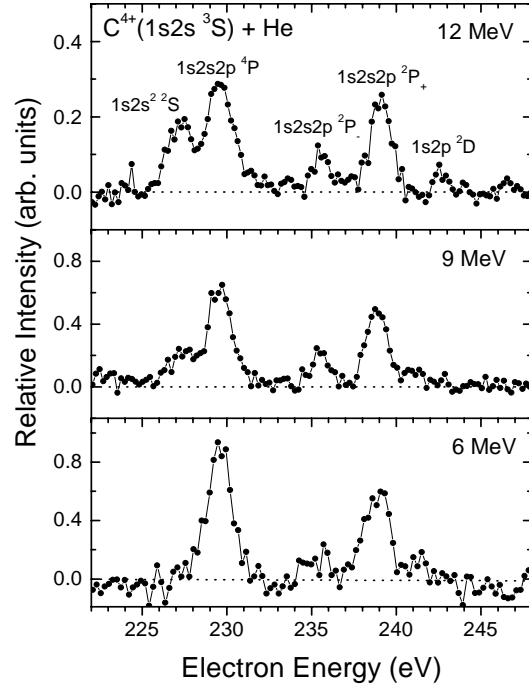
Previously, anomalously large Auger emission intensities were observed for the  $1s2s2p\ ^4P$  state compared to the similarly configured  $1s2s2p\ ^2P$  and  $1s2s2p\ ^2P_+$  states in electron transfer interactions involving 1.1 MeV/u collisions of He-like and H-like F ions with He and Ne targets [1]. Enhancement of the measured  $^4P$  intensities was determined from the ratio  $R = ^4P/(^2P + ^2P_+)$ , for which a value of two is expected based on spin statistics [2]. Determination of R requires corrections for geometrical factors due to the long lifetimes of the  $^4P$  state ( $J = 5/2, 3/2, 1/2$ ), which have values in the range  $10^{-9} \text{ s} < t < 10^{-7} \text{ s}$  in  $F^{6+}$  [3]. The resulting large  $^4P$  intensities, which could not be explained on the basis of spin statistics, were attributed to a dynamical Pauli exchange mechanism involving projectile and target electrons having the same spin alignment in the electron transfer interaction. More recently, it has been suggested that the  $^4P$  intensity might be significantly enhanced due to cascading effects following electron transfer to states with  $n \geq 3$  [4], thereby eliminating the need to invoke a dynamic mechanism such as Pauli exchange.

To shed light on these conflicting interpretations, and to gain further insight into the origin of the observed  $^4P$  enhancement, new measurements have been undertaken for 0.5 – 1.0 MeV/u  $C^{4,5+}$  ions colliding with He and Ne targets. It is expected that if cascading effects are important then enhancement of the  $^4P$  state should decrease with increasing collision velocity. In the present work, Auger spectra for single transfer to incident  $C^{4+}$  spectra were collected for both ground-state  $C^{4+}(1s^2)$ , formed directly by gas-stripping  $C^-$  ions at the terminal of the accelerator, as well as mixed-state  $C^{4+}(1s^2 + 1s2s\ ^3S)$  formed by post-stripping  $C^{3+}$  ions following acceleration. In this way, the measured spectra for the mixed-state beam could be corrected for the ground-state contribution to give the  $1s2s2p$  intensities due solely to the  $C^{4+}(1s2s\ ^3S)$  component. A limitation of the earlier measurements for 1.1 MeV/u  $F^{7,8+}$  ions [1] was the fact that the single transfer measurements were conducted only for the mixed-state beam  $F^{7+}(1s^2+1s2s\ ^3S)$  formed by post-stripping accelerated F ions of lower charge states. Thus, it was not clear what fraction of the observed  $^4P$  intensity was due solely to single transfer to the metastable  $1s2s\ ^3S$  beam component.

Figure 1 shows the electron spectra obtained for the mixed-state and ground-state  $C^{4+}$  beams for the He target for each of the collision energies investigated. The energy scale of the spectra in Figure 1 has been transformed to the rest frame of the projectile. To determine the contribution due solely to the metastable  $1s2s\ ^3S$  beam component the ground-state  $(1s2p^2)\ ^2D$  intensity was normalized to that of the metastable state, since the  $^2D$  is produced almost entirely from the ground state [5], giving metastable fractions of  $\sim 25\%$ . The resulting metastable-state spectra, obtained by subtracting the ground-state contributions are shown in Figure 2.



**Figure 1** Measured zero-degree Auger emission spectra following single electron transfer to mixed state  $C^{4+}(1s^2 + 1s2s^3S)$  and ground state  $C^{4+}(1s^2)$  in 6, 9, and 12 MeV collisions with He. The ejected electron energy has been transformed to the rest frame of the projectile and the electron yield has been normalized to the incident beam current.

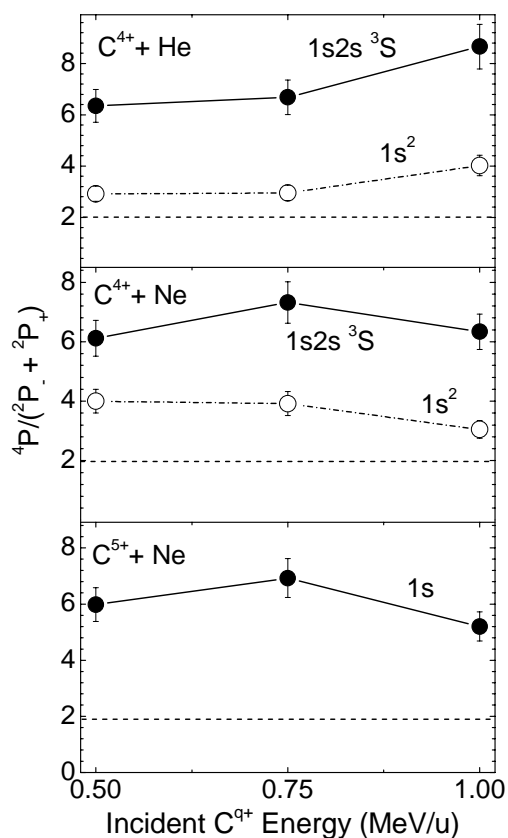


**Figure 2** Measured Auger emission spectra for single transfer to metastable  $C^{4+}(1s2s^3S)$  in He after correction for the contribution due to ground-state  $C^{4+}(1s^2)$  using the data of Figure 1.

Geometrical correction factors for the observed  $^4P$  intensities resulting from in-flight decays were calculated by numerical integration to account for the long lifetimes, which have a range  $10^{-9} \text{ s} < t < 10^{-7} \text{ s}$  in  $C^{3+}$  [3]. The correction factors for 0.5, 0.75, and 1.0 MeV/u carbon ions were found to be 7.3, 8.8, and 10.2, respectively. Intensities of the autoionizing metastable  $(1s2s2p)^4P$  state were found to be strongly enhanced relative to the similarly configured  $(1s2s2p)^2P$  and  $(1s2s2p)^2P_+$  states in single and double electron transfer to  $C^{4+}(1s2s^3S)$  and  $C^{5+}(1s)$  as shown in Fig. 3.

Values for the ratio  $^4P/(^2P + ^2P_+)$  significantly exceed the expected ratio of 2 based on spin statistics and show little energy dependence. The lack of energy dependence in the ratios suggests that cascading is not primarily responsible for enhancement of the  $^4P$  state. Thus, we are led to conclude that Pauli exchange is a viable mechanism to explain the large  $^4P$  enhancement. In this mechanism, for single capture to  $1s2s^3S$  it was proposed [1] that an incoming target electron with the same spin alignment as the projectile  $1s$  electron gives rise to an exchange interaction such that one of them is transferred to  $2p$  to form the  $1s(2s2p^3P)^4P$  state, since both electrons cannot occupy  $1s$  due to the Pauli exclusion principle (see Fig. 2 of Ref. [1]). Hence, by means of this exchange, the  $^4P$  state can be enhanced beyond the intensity expected for direct transfer of an aligned target electron to the  $2p$  orbital, and the ratio  $^4P/(^2P + ^2P_+)$  provides a measure of the magnitude of this effect. Nevertheless, quantitative calculations of both cascading effects as well as Pauli exchange are needed to better assess the origin of the nonstatistical enhancement of the  $^4P$  state.





**Figure 3** Measured ratios of the  $1s2s2p\ ^4P$  intensities to the sum of the  $1s2s2p\ ^2P_-$  and  $1s2s2p\ ^2P_+$  intensities as a function of the incident projectile energy for the indicated collision systems. The observed  ${}^4P$  intensities were corrected for lifetime effects and, in the case of single transfer to  $C^{4+}(1s2s\ ^3S)$ , contributions from the  $C^{4+}(1s^2)$  ground state (see text). The horizontal dashed line at  ${}^4P/({}^2P_- + {}^2P_+) = 2$  represents the value expected from spin statistics.

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## 4.13 Inelastic Guiding of Electrons in Insulating Nanocapillary Foils

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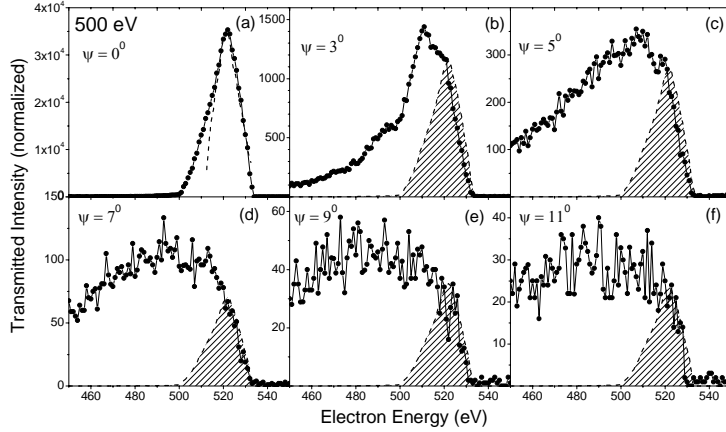
The interaction of highly-charged ions (HCI) with surfaces has been the subject of extensive research both experimentally and theoretically not only because of its potential application in the field of nanotechnology but also from the point of view of fundamental understanding [1,2]. In recent years attention has centered on the transmission of HCI through nanocapillaries, with the reported *guiding* of slow positive ions (3 keV Ne<sup>7+</sup>) through insulating nanocapillary foils of polyethylene terephthalate (PET) by Stolterfoht *et al.* [3]. Surprisingly, ion transmission with negligible charge change was observed for foil tilt angles up to  $\psi = 20^\circ$  with respect to the incident beam direction, indicating distant encounters with the capillary walls. It was proposed that this result was due to a self-organizing charge-up of the inner walls of the capillaries [3] that, after a characteristic charging time, deflects the traversing ions causing them to be “guided” through the sample along the capillary axis. In subsequent work by these authors additional properties of slow ion guiding in PET foils were investigated [4,5].

Experimental and theoretical works by other investigators have been conducted for slow (~1-10 keV) positive ions [6-11], and in one instance fast 200 MeV Ti<sup>12+</sup> ions [12] were used to determine the alignment of nanocapillaries in a sample. Notably, for slow H<sub>2</sub> molecular ions [13] negligible fragmentation occurred as a result of passage through the nanocapillary foils, indicating the strength of the guiding effect. In addition to polymer foils, ion guiding has been studied for nanocapillary samples of SiO<sub>2</sub> [7], alumina [10,12] and tapered glass [11]. In all cases, the surfaces of the insulating nanocapillary samples were coated with a thin conducting layer, e.g., gold or aluminum, to prevent charging of the sample during the measurements. More recently, guiding for lower energy 200-350 eV electrons in Al<sub>2</sub>O<sub>3</sub> nanocapillary foils has been reported [14].

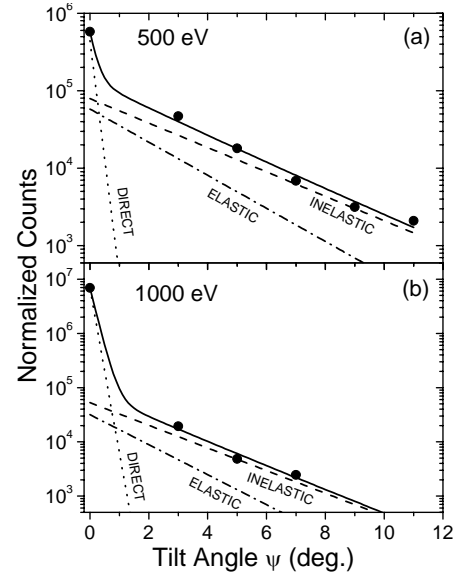
In this work, the transmission and guiding of 500 and 1000 eV electrons through insulating PET nanocapillaries of diameter 200 nm and aspect ratio 50 [3] have been investigated. The experiment was performed at Western Michigan University. The sample was mounted in a goniometer that allowed precise two-dimensional positioning with respect to the incident beam. The electrons were produced using an electron gun containing a simple filament source and collimated to a diameter of 1.5 mm. The transmitted electrons were analyzed with a parallel-plate spectrometer located a few centimetres behind the sample and counted with a channel electron multiplier (CEM).

To investigate guiding phenomena the sample was tilted with respect to the straight-through position and the observation angle changed accordingly. Significant intensities of transmitted electrons were found for tilted sample angles, and correspondingly shifted observation angles as shown in Fig. 1 for incident 500 eV electrons. However, unlike positive ions the energy spectra of guided electrons exhibit significant energy losses, indicating that electrons undergo both *elastic*

and *inelastic* scattering with the surfaces of the capillaries. From the figure it can be seen that the inelastic contribution dominates the transmitted electron spectrum and increases significantly with the capillary tilt angle.



**Figure 1** Measured electron energy spectra showing the increasing fractional electron energy loss vs. tilt angle  $\psi$  for incident 500 eV electrons. The dashed curve in (a) shows the energy spectrum obtained for electron emission from the bare filament normalized to the spectrum for  $\psi = 0^\circ$ . The shaded areas in (b) – (f) show the spectrum for  $\psi = 0^\circ$ , normalized to the spectra for  $\psi > 0^\circ$ , indicating the elastic contribution to the individual spectra.



**Figure 2** Relative transmission intensities vs. tilt angle for incident 500 and 1000 eV electrons. The elastic and inelastic decay curves were determined by fitting exponential functions to their respective contributions. The direct contribution represents the large measured transmission fraction near  $\psi = 0^\circ$ .

While the overall transmitted electron intensity decreases exponentially as observed for positive ions, the existence of the inelastic contribution requires modification of the concept of the *guiding power* proposed by Hellhammer *et al.* [15], in which the *critical angle*  $\psi_c$  is defined as the tilt angle for which the transmitted intensity falls to  $1/e$ . The elastic and inelastic scattering contributions were evaluated separately by superimposing the  $\psi = 0^\circ$  spectrum, which has same profile and width as the bare filament spectrum (dashed curve in Fig. 1a), onto the  $\psi \neq 0^\circ$  spectra and normalizing it to the intensities of these latter spectra as shown in Figs. 1b-f. The decay rates, i.e.,  $\psi_c$ , were then determined by fitting an exponential function to the elastic and inelastic contributions, giving the results shown in Figs. 2a and 2b. To represent the integrated measured intensity for all tilt angles including  $\psi = 0^\circ$ , a *direct* contribution corresponding to the large transmitted electron intensity at  $\psi = 0^\circ$  must also be included. This contribution is due to the convolution of the capillary aspect ratio, the beam collimation, and capillary nonparallelism.

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## 4.14 Interference Effects in Electron Emission from 30 MeV $O^{8+} + O_2$ Collisions

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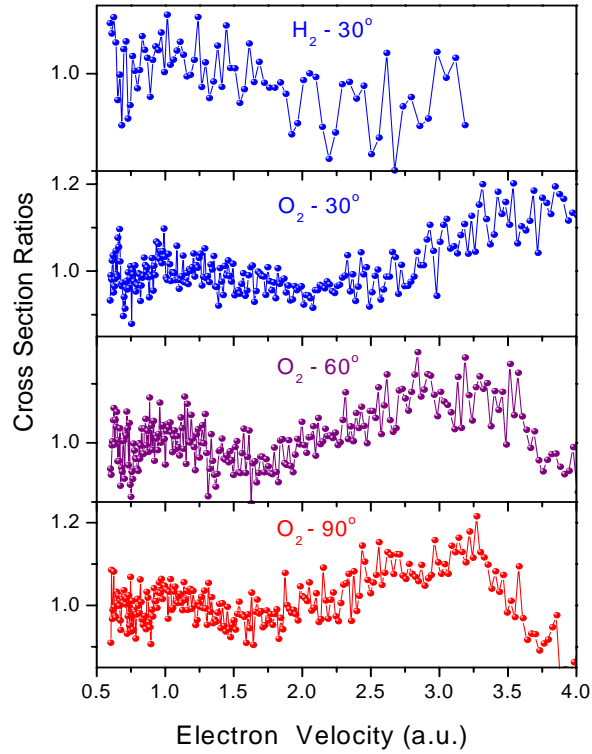
As noted in Sec. 4.11, previous investigations of interference phenomena associated with electron emission from  $H_2$  by (1-5)-MeV  $H^+$  impact have revealed both primary Young-type interferences due to coherent electron emission from the identical atomic centers as well as secondary interferences caused by intramolecular scattering [1]. The primary interferences showed a strong dependence on the electron observation angle, while the secondary structures with higher frequencies superimposed on the main interference structures did not. More recently, interferences for (1-5)-MeV ( $H^+$ ) +  $N_2$  were investigated apparently revealing only secondary oscillations [2].

In the present work, the experimental studies were extended to 30 MeV  $O^{8+}$  impact with  $O_2$  and  $H_2$ . In addition to primary and secondary interferences, the resulting electron spectra were examined for evidence of the much higher-frequency oscillations observed in Ref. [1].

The measurements were conducted at Western Michigan University using the tandem Van de Graaff accelerator. A collimated beam of 30 MeV  $O^{8+}$  ions was directed into the scattering chamber onto  $H_2$  and  $O_2$  targets which were supplied by a gas jet. The flow rate of the gas was adjusted to maintain a pressure of  $\sim 4 \times 10^{-5}$  Torr in the scattering chamber with a background pressure of  $\sim 1.0 \times 10^{-6}$  Torr. A parallel-plate electron spectrometer equipped with a channel electron multiplier was used to measure the energy spectra of electrons emitted from the target for observation angles ranging from  $30^\circ$  to  $150^\circ$  with respect to the incident beam and ejected electron energies between 5 and 400 eV.

The measured electron yields were fit to a second-order decreasing exponential function and then divided by this function to obtain the cross section ratios shown in Figure 1. The resulting ratios for  $O_2$  show structures that are suggestive of secondary interferences as in the case of  $H^+ + N_2$  [2], whereas the observed behavior for  $H_2$  indicates only the primary interference. The  $O_2$  ratios for  $60^\circ$  and  $90^\circ$  also show some evidence for higher frequency oscillations near 3 a.u. but better statistics are needed to verify this.

To better reveal interference structures for  $O_2$ , calculations of the non-oscillatory atomic oxygen cross sections are needed. These calculations are currently being carried out. Additionally, measurements will be made for  $H^+ + O_2$  to determine the differences, if any, compared to oxygen projectiles.



**Figure 1** Cross-section ratios for 30 MeV  $O_8^+$  plotted as a function of ejected electron velocity for  $H_2$  and  $O_2$  at the indicated observation angles.

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# 5 NUCLEAR PHYSICS

## 5.1 Proton Capture by $^{14}\text{N}$ at Astrophysical Energies

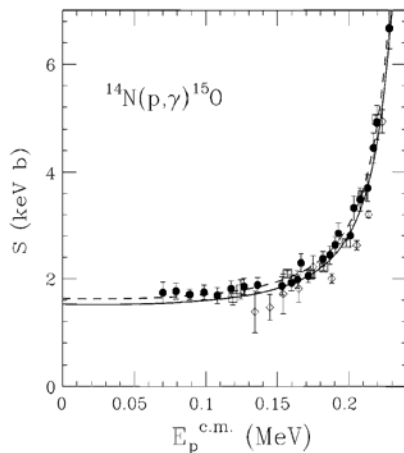
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Nucleon capture reactions play a critical role in astrophysical processes. Direct low energy cross section measurements for proton capture are often unavailable due to the Coulomb barrier. Predictions for these cross sections on light nuclei have been calculated using a recoil corrected continuum shell model. Current calculations were done for the  $^{14}\text{N}(p,\gamma)^{15}\text{O}$  reaction. New measurements of this reaction in the Gamow window demonstrate the method to be reliable for extrapolating cross sections to low energies.  $^{14}\text{N}(p,\gamma)^{15}\text{O}$  is a bottleneck reaction in the CNO cycle. It controls duration of hydrogen burning, determines main sequence turnoff and hence globular cluster ages. It also determines CNO neutrino flux in the Sun. Therefore extensive measurements and theoretical predictions have been made. Previous theoretical calculations used R-matrix fits [1] or direct and resonant capture methods.

The advantage of the RCCSM formalism [2] is that it provides coupled-channel solutions for bound and unbound wave functions. It uses oscillator size parameter, desired states of A-1 core nuclei and a realistic, translationally invariant interaction. Calculations are transformed to the center-of-mass system; hence, the wave functions are antisymmetric and contain no spurious components. Also the bound and continuum states are orthogonal.

Agreement for  $^{14}\text{N}(p,\gamma)^{15}\text{O}$  proton capture to the  $3/2^+$  state is good. However, the weak transition from the  $1/2^+$  resonance to the ground state is very sensitive to the components of the ground state wave function. No evidence is found for a contribution to the subthreshold state, and the S-factor is essentially flat as energy approaches zero. The consistency between the data of Ref. 3 and the dashed line in Fig. 1 make this combination the preferred result. The calculation predicts  $S(0)=1.632$  and  $S(30)=1.625$  keV b.



**Figure 1** Sum of the scaled the  $3/2^+$ ,  $1/2^+$ ,  $5/2^+$ ,  $1/2^-$ , and  $3/2^-$  S-factors from interaction A plotted as the solid line. The dashed line is the solid line times 1.08. The solid circles are the data of Ref. 3; the squares are the data of Ref. 4 and the diamonds are the data of Ref. 5 as given in Ref. 3.

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## 5.2 The ${}^2\text{H}({}^{12}\text{B},p){}^{13}\text{B}$ Reaction

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The positions of positive parity orbitals in neutron rich light nuclei are of interest due to their role in the development of neutron halos. The nucleus  ${}^{13}\text{B}$  contains 8 neutrons and thus corresponds to a closed neutron  $p$  shell. While the energies of a number of levels are known in  ${}^{13}\text{B}$ , little information is available about the spins and parities of these states. The shell model should be well suited to describe this nucleus, but the influence of  $(s_{1/2})^2$  configurations in this region has been noted in nearby nuclei. Also, intruder orbitals from the  $sd$  shell are increasingly important in neutron-rich light nuclei in this region. Of particular interest is the cluster of excited states near  $E_x({}^{13}\text{B})=3.5$  MeV. The angular distributions of protons from the  ${}^2\text{H}({}^{12}\text{B},p){}^{13}\text{B}$  reaction can clarify the order of these levels, and identify  $l=0$  and  $l=2$  states. The results in  ${}^{13}\text{B}$  may also be compared with those from the less well understood mirror nucleus  ${}^{13}\text{O}$ .

A first measurement of the  ${}^2\text{H}({}^{12}\text{B},p){}^{13}\text{B}$  reaction has been carried out in inverse kinematics using a  ${}^{12}\text{B}$  beam produced with the Argonne National Laboratory In-Flight radioactive beam production facility. The most crucial element in the experiment is resolution, in both angle, and proton energy, due to the small separation between the states of interest in  ${}^{13}\text{B}$ . While the detector setup functioned well, the average beam intensities were approximately 5000 particles per second, although the peak intensities were near  $10^5$  particles per second. The statistics obtained during this measurement were insufficient to address the physics goals. However, additional accelerator time has already been allocated for another measurement of this reaction, and the measurement will be carried out in the near future.

### 5.3 Carbon Production in Stars and the Triple $\alpha$ Reaction

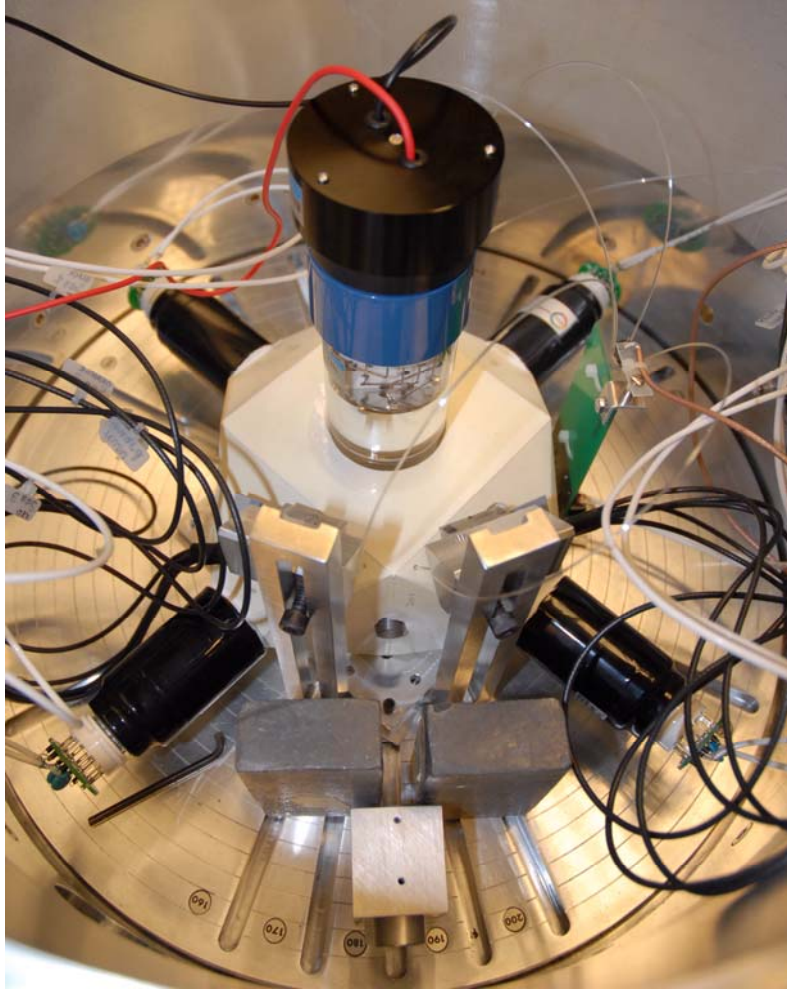
C. Tur,<sup>1</sup> S. M. Austin,<sup>1</sup> A. H. Wuosmaa,<sup>2</sup> J. Lighthall,<sup>2</sup> S. Marley,<sup>2</sup> N. Goodman,<sup>2</sup> J. Bos,<sup>2</sup> J. Snyder<sup>2</sup>

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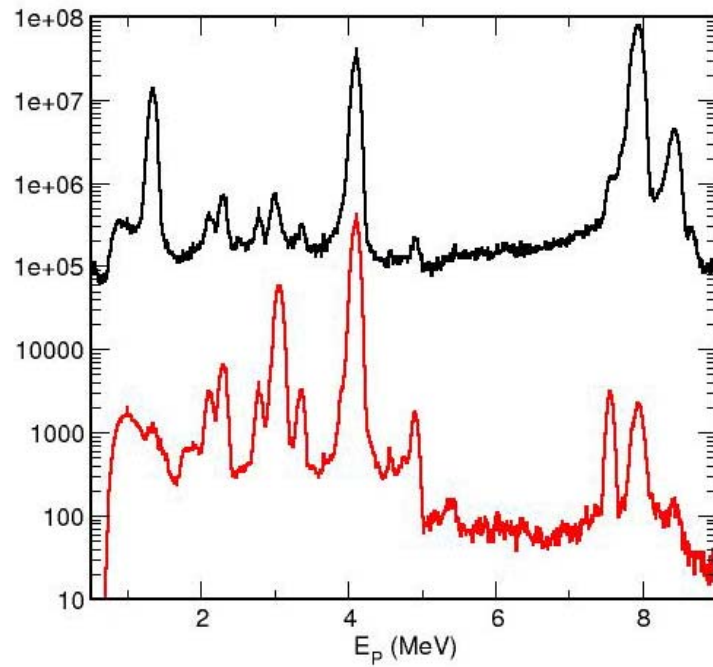
One piece of information limiting the precision of calculations of carbon and oxygen production in stars nearing the end of their lives is the rate of the “triple- $\alpha$ ” reaction whereby three alpha particles combine to form  $^{12}\text{C}$  through two short-lived, resonant states: the ground state of  $^8\text{Be}$  and the excited  $0^+$  state in  $^{12}\text{C}$ . The crucial information is the branching ratio between the  $\alpha$ - $^8\text{Be}$  decay of the  $^{12}\text{C } 0^+_2$  state, and the radiative decays that lead to the  $^{12}\text{C}$  ground state that produce stable carbon. This rate is known to an uncertainty of approximately 12%. This rate is obtained from three separate experimentally determined quantities: the radiative branching ratio of the  $0^+_2$  state, the total pair-decay width, and the  $e^+e^-$  pair decay branching ratio. Of these, the least well known is the  $e^+e^-$  pair branching ratio, most recently measured by Robertson *et al.* to be  $6 \pm 0.6 \times 10^{-6}$  [1].

A collaboration between the WMU group and Michigan State University (MSU) has worked to reduce this uncertainty and re-measure the  $e^+e^-$  pair decay branch using a specially designed  $e^+e^-$  pair detector. The experiment utilizes a 10.6 MeV proton beam produced at the WMU Tandem Accelerator Laboratory. The  $0^+_2$  state is excited via proton inelastic scattering, and the protons are detected at backward angles using 1mm thick silicon detectors. The  $e^+e^-$  decay events are identified using a segmented plastic scintillator detector that combines a thin (3mm) plastic scintillator tube with four thick plastic scintillator blocks. The thin tube is insensitive to  $\gamma$  radiation, and thus the registration of coincidences between signals in the tube, quadrants, and silicon detectors serve to identify events corresponding to pair decays of the  $0^+_2$  state. Following a test run in August 2006, modifications to the detector were made to improve the energy response of the plastic scintillators, and a new, three-week long experiment was conducted in April 2007. Figure 1 shows a photograph of the device installed in the scattering chamber at one beam line at the WMU Tandem Accelerator Laboratory. The results of the experiment are still being analyzed. However, it is clear that the performance of the detector has been very significantly improved.



**Figure 1** Photograph of  $e^+e^-$  pair detector in scattering chamber at the WMU Tandem Accelerator Laboratory.

Figure 2 shows proton energy spectra for  $(p,p')$  inelastic scattering from the  $^{12}\text{C}$  target, which contained a small  $^{16}\text{O}$  impurity. The inelastic-scattering peak for the  $^{16}\text{O}(0^+_{2,3})$  states near 6 MeV is barely discernable in the singles spectrum. The pair-decay branching ratio for the  $^{16}\text{O}(0^+_{2})$  state is 1, however, and the  $^{16}\text{O}(0^+_{2})$  peak stands out clearly when the coincidence is imposed and randoms are subtracted. The  $^{12}\text{C}(2^+; 4.443 \text{ MeV})$  peak in the random-subtracted coincidence spectrum provides a measure of the gamma-ray sensitivity of the device which is very small, only approximately  $\epsilon_{\gamma} \sim 0.3\%$ . For the test run, the beam intensity was limited due to the random coincidence rate from scattered beam in the scintillator, and the statistics were insufficient to determine  $\Gamma_{\pi}/\Gamma$  for the  $^{12}\text{C}(0^+_{2})$  state. Modifications are currently underway to correct this problem and another run is planned in calendar year 2007 to complete the measurement.



**Figure 2** Proton energy spectra from  $^{12}\text{C},^{16}\text{O}(p,p')$  inelastic scattering. The black histogram represents proton singles events, and the red histogram corresponds to random-subtracted proton-scintillator coincidences.

Work supported by the U.S. Department of Energy, Nuclear Physics Division under Contract number DE-FG02-04ER41320, and the U.S. National Science Foundation grant PHY01-10253.

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## 5.4 *HELIOS*: The HELIcal ORbit Spectrometer

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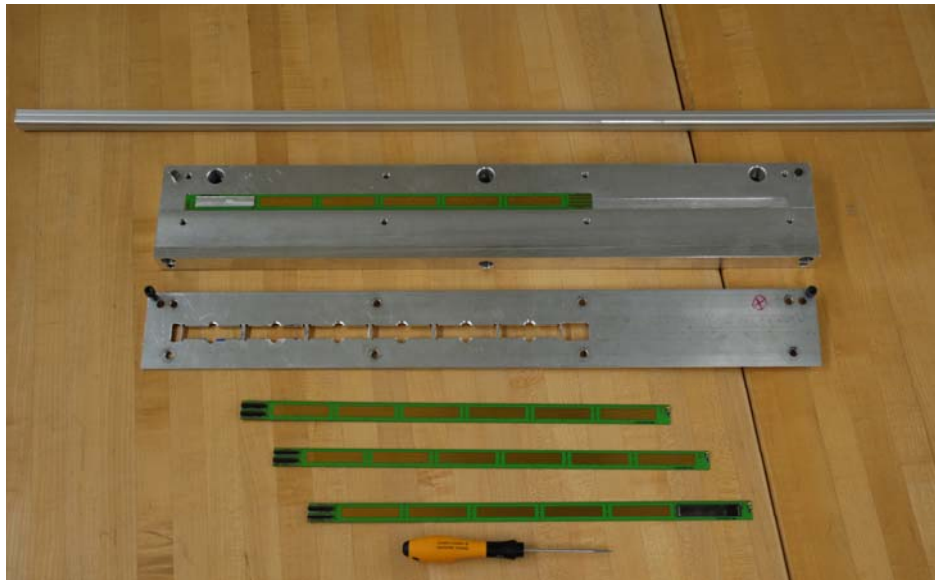
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The HELIOS device is a novel new spectrometer, based on a large-volume high-field magnetic solenoid, designed to study nucleon transfer and other reactions in inverse kinematics. A detailed technical description of the device and its expected capabilities are contained in Ref. [1]. HELIOS plays a prominent role in the future Strategic Plan for the ATLAS facility, as it is well matched to the ongoing CARIBU radioactive beam source development project. Over the past year, significant progress has been made in the HELIOS project. Most importantly, the large-bore high-field superconducting solenoid that is the heart of HELIOS has been delivered to the ATLAS facility at Argonne National Laboratory, and has been energized to a field of 2 Tesla. WMU graduate student Jonathon Lighthall and undergraduate student Jack Winkelbauer have designed and installed the apparatus that is used to map the magnetic field of the solenoid (see Fig. 1). The design of the target area, including the layout of the beam-line are underway, and installation of beam-line components will begin when field mapping is concluded. Many of the other mechanical components of the spectrometer have either been fabricated or are under construction.

At WMU, we have evaluated a set of position-sensitive silicon detectors that can be used in a prototype HELIOS detector array. While these detectors do not possess an optimal geometry for the final HELIOS array they will be useful for development and performance evaluation as the design for the final detectors is completed. The silicon detector array requires precision assembly, and to accomplish that task a precision assembly jig has been designed and built by WMU graduate student Scott Marley (see Fig. 2). The detector arrays are currently under construction, and should be ready for installation in the HELIOS magnet by the end of December 2007.



**Figure 1** Western Michigan University graduate student Jonathon Lighthall (right) and undergraduate student Jack Winkelbauer (left) adjust a field mapping apparatus in the HELIOS spectrometer magnet at the ATLAS accelerator facility at Argonne National Laboratory.



**Figure 2** Assembly apparatus for the HELIOS silicon-detector array.

## 6 PHYSICS EDUCATION

### 6.1 Promoting Instructional Change in New Faculty: An Evaluation of the Physics and Astronomy New Faculty Workshop

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#### *Introduction*

An important finding of Physics Education Research (PER) is that traditional, transmission-based instructional approaches are generally not effective in promoting meaningful student learning. Instead, PER advocates that physics be taught using more interactive instructional methods. Although the research base and corresponding pedagogies and strategies are well-documented and widely available to physics faculty, widespread change in physics teaching at the college level has yet to occur. Since 1996, the Workshop for New Physics and Astronomy Faculty has been working to address this problem. This workshop, jointly administered by the American Association of Physics Teachers, the American Astronomical Society, and the American Physical Society, has attracted approximately 25% of all new physics and astronomy faculty each year to an intensive 4-day workshop designed to introduce new faculty to PER-based instructional ideas and materials. This paper describes the impact of the New Faculty Workshop (NFW) as measured by web-based surveys of 527 workshop participants and 206 physics and astronomy department chairs.

The primary goals of the NFW are to, (1) reach a large fraction of the physics and astronomy faculty in tenure-track appointments prior to their receiving tenure, (2) help participants develop knowledge about recent developments in physics pedagogy and the assessment of changes in pedagogy, and (3) have participants integrate workshop ideas and materials into their classrooms in a way that has a positive impact on their students and their departments.

#### *Description of the NFW*

During its first 11 years in operation, 759 faculty have participated in the NFW. This represents 24.3% of the estimated 3,124 assistant professor faculty hires during these years [1-4]. NFW participants represent 344 distinct colleges and universities. This is 43% of the 797 degree-granting physics and astronomy departments in the US [1]. In addition, 170 departments (21% of all departments in the US) have had more than one faculty member attend the NFW.

Attendees at the NFW must be nominated by their department chair and the only cost to the department is transportation to College Park, MD. The workshop runs from approximately 4:00 p.m. on a Thursday to noon the following Sunday and contains roughly 12 hours of programming each full day. Presentations and discussions include a mix of large group sessions and small group sessions. It is important to note that the workshop presenters are leading and well-

respected curriculum developers since research suggests that the reputation of the reformer and/or their institution can have an important impact on how a reform message is received [5].

The NFW was funded with two grants from the National Science Foundation (NSF #0121384 and NSF #9554738). A total amount of \$742,000 was spent during the first 11 years reported on in this paper [6]. This works out to a cost per participant of \$978 (not including transportation cost to College Park, MD).

### Data Collected

During spring 2007, a web survey was administered to the 690 NFW participants who could be located and who were still in academia. Of these, 527 (76%) completed the web survey before analysis began. Also, during spring 2007, a web survey was administered to all 794 US physics and astronomy department chairs using an email list provided by the American Institute of Physics. The survey was completed by 206 department chairs (26%). Approximately 53% of survey respondents reported having a faculty member from their department attend the NFW.

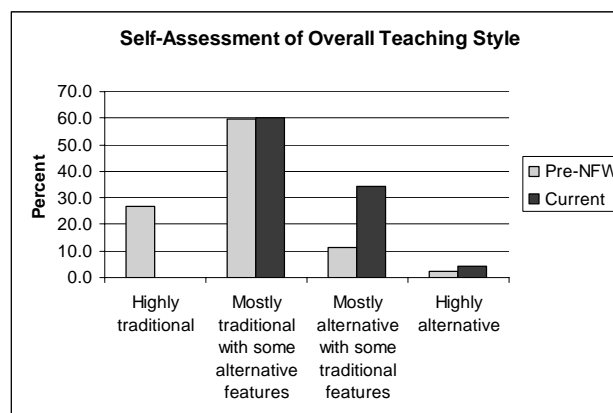
### Results

The NFW improves participants' knowledge of PER-based teaching techniques and interests participants in trying these techniques. Table 1 shows that most NFW participants indicate familiarity with the specific PER-based approaches discussed at the NFW after the workshop. In addition, nearly all (93.7%) of the NFW participants report being interested in incorporating some of the workshop ideas into their teaching right after the workshop. This suggests that they had formed a positive opinion of the instructional techniques presented at the workshop.

Participants report instructional changes to more alternative modes of instruction. Department chairs agree. Figure 1 shows that there was a large shift to more alternative teaching styles after the NFW. In addition, 70.7% of participants rate their teaching style as more alternative than

**TABLE 1.** Summary of participant responses to web survey question #17.

17. Please rate the following:				
	I currently use it	I have used it in the past	I am familiar with it but have never used it	Little or no Knowledge
Astronomy Tutorials	8.7%	5.0%	30.2%	<b>56.1%</b>
Collaborative Learning	<b>39.2</b>	17.2	23.0	20.6
Cooperative Group Problem Solving	<b>47.2</b>	21.9	22.9	8.0
Interactive Lecture Demonstrations	<b>46.1</b>	24.2	23.4	6.3
Just-In-Time Teaching	22.9	18.0	<b>50.9</b>	8.2
Peer Instruction	<b>54.1</b>	21.4	22.4	2.1
Realtime Physics	5.2	7.5	<b>46.6</b>	40.7
Personal Response Systems	32.6	15.0	<b>43.7</b>	8.7
Physlets	19.7	21.4	<b>41.3</b>	17.5
Tutorials in Introductory Physics	13.1	20.9	<b>45.8</b>	20.3



**Figure 1** Participant self-assessment of their overall teaching style.



other faculty in their department. The department chair survey corroborates the participant self-report data -- 58.6% of department chairs rate NFW participants as having a more alternative teaching style than other faculty in the department.

Finally, 96.5% of participants reported at least some change in their teaching style. Department chairs again corroborate the participant self-report data. Most department chairs (72.4%) report that NFW participants have made changes to their teaching as a result of the workshop. It is reasonable that this percentage is smaller than the percentage of faculty who reported making a change in their teaching since a department chair is unlikely to be aware of all changes made in the teaching practices of faculty in their department.

Participants report improved student learning. Department chairs agree. Most participants (64.7%) believe that the NFW has had a considerable or larger positive impact on their students. Similarly, most department chairs (72.6%) who have sent faculty to the NFW indicate that the workshop has led to improved student learning in classes taught by workshop participants.

Faculty report discussing NFW ideas with their colleagues and that some colleagues have made changes as a result of these discussions. Department chairs agree. If one of the ultimate goals of the NFW is to change the culture of physics teaching in the US, it is not enough for NFW participants to just learn about PER-based instructional materials and strategies and make changes to their own teaching. They must also bring these ideas into interactions with colleagues in their home departments. There is evidence that this has taken place. Most participants (86.8%) say that they have discussed NFW ideas with their colleagues. Many NFW participants (39.8%) report that their colleagues have made changes in their teaching as a result of these discussions. Many department chairs (51.0%) also believe that NFW attendees have influenced other faculty in the department.

### The Danger of Self-Reported Data

Table 1 shows that participants report high levels of use of one or more PER-based instructional strategy. One danger of the use of such self-report data is that a respondent may say that they are using a particular instructional strategy when an outside observer would think otherwise. One way to estimate the degree of over-reported use is to compare the general statements of instructional style made on Table 1 with more detailed descriptions of instructional activities. In one part of the web survey, NFW participants were asked to select a particular class that they had taught frequently since the NFW and to identify the frequency with which they engaged in particular instructional activities. Table 2 shows

**TABLE 2.** Summary of self-described instructional activities of NFW participants who are teaching an introductory course and indicated that they currently use Peer Instruction.

	Never	Once or twice per semester	Several times per semester	Weekly	Nearly every class	Multiple times every class
22. During the most recent time you taught the course, over the semester or quarter, how frequently did/do you use the following teaching strategies during the lecture portion of your course?						
Instructor solves/discusses quantitative problem	3%	5%	13%	33%	<b>36%</b>	10%
Instructor solves/discusses qualitative problem	4	2	10	25	<b>37</b>	24
Students solve/discuss quantitative problem	9	9	16	<b>33</b>	23	10
Students solve/discuss qualitative problem	3	1	12	25	<b>33</b>	27
Pair or small group discussion	4	2	15	24	25	<b>30</b>
Instructor questions answered simultaneously by entire class	8	2	8	15	26	<b>40</b>

the responses for the 192 participants (36.4%) who said that they used Peer Instruction on question #17 (Table 1) and also opted to report on the details of an introductory level class that they had taught. These instructors report instructional patterns quite different from traditional instruction, which would rarely, if ever, involve students working on quantitative or qualitative problems nor would students ever engage in pair or small group discussions. But, to what extent are the reported instructional styles indicative of Peer Instruction?

Three of the instructional activities are particularly relevant for the non-traditional aspects of Peer Instruction: “Students solve/discuss qualitative problem”, “Pair or small group discussion”, and “Instructor questions answered simultaneously by entire class”. In Peer Instruction, each 1-hour class session involves three or four lecture-ConceptTest segments [7]. During each segment the instructor first lectures on a particular topic. Students then work individually on a multiple-choice ConceptTest (a qualitative problem) followed by a pair or small group discussion with nearby classmates. Finally, the students simultaneously report on their answers using a show of hands, flash cards, or a classroom response system (i.e., clickers). Thus, we would expect faculty engaging in the “pure” form of Peer Instruction to report each of the three relevant activities occurring multiple times each class. This was true for only 37 (19%) of the subsample of 192 participants. If the criteria is loosened a bit to include faculty who report each of these three activities “nearly every class”, the number increases to 73 (38%). Thus, only 19%-38% of faculty who say they are using Peer Instruction report instructional activities that could be consistent with Peer Instruction. There is not enough evidence available in the survey data to judge whether the variations of Peer Instruction used by NFW participants are likely to be productive or not.

## Conclusions

Evidence presented suggests that the NFW has been effective in meeting its goals of introducing new faculty to PER-based ideas and materials and motivating faculty to try these ideas and materials. There is some evidence that NFW participants have also had an influence on other faculty in their departments. Thus, the NFW appears to be contributing significantly to the spread of PER ideas.

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## 6.2 Modeling Success: Building Community for Reform

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### Introduction

The education research community has produced a substantial body of research demonstrating the weaknesses of traditional instructional approaches and has developed a large number of proven alternative methodologies and curricular packages which are widely available [1]. Despite significant dissemination efforts these products are only weakly integrated into mainstream physics teaching [2]. Therefore, attention needs to be given to issues of dissemination.

Within physics education, one approach that has impacted large numbers of physics classrooms is Arizona State University's Modeling Instruction in High School Physics Project [3]. In an effort to understand the success of this approach we conducted open-ended telephone interviews with five leaders of the Modeling Project. We asked them about the history, goals, philosophies, successes, failures, and evolution of the project. Although analysis of these interviews is ongoing, in this paper we report some preliminary findings.

### History and Successes of the Modeling Project

Modeling, as a theory-based instructional technique was conceived between 1980-85 with the goal of making instruction in physics reflect the activities of practicing physicists. The instructional techniques were established by Malcom Wells and formalized by David Hestenes [4]. These instructional techniques formed the foundational curriculum for the Modeling Workshop Project. Evidence for the success of the Modeling approach to physics came from the development of the Force Concept Inventory and led to a pilot workshop project. Modeling gained support from the National Science Foundation during 1990 and held the first Modeling Workshop for high school physics teaching during 1991. Malcom Wells led the initial workshop, which lasted six weeks and included teachers from Arizona. During the summer of 1992, the project expanded to two workshops and included a follow-up workshop for the initial participants.

As the number of workshops grew, so did the scope and emphasis. The group of initial workshop participants in 1991 made a commitment to participate in three successive years. The initial workshop focused on Modeling in mechanics, using technology to support teaching and help manage classroom discourse. In subsequent years, the participants began to develop curricular materials that covered electricity and magnetism as well as refining materials for the mechanics curriculum. Many of the participants in the initial workshops went on to become workshop leaders in subsequent years. The training of workshop leaders through the national dissemination grant expanded the reach of the project. In 1998, an initial leadership workshop helped train new workshop leaders, and initiated an on-going effort to develop new curriculum, including Modeling Chemistry and Modeling for Physical Science.

Modeling workshops helped teachers gain a better understanding of the content of physics by acting as both participant and teacher in the physics curriculum [5]. By training workshop leaders and encouraging them to submit proposals for local workshops, the leadership team allowed local leaders to adapt the workshops to their particular circumstances and needs. This gave leaders a sense of ownership and encouraged strong allegiance to the workshop project. As a result, over 1500 teachers have participated in a Modeling Workshop, which represents over 8% of all physics teachers nationally. The numbers are even greater in Arizona, where over 70% of teachers in the state have participated in Modeling Workshops [6]. In recognition of the conceptual gains for both teacher and student, and the broad participation in the workshops, in 2002 the U.S. Department of Education cited the Modeling Workshop Project as one of two outstanding educational reform efforts nationally [7].

### **Data Collection and Analysis**

Open-ended telephone interviews were conducted with five leaders of the Modeling Project: Larry Dukerich, David Hestenes, Jane Jackson, Colleen Megowan, and Greg Swackhamer. All interviews were conducted by Eric Brewe and then transcribed for analysis. Although a detailed analysis is ongoing, the preliminary analysis reported here is based on identification of dissemination-related patterns and themes in the interview transcripts. All three authors engaged in this process.

### **What makes modeling different?**

In many respects the Modeling Project is similar to other reform efforts. It is based on a good idea, backed up by research which indicates that the modeling approach helps students deepen their conceptual understanding, improve their problem solving skills, and develop more positive attitudes toward science. Additionally, the modeling project faced many of the barriers so common to dissemination in general. Our interviewees indicated that the Modeling Project was significantly impeded by lack of sufficient funding, resistant teachers, and either a lack of administrative support for the reforms or, in some cases, outright resistance on the part of administrators and policy makers. However, the Modeling Project was able to overcome these barriers.

Although every dissemination approach is unique, there are many aspects that are common. For the purposes of this paper, when we speak of the standard dissemination approach we refer to an approach similar to the model of reform advocated by the NSF CCLI program [8]. In this model of dissemination ideas and/or curriculum are developed by educational researchers and then distributed to teachers with some sort of training or guidance in their use.

### **The Modeling Project Focused on Building Community**

Modeling differs from this standard approach. Standard curriculum development and dissemination is focused on a specific idea, methodology or curriculum. Although the Modeling Project appears on the surface to be focused on a specific set of “Modeling” curricular materials and strategies, the interviewee’s descriptions reveal that the Modeling Project was actually largely focused on the building of a community of “Modelers”. Instead of developing and disseminating a product. Ownership of the project does not fall with any one person or small group, it is shared by all and newcomers are welcoming and encouraged. Recently, the modeling community has established The American Modeling Teachers Association as a means to support the community of modeling teachers [9]. The establishment if this association was done independent of the

original leaders of the Modeling Project. This theme of community building manifested itself in both the curriculum development and dissemination activities used by the modeling program. Each is discussed below.

Community-Based Curriculum Development. Although some curriculum was developed by the original implementers of the project they did not attempt to distribute the curriculum as is. Instead they deliberately encouraged workshop participants to work on refining existing curricular materials as well as developing their own new materials. By encouraging potential adopters to become involved in the development process, teachers came to feel a sense of ownership in the project which appears to have increased their interest and commitment toward adoption. This community-based approach is still ongoing in the Modeling community with no plans to cease this community-based development.

Community-Based Dissemination. In the standard dissemination approach there are usually a few leaders who take nearly all the responsibility for writing articles, giving talks, and most importantly, running workshops. The Modeling Project has always encouraged others to join in the dissemination effort, to assume leadership positions, and, just as with the curriculum development, to build ownership in the project. Another feature of the community-based dissemination is the availability of the Modeling materials in editable Microsoft Word format. This is, of course, contrary to some dissemination efforts that do not think it is appropriate for teachers to make modifications to the curricular materials.

## **Conclusion**

The standard approach to dissemination is hierarchical, with a small group of individuals developing an idea or curriculum to be disseminated and then providing a product to adopters, while retaining ownership of the product and its dissemination. It is an approach that can be characterized as top-down. The Modeling Project did not follow this approach. Their approach was more grassroots and focused on the building of community and the giving away of ownership. It appears that this grassroots approach offered numerous advantages. By giving ownership to the adopters, in addition to curriculum and ideas, the project has developed and has benefited from a large and still growing group of highly enthusiastic implementers/leaders, which has positioned it to survive and grow well into the future.

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## 7 PUBLICATIONS

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**O. Abu-Haija, J. A. Wardwell and E. Y. Kamber**, *Electron Capture by  $O^{3+}$  Ions from He,  $H_2O$  and  $CO_2$* , Journal of Physics: Conference Series **58**, 195 (2007).

**J. L. Baran, S. Das**, F. Járαι-Szabó, L. Nagy, and **J. A. Tanis**, *Interferences in Electron Emission Spectra from 1, 3 and 5 MeV  $H^+ + N_2$  Collisions*, Jour. Phys.: Conf. Series **58**, 215 (2007).

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**Arthur R. McGurn**, *Interaction of Two Different Photonic Crystal Waveguide Modes through the Resonant Excitation of Modes on Off-channel Kerr Nonlinear Media*, Organic Electronics **8**, (2007).

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**J. A. Tanis**, J.-Y. Chesnel, B. Sulik, B. Skogvall, P. Sobocinski, A. Cassimi, J.-P. Grandin, L. Adoui, D. Hennecart, and N. Stolterfoht, *Angular and High-frequency Analysis of Electron Interference Structures in  $\sim 60$  MeV/u  $Kr^{34+} + H_2$  Collisions*, Phys. Rev. A **74**, 022707 (2006).



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**G. Turri**, B. Lohmann, B. Langer, **G. Snell**, U. Becker and **N. Berrah**, *Spin Polarization of the  $Ar^* 2p^{-1}_{1/2}4s$ , and  $2p^{-1}_{1/2}3d$  Auger Decay*, J. Phys. B **40**, 3453 (2007).

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## 7.2 Papers in Press

**R. C. Bilodeau**, J. D. Bozek, G. D. Ackerman, N. D. Gibson, C. W. Walter, A. Aguilar, **G. Turri**, **I. Dumitriu**, and **N. Berrah**, *Multi-Auger Decay in Negative Ion Photodetachment*, AIP.

**S. Das**, **B. S. Dassanayake**, **M. Winkworth**, **J. L. Baran**, N. Stolterfoht, and **J. A. Tanis**, *Inelastic Guiding of Electrons in Polymer Nanocapillaries*, Phys. Rev. A **76** (2007).

**M. A. Famiano**, R.N. Boyd, T. Kajino, K. Otsuki, M. Terasawa, and G. J. Mathews, *Effects of Beta-Decays of Excited-State Nuclei on the Astrophysical  $r$ -Process*, J. Phys. G (2007).

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M. S. Wallace, **M. A. Famiano**, F. Delauney, A. Rogers, et al., *The High Resolution Array (HiRA), a New Charged Particle Detector for Rare-Isotope Experiments*, Nucl. Instr. and Meth. in Phys. Res. A (2007).

**D. Halderson**, *A Hypernuclear Single Particle Energies with the ESC04 Baryon-Baryon Potential*, Phys. Rev. C (2008).

A. Beach, **C. Henderson**, and **M. Famiano**, *Co-Teaching as a Faculty Development Model*, To Improve the Academy (2008).

**C. Henderson** and M. Dancy, *Barriers to the Use of Research-Based Instructional Strategies: The Dual Role of Individual and Situational Characteristics*, Physical Review Special Topics: Physics Education Research (2008).

### 7.3 Papers Submitted

**N. Berrah, R. C. Bilodeau, I. Dumitriu, J. D. Bozek, N. D. Gibson, C. W. Walter, G. D. Ackerman, O. Zatsarinny, and T. W. Gorczyca**, *Shape Resonances in the Absolute K-Shell Photodetachment of B-*, Phys. Rev. A.

Y. X. Zhang, P. Danielewicz, **M. A. Famiano**, Z. Li, W. G. Lynch, and M. B. Tsang, *Exploring the Symmetry Energy with Emitted Neutrons and Protons*, Phys. Rev. C.

**J. Grineviciute and D. Halderson**, *Proton Capture by  $^{14}\text{N}$  at Astrophysical Energies*, Phys. Rev. C.

**C. Henderson**, A. Beach, and **M. Famiano**, *Promoting Instructional Change via Co-Teaching*, American Journal of Physics (Physics Education Research Section).

**D. Rolles, Z. D. Pešić, H. Zhang, R. C. Bilodeau, J. D. Bozek, and N. Berrah**, *Study of Variable Clusters using Photoelectron Spectroscopy and Ion Imaging Techniques*, ICPEAC 07 proceedings.

**Lihua Wang and S. G. Chung**, *Precise Implementation of Cluster Transfer Matrix Method in the Single Electron Box*, Phys. Rev. B.

## 8 DISSERTATIONS

### 8.1 Ph.D.

Chaminda N. Kodituwakku, *Inelastic X-ray Scattering Studies on Organic Semiconductors and Organic Superconductors*, June 2007. Advised by **Clement Burns**.

## 9 PRESENTATIONS

### 9.1 Research Talks at Professional Meetings and Other Institutions

#### 9.1.1 Invited

**N. Berrah**, *AMO Physics using the ALS Slicing Source*, Advanced Light Source Workshop, July 24, 2006.

**N. Berrah**, *Studies of Negative Ions using an FEL*, Vuv-FEL Workshop 2006, Madison, Wisconsin, October 2006.

**N. Berrah**, *Opportunities for Future AMO Science at the ALS with FELs*, Prospects for Studies of Exotic, Transient, and Ultradilute Gas-Phase Targets ALS AMO workshop, ALS, LBNL, October 9-10, 2006.

**N. Berrah**, *Impact of AMO Science using FEL: Atmospheric and Intergalactic Gases*, Introduction to organized AMO session at the SRC FEL workshop, Madison, WI, October 18-19, 2006.

**N. Berrah**, *Probing Molecules and Clusters using the ALS*, International Atomic Workshop, Dresden, Germany, November 28, 2006.

**R. Bilodeau**, *Unexpected Inner-Shell Photodetachment Threshold Laws and Near-threshold Structure*, ALS Users' Meeting, October 2006.

**S. G. Chung**, *New Method for the Quantum Ground States in One Dimension*, at the International Conference Quantum Mechanics from Fundamental Physics to Applications, Bertinoro, Italy, December 4-7, 2006.

**S. G. Chung**, *New Method for the 3D Ising Model*, Pusan National University, Pusan, Korea, December 19, 2006.

**S. G. Chung**, *New Method for the Quantum Ground States in One Dimension*, Pusan National University, Pusan, Korea, December 19, 2006.

**S. G. Chung**, *Cluster Transfer Matrix Method: A Novel Many-body Method in Nano-electronics*, Ball State University, Muncie, IN, April 5, 2007.

**S. G. Chung**, *Novel Many-Body Method in Statistical Mechanics and Strongly Correlated Condensed Matter Systems*, Inha University, Incheon, Korea, June 7, 2007.

**S. G. Chung**, *Novel Many-Body Method in Statistical Mechanics and Strongly Correlated Condensed Matter Systems*, Pohang University of Science and Technology, Pohang, Korea, June 8, 2007.

**S. G. Chung**, *Novel Many-Body Method in Statistical Mechanics and Strongly Correlated Condensed Matter Systems*, Korea Advanced Institute for Science and Technology, Taejeon, Korea, June 13, 2007.

**S. G. Chung**, *Novel Many-Body Method in Statistical Mechanics and Strongly Correlated Condensed Matter Systems*, Yonsei University, Seoul, Korea, June 14, 2007.

**S. G. Chung**, *Novel Many-Body Method in Statistical Mechanics and Strongly Correlated Condensed Matter Systems*, Pusan National University, Pusan, Korea, June 15, 2007.

**S. G. Chung**, *Novel Many-Body Method in Statistical Mechanics and Strongly Correlated Condensed Matter Systems*, Korea Institute for Advanced Study, Seoul, Korea, June 21, 2007.

**M. A. Famiano**, *Experimental Investigations of the Asymmetry Term in the Nuclear Equation-of-State*, Horia Hulubei Institute of Nuclear Physics Invited Seminar, Magurele, Romania, March 8, 2007.

**M. A. Famiano**, *Experimental Progress in Nuclear Asymmetry and the Equation-of-State*, Valparaiso University, January 12, 2007.

**T. W. Gorczyca**, *Autoionization in Astrophysics*, Workshop on *High Accuracy Atomic Physics in Astronomy*, Institute for Theoretical Atomic and Molecular Physics, Harvard-Smithsonian Center for Astrophysics, Cambridge, MA, August 2006.

**T. W. Gorczyca**, *The Role of Atomic Physics in Understanding the Cosmos*, Kellogg Community College, Battle Creek, MI, April 2007.

**C. Henderson**, *From Research to Practice: Why Hasn't Physics Education Research Had More of an Influence on Physics Teaching and What can We Do About It?*, Physics Education Research Colloquium, University of Maryland, College Park, MD, May 23, 2007.

**C. Henderson**, *Barriers to the Implementation of 'Reformed' Instruction*, Physics Colloquium, Southern Illinois University, Edwardsville, IL, April 19, 2007.

**C. Henderson**, *From Research to Practice: Why Hasn't Educational Research Had More of an Influence on Teachers and What Can We Do About It?*, Invited Workshop, PTEC 2007 Conference, Boulder, CO, March 3, 2007.

**C. Henderson**, *Putting Values into Practice: The Mismatch Between Faculty Beliefs and Practices*, Physics Colloquium, Central Michigan University, Mount Pleasant, MI, February 8, 2007.

**C. Henderson**, *Putting Values into Practice: The Mismatch Between Faculty Beliefs and Practices*, Physics Colloquium, Emory University, Atlanta, GA, January 26, 2007.

**C. Henderson** and M. Dancy, *Build It and They Will “Come,” and Other Myths About Science Education Reform*, invited talk, 19th Biennial Conference on Chemical Education, West Lafayette, IN, August 2, 2006.

E. Yerushalmi, **C. Henderson**, K. Heller, and P. Heller, *Faculty Cognitive Conflict About Instruction: Opportunities for Improving Dissemination Efforts*, Invited Poster, Targeted Poster Session TP-D: Bridging the Gap Between Instructors and Curriculum Developers: Facilitating Successful Communication and Promoting Customization, 2006 Physics Education Research Conference, Syracuse, NY, July 27, 2006.

**C. Henderson** and M. Dancy, *Divergent Expectations between Physics Faculty and Educational Researchers about the Use of Educational Research*, Invited Poster, Targeted Poster Session TP-D: Bridging the gap between instructors and curriculum developers: Facilitating successful communication and promoting customization, 2006 Physics Education Research Conference, Syracuse, NY, July 27, 2006.

**Arthur R. McGurn**, *Impurity Mode Techniques Applied to the Study of Light Sources*, Conference on Building Bridges Between Lithuanian and U.S. Scientists, Vilnius University, January 26, 2007.

**Z. Pešić**, *Studies of Molecules using a Velocity Map Imaging Detector*, International Conference on the Application of Accelerators in Research and Industry, Denton, Texas, November 2006.

**D. Rolles**, *Size Effects in Angle-Resolved Photoelectron Spectroscopy of Free Rare-Gas Clusters*, International Symposium on Scattering, Coincidence and Absorption Studies of Molecules (SCASM), Rio de Janeiro, Brazil, September 2006.

**J. A. Tanis** and **S. Hossain**, *Electron Interferences in the Ionization of  $H_2$* , Nineteenth International Conference of the Application of Accelerators in Research and Industry, Fort Worth, TX, August 2006.

**J. A. Tanis**, *Evidence for Pauli Exchange in Electron Transfer by He-like and H-like Ions*, Topical Workshop of the SPARC Collaboration, Paris, France, February 2007.

**A. H. Wuosmaa**, *Nuclear Clusters in Astrophysics*, Division of Nuclear Physics Meeting of the American Physical Society, Nashville TN, October 2006.

**A. H. Wuosmaa**, *APEX – A Search for Things That Weren’t*, Symposium on Nuclear Physics, University of Illinois at Chicago, Chicago, IL, May 2007.

**A. H. Wuosmaa**, *Studies of Exotic Light Nuclei with Nucleon Transfer Reactions*, Gordon Research Conference, New London, NH, June 2007.

### 9.1.2 Contributed

**Sh. A. Abdel-Naby, D. Nikolic, T. W. Gorczyca**, N. R. Badnell, and D. W. Savin, *Dielectronic Recombination of Al-Like Sulfur*, 2007 American Physical Society Division of Atomic, Molecular, and Optical Physics Meeting, June, 2007, Calgary, Alberta; Bull. Am. Phys. Soc. **52**, 39 (2007).

**O. Abu-Haija, J. A. Wardwell and E. Y. Kamber**, *Electron Capture by  $O^{3+}$  Ions from He,  $H_2O$  and  $CO_2$* , 13<sup>th</sup> International Conference on the Physics of Highly Charged Ions, August 28-September 1, 2006, Belfast, Northern Ireland, UK.

**N. Berrah, D. Rolles, Z. Pešić, H. Zhang, R. Bilodeau, Ileana Dumitriu, W. Johnson, J. D. Bozek**, and G. Ackerman, *Studies of Molecules and of van-der-Waals Clusters*, ICESAT Satellite on Molecular Fragmentation, Rio de Janeiro, Brazil, September 4, 2006.

**N. Berrah**, *Probing AMO Science from Within*, 2006 AMOS DOE Workshop, Airlie Center, Warrenton, VA, September 2006.

D. Cubaynes, J-M. Bizau, S. Diehl, F. J. Wuilleumier, H. L. Zhou, S. T. Manson, A. Hibbert, **N. Berrah, S. Canton**, J. D. Bozek, E. T. Kennedy, L. Voky, and X. Y. Han, *Dynamical and Relativistic Effects in Experimental and Theoretical Studies For Inner-Shell Photoionization of Sodium*, DAMOP (Bulletin of the American Physical Society), p. 152, Calgary, Alberta, Canada, June 5-9, 2007.

**R. C. Bilodeau, D. Rolles, Z. Pesic, J. D. Bozek**, and **N. Berrah**, University of Wisconsin FEL Workshop, Madison, Wisconsin, October 18, 2006.

**R. C. Bilodeau, J. D. Bozek, N. D. Gibson, C. W. Walter, G. D. Ackerman, I. Dumitriu**, and **N. Berrah**, *Unexpected Inner-Shell Photodetachment Threshold Laws and Near-Threshold Structure*, ALS users meeting, Lawrence Berkeley National Laboratory, October 2006.

**R. C. Bilodeau, C. W. Walter, I. Dumitriu, N. D. Gibson, G. Ackerman, J. D. Bozek, B. S. Rude, R. Santra, L. S. Cederbaum**, and **N. Berrah**, *Photo Double Detachment of  $CN^-$ : Electronic Decay from an Inner-Valence Hole in Molecular Anions*, DAMOP (Bulletin of the American Physical Society), p. 153, Calgary, Alberta, Canada, June 5-9, 2007.

**R. C. Bilodeau, I. Dumitriu, N. D. Gibson, C. W. Walter, J. D. Bozek, Z. Pesic, D. Rolles**, and **N. Berrah**, *Inner-Shell Studies in Transition Metal Negative Ions: d-Shell Photoexcitation and Detachment*, DAMOP (Bulletin of the American Physical Society), p. 153, Calgary, Alberta, Canada, June 5-9, 2007.

**B. S. Dassanayake, M. Winkworth, J. A. Tanis**, and N. Stolterfoht, *Electron Guiding through Nanocapillaries in Insulators*, 16<sup>th</sup> International Workshop on Inelastic Ion-Surface Collisions (IISC-16), Schloss Hernstein, Austria, September 2006.

**M. A. Famiano**, *Experiments with Hot Nuclei and Dense Matter*, Long Range Plan Town Meeting on Nuclear Astrophysics/Study of Nuclei, Chicago, IL, January 19 - 21, 2007.

**T. W. Gorczyca**, **M. F. Hasoglu**, **S. A. Abdel Naby**, **D. Nikolic**, **J. Fu**, **K. T. Korista**, N. R. Badnell, B. M. McLaughlin, D. W. Savin, and S. T. Manson, *New and Improved Atomic Data for Accurate Plasma Modeling*, 15th International Conference on Atomic Processes in Plasmas, Gaithersburg, MD, March 2007; eds. J. D. Gillaspay, J. J. Curry, and W. L. Wiese (American Institute of Physics Conference Proceedings 926, New York, 2007).

**T. W. Gorczyca**, **K. T. Korista**, **J. Fu**, **D. Nikolic**, **M. F. Hasoglu**, **I. Dumitriu**, N. R. Badnell, and D. W. Savin, *Calculation of Atomic Data for NASA X-Ray Astrophysics*, 2006 American Astronomical Society High Energy Astrophysics Division Meeting, October, 2006, San Francisco, California; Bull. Am. Astr. Soc. **38**, 387 (2006).

P. Bryans, N. R. Badnell, **T. W. Gorczyca**, J. M. Laming, W. Mitthumsiri, and D. W. Savin, *Updated Ionization Balance Calculations for Collisionally Ionized Plasmas*, 2006 American Astronomical Society High Energy Astrophysics Division Meeting, October, 2006, San Francisco, California; Bull. Am. Astr. Soc. **38**, 387 (2006).

**D. Halderson**, *A Hypernuclear Single Particle Energies with the ESC04 Baryon-Baryon Potential*, Midwest Nuclear Theory Get-Together, Argonne National Laboratory, October, 2006.

S. T. Manson, **M. F. Hasoglu**, **T. W. Gorczyca**, N. R. Badnell, and D. W. Savin, *K-shell Fluorescence Yields of Li- to F-like Ions*, 2007 American Physical Society Division of Atomic, Molecular, and Optical Physics Meeting, June, 2007, Calgary, Alberta; Bull. Am. Phys. Soc. **52**, 39 (2007).

**M. F. Hasoglu**, **Sh. A. Abdel-Naby**, **D. Nikolic**, **T. W. Gorczyca**, and B. M. McLaughlin, *X-Ray Absorption in Carbon Ions Near the K-Edge*, 2007 American Physical Society Division of Atomic, Molecular, and Optical Physics Meeting, June, 2007, Calgary, Alberta; Bull. Am. Phys. Soc. **52**, 129 (2007).

**C. Henderson** and M. Dancy, *Reform Barriers for University Faculty*, American Educational Research Association Annual Meeting, Chicago, IL, April 9, 2007.

**C. Henderson** and M. Dancy, *When One Instructor's Interactive Classroom Activity is Another's Lecture*, MIAAPT 2007 Spring Meeting, Grand Rapids, MI, March 17, 2007.

H. Fynewever and **C. Henderson**, *Unobservable Educational Choices Rubric (UECR) Project*, MSTA Annual Meeting, Grand Rapids, MI, March 16, 2007.

**C. Henderson**, M. Dancy, and A. Beach, *Promoting Instructional Change: Beyond an Emphasis Curriculum*, AAPT 2007 Winter Meeting, Seattle, WA, January 9, 2007.

**C. Henderson**, A. Beach and **M. Famiano**, *Diffusion of Educational Innovations via Co-Teaching*, MIAAPT 2006 Fall Meeting, Dearborn, MI, October 14, 2006.



**C. Henderson**, A. Beach and **M. Famiano**, *Creating Lasting Reform: Diffusion of Educational Innovations via Co-Teaching*, AAPT 2006 summer meeting, Syracuse, NY, July 24, 2006.

M. Dancy and **C. Henderson**, *A Post-Positivist Perspective on Physics Education*, AAPT 2006 Summer Meeting, Syracuse, NY, July 24, 2006.

**D. Nikolic**, **T. W. Gorczyca**, D. W. Savin, and N. R. Badnell, *Signature of Quantum Interference in Photorecombination of Ar-Like Ions*, 2007 American Physical Society Division of Atomic, Molecular, and Optical Physics Meeting, June, 2007, Calgary, Alberta; Bull. Am. Phys. Soc. **52**, 39 (2007).

**D. Nikolic**, **T. W. Gorczyca**, **J. Fu**, D. W. Savin, and N. R. Badnell, *Steps Toward Dielectronic Recombination of Argon-Like Ions: A Revisited Theoretical Investigation of  $Sc^{3+}$  and  $Ti^{4+}$* , Proceedings of CAARI 2006: The 19th International Conference on the Application of Accelerators in Research and Industry, Forth Worth, Texas, Aug. 2006.

**Z. Pešić**, **D. Rolles**, **R. Bilodeau**, **I. Dumitriu**, G. Ackerman J. Bozek, and **N. Berrah**, *Velocity Map Imaging of Molecular Photoionization Fragment*, International Conference on the Application of Accelerators in Research and Industry, CAARI 2006, Dallas, TX, August 2006.

**D. Rolles**, **Z. D. Pešić**, **R. Bilodeau**, **I. Dumitriu**, G. Ackerman, J. Bozek, and **N. Berrah**, *Velocity Map Imaging of Fragments Subsequent to Photoionization of Molecules*, ICESS Satellite on Molecular Fragmentation, Rio, de Janeiro, Brazil, September 4, 2006.

**D. Rolles**, **Z. D. Pešić**, **M. Perri**, **R. Bilodeau**, G. Ackerman, B. Rude D. Kilcoyne, J. D. Bozek, and **N. Berrah**, *Molecular Fragmentation Dynamics Studied by Velocity Map Imaging*, ALS Users Meeting, Lawrence Berkeley National Laboratory, October 2006.

**A. Rosenthal**, **C. Henderson**, **D. Isola** and **D. Schuster**, *Development of a Wave Concept Survey*, AAPT 2006 Summer Meeting, Syracuse, NY, July 25, 2006.

**D. Strohschein**, **J. Baran**, and **J. A. Tanis**, *Nonstatistical Enhancement of the  $1s2s2p^4P$  State in Electron Transfer for 0.5-1 MeV/u  $C^{4,5+} + He$  and  $Ne$  Collisions*, Thirteenth International Conference on the Physics of Highly Charged Ions, Belfast, Northern Ireland, UK, August 2006.

**J. A. Tanis**, **J. L. Baran**, F. Járαι-Szabó, and L. Nagy, *Interferences in Electron Emission Spectra from 1, 3, and 5 MeV  $H^+ + N_2$  Collisions*, Thirteenth International Conference on the Physics of Highly Charged Ions, Belfast, Northern Ireland, UK, August 2006.

## 9.2 Research and Public Lectures at WMU

The Department of Physics sponsors lectures on physics research intended mainly for graduate students and faculty. These talks inform faculty and students at Western of research efforts here and at other institutions as well as acquaint visiting speakers with our research and academic programs at Western. The Department of Physics also sponsors public lectures on physics topics of general interest. These talks are intended for faculty, physics graduate students, physics undergraduate students, and non-physicists. The research and public lectures are listed below.

*Guided Transmission of Highly Charged Ions through Nanocapillaries in Polyethylene Terephthalate (PET)*, Rolf Hellhammer, Hahn-Meitner-Institut, Berlin, Germany, August 17, 2006.

*Experimental Investigations of Negative Ions*, **René Bilodeau**, Western Michigan University and Lawrence Berkeley Laboratory, Berkeley, CA, September 11, 2006.

*Autoionizing States and Their Relevance in Electron-Ion Recombination*, **Dragan Nikolić**, Department of Physics, Western Michigan University, September 18, 2006.

*Nuclear Shell Structure Above CA-48 Probed by Beta Decay*, Paul Mantica, NSCL and Department of Chemistry, Michigan State University, September 25, 2006.

*Atoms and Molecules in Extreme Light Fields*, Joachim Ullrich, Max-Planck-Institut, Heidelberg, Germany, October 2, 2006.

*Nonperturbative Electron Dynamics in Field-Free and Laser-Assisted Atomic Collisions*, Tom Kirchner, Institute of Theoretical Physics, Clausthal University of Technology, Germany, October 3, 2006.

*Learning about Enzymes with Molecular Dynamics*, Robert I. Cukier, Dept. of Chemistry and the Quantitative Biology Modeling Initiative, Michigan State University, October 9, 2006.

*Nuclear Terrorism – What is Being Done*, Larry Satkowiak, Director, Nuclear Nonproliferation Program, Oak Ridge National Laboratory, October 13, 2006.

*Because Physics Majors Have Conceptual Difficulties Too: Refining an Inquiry-Based Approach to Teach Intermediate Mechanics*, Bradley S. Ambrose, Department of Physics, Grand Valley State University, October 16, 2006.

*Red Giants to Planetary Nebulae: A Study of the Transitional Objects*, Dr. Bruce Hrivnak, Department of Physics and Astronomy, Valparaiso University, October 23, 2006.

*Fractures as Time-Dependent Structures: Characterizing Alterations and Changing Length Scales*, Laura J. Pyrak-Nolte, Department of Physics/Department of Earth and Atmospheric Sciences, Purdue University, October 30, 2006.

*New Developments in Liquid Interfacial Nanoscience*, Mark Schlossman, Department of Physics University of Illinois at Chicago, November 6, 2006.

*Big-Bang, Little-Bang Nucleosynthesis Studied with Short-Lived (Radioactive) Nuclear Beams and the "Missing Mass" Problem*, Fred Becchetti, University of Michigan, November 13, 2006.

*Environmental Science on the Molecular Scale: How Can a Physicist Help?*, Bruce A. Bunker, Department of Physics, University of Notre Dame, November 20, 2006.

*The Search for Dark Matter with Superheated Fluids*, Ilan Y. Levine, Department of Physics and Astronomy, Indiana University, November 27, 2006.

*Guiding of Highly-Charged Ions through Insulating Nanocapillaries*, M. B. Sahana, Department of Astronomy and Physics, Wayne State University, December 4, 2006.

*Protein Dynamics Near the Unfolding/Refolding Transition State*, Warren F. Beck, Department of Chemistry, Michigan State University, December 11, 2006.

*Einstein, Ethics, and Physics*, Lewis Pyenson, Ph.D., FRSC (Academy II), Membre Correspondant, Académie Internationale d'histoire des Sciences (Paris), Dean of the Graduate College, Professor of History, Western Michigan University, January 8, 2007.

*High Pressure Mineralogy: An Experimental Window into Planetary Interiors*, Henry Scott, Indiana University - South Bend, January 22, 2007.

*New Directions in Multiphoton Microscopy*, Jennifer Ogilvie, University of Michigan, January 29, 2007.

*Spartan Infrared Camera, High Resolution Imaging for the Soar Telescope*, Ed Loh, Michigan State University, February 5, 2007.

*Impurity Mode Techniques Applied to the Study of Light Sources*, **Arthur McGurn**, Department of Physics, Western Michigan University, February 12, 2007.

*Electron Transport Through the Coupled Quantum-Dots in Nanoscale Systems*, Yong S. Joe, Center for Computational Nanoscience, Department of Physics and Astronomy, Ball State University, February 19, 2007.

*Why is there Mass? The Search for the Higgs*, Mark Adams, University of Illinois at Chicago, February 26, 2007.

*Geophysics at WMU, and an Application to Groundwater Exploration in Egypt*, William Sauck, Department of Geosciences, Western Michigan University, March 12, 2007.

*Higher Education for a Higher Purpose: Research and Education for Ecocultural Sustainability*, Harold Glasser, Department of Environmental Studies, Western Michigan University, March 19, 2007.

*Improving the Education of Physics Teachers: A Five Year Summary of the PhysTEC Project at WMU*, **Alvin Rosenthal** and **Drew Isola**, Department of Physics, Western Michigan University, March 21, 2007.

*The Neutrino Oscillation Industry*, Maury Goodman, Argonne National Laboratory, March 26, 2007.

*Photoionization Studies of Atomic Systems*, Steven T. Manson, Georgia State University, Department of Physics and Astronomy, Atlanta, GA, April 2, 2007.

*Superconductivity: Challenges and Opportunities*, George Crabtree, Materials Science Division, Argonne National Laboratory, April 9, 2007.

*Alternative Approaches to Dark Matter and Dark Energy*, Grant J. Mathews, Department of Physics, Center for Astrophysics, University of Notre Dame, April 23, 2007.

## 10 PROPOSALS AND GRANTS

**N. Berrah**, Advanced Light Source Support toward a postdoctoral fellow Rene Bilodeau, awarded, \$12,000 for 2006-2007.

**N. Berrah**, Advanced Light Source Support toward a postdoctoral fellow Daniel Rolles, awarded \$12,000 for 2006-2007.

**N. Berrah** (PI), DOE, Office of Science, BES, Division of Chemical Sciences, Geosciences and Biosciences grant, Project title: *Probing Complexity using the ALS*, funded \$564,000 for period March 2005-2008.

**N. Berrah**, Fellowship for Ms. Ileana Dumitriu from the ALS, LBNL, awarded \$16,000.

**N. Berrah** (PI), NSF international grant for US/CNRS research, project title: *Two Color Experiments in Open Shell Atoms*, funded \$29,600 for the period May 2005-2008.

**N. Berrah** (PI), Applied for 12% of beamtime, every six months, for three years on undulator Beamline 10.0.1 of the Advanced Light Source, Lawrence Berkeley National Laboratory, CA. Beamtime to carry out research experiments was granted for 2007.

**N. Berrah** (PI), applied for beamtime at a higher energy undulator Beamline (8.0.1) at the Advanced Light Source, beamtime granted for 3 weeks (2007).

**N. Berrah** (Co-PI), and Subra Mural, WMU Chemistry Department, Presidential Innovation Fund, WMU to establish a Center for Nano-Enabled Instrumentation and Nanofabrication (CNIN), award \$383,000, for the period 03/06-02/08.

**N. Berrah** (PI), Artie Bienenstock, Stanford University and Judy Franz, APS, (Co-PI) *Gender Equity: Strengthening the Physics Enterprise in Physics Departments and National Laboratories*, DOE, Office of Science, awarded \$90,000 for the period April 2007-March 2008.

**S. Chung**, *A Novel Many-Body Method in Condensed Matter Physics*, requesting 10,000 SU of IBM P690 supercomputer at the University of Illinois at Urbana-Champaign, submitted to National Science Foundation, granted to February 28, 2007 and extended to August 28, 2007.

**M. A. Famiano**, *Experimental and Theoretical Determination of Nuclear Data of Interest for Nuclear Safety*, NATO Expert Visit Grant, Visit to the HH-NIPNE for collaborative work. Amount: €7,000, awarded for period Fall 2006 – Fall 2007.

**M. A. Famiano** and M. B. Tsang (PI), *PIRE: U.S.-Japan-Western Europe Cooperative Research and Education: Determination of the Equation of State of Neutron Rich Matter*, submitted to NSF Office of International Science and Education Collaborative Research Office, November 28, 2006, declined.

**M. A. Famiano**, *Experimental Investigations of the Asymmetry Term of the Nuclear Equation of State*, PI: Michael Famiano, submitted to DOE Office of Nuclear Physics Outstanding Junior Investigator Program, November 8, 2006, declined.

**M. A. Famiano (PI)**, *Applications of Nuclear Structure and the Nuclear Equation-of-State*, submitted to NSF Program 05-036 Nuclear Physics Solicitation, September 27, 2006, declined.

**T. W. Gorczyca (PI)**, NASA Solar and Heliospheric Research and Technology Program, for project entitled *Calculations of High Temperature Dielectronic Recombination Rate Coefficients in Support of NASA's Sun-Earth Connection Program*, funded \$461,693 for period 2/1/2005-1/31/2008.

**T. W. Gorczyca (PI)** and **K. T. Korista**, NASA Astrophysics Research and Analysis Program, for project entitled *Improved Simulations of Astrophysical Plasmas: Computation of New Atomic Data*, funded \$435,000 for period 1/1/2004-12/31/2006.

**T. W. Gorczyca (PI)** and **K. T. Korista**, NASA Astrophysics Research and Analysis Program, for project entitled *Improved Simulations of Astrophysical Plasmas: Computation of New Atomic Data*, funded \$369,999 for period 4/1/2007-3/31/2010.

**D. Halderson**, National Science Foundation, *Microscopic Theory of Nuclear and Hypernuclear Structure and Reactions*, awarded \$26,820 for the period of 8/1/05 to 7/31/08.

**C. Henderson (PI)**, A. Beach, N. Finkelstein, and R. S. Larson (Co-PIs), National Science Foundation, *Facilitating Change in Higher Education: A Multidisciplinary Effort to Bridge the Individual Actor and System Perspectives*, awarded \$97,011 for the period 1/1/07 to 12/31/09.

H. Fynewever (PI), **C. Henderson** and H. Petcovic (Co-PIs), Michigan Department of Education, *Alignment of Secondary Science Teacher Practice and Materials in the Battle Creek Region*, \$195,458 requested, pending.

H. Fynewever (PI), **C. Henderson**, M. Jenness, R. Lindell, and H. Petcovic (Co-PIs), National Science Foundation, *Unobservable Education Choices Rubric (UECR): A Tool for Self and External Assessment of Teacher Alignment with Standards*, \$796,261 requested, pending.

A. Beach (PI), **C. Henderson**, and N. Finkelstein (Co-PIs), National Science Foundation, *STEM Educational Change Efforts in Higher Education: A Meta-Synthesis of Activities, Strategies, Concepts, and Theories across Disciplines*, \$198,379 requested, pending.

**C. Henderson (PI)** and M. Dancy (Co-PI), National Science Foundation, *Understanding Instructor Practices and Attitudes Towards the Use of Research-Based Instructional Strategies In Introductory College Physics*, \$331,143 requested, pending.

**C. Henderson (PI)**, H. Fynewever, S. Lentz, and H. Petcovic, (Co-PIs), *Rethinking the Science PhD as Preparation for a Community College Science Teaching Career: An Empirical Research and Evaluation Project*, National Science Foundation, \$787,377 requested, not funded.

**E. Y. Kamber**, NASA Planetary Atmosphere (PATM 2005), *State-Selective Charge Transfer Studies Relevant to Astrophysical Plasmas and Solar Wind-Comet Interactions*, requested \$321,401, not funded.

**A. Kayani** (PI), **E. Y. Kamber** (Co-PI), **J. A. Tanis** (Co-PI), **A. Wuosmaa** (Co-PI), DOD – Defense University Research Instrumentation Program (DURIP), *Equipment Acquisition for Accelerator Lab and Machine Shop*, \$509,724 pending.

**A. Kayani** (PI), **M. Famiano** (Co-PI), **E. Y. Kamber** (Co-PI), **J. A. Tanis** (Co-PI), **A. Wuosmaa** (Co-PI), National Science Foundation – Major Research Instrumentation (MRI) Program, *Equipment Acquisition for Accelerator Lab and Machine Shop*, \$508,634 declined.

**J. A. Tanis** (PI), Fulbright Scholar Program (France), *Investigation of Electron Interferences in Atomic Collisions*, Support level: ~ \$3000/mo. for 4 months, recommended at the peer review stage; declined at the administrative review stage.

**J. A. Tanis** (PI), R. D. DuBois (Co-PI), D. Schneider (Co-PI), E. H. Silver (Co-PI), and C. Whelan (Co-PI), National Science Foundation-Partnerships for International Research and Education. *PIRE: US-German Partnership for Atomic Physics Research at the New Facility for Antiproton and Ion Research (FAIR) at GSI-Darmstadt*, \$500,000/yr. for 5 years, declined at pre-proposal stage.

**J. A. Tanis**, Research Corporation, *Guiding of Fast Electrons and Positive Ions in Nanocapillaries*, awarded \$50,000 (sponsor) + \$25,000 (matching) for the period 6/30/07-6/29/09.

**J. A. Tanis** (PI), National Science Foundation – Atomic and Molecular Dynamics Program, *Travel Grant for US-based Student and Postdoctoral Participants to Attend ICPEAC XXV*, awarded \$7500 for the period 6/15/07 – 5/31/08.

**J. A. Tanis**, Applied Ion Beam Physics Laboratory, Fudan University, Shanghai (China), *Visiting Lecturer/Researcher*, awarded \$7500 for a 2-month appointment.

**J. A. Tanis** (PI), College of Arts & Sciences Teaching and Research Award (ASTRA), *Fragmentation of Water Molecules by Fast Ions/Funds to Purchase Microchannel Plates*, requested \$1000, awarded \$500 for Fall 2006.

**J. A. Tanis** (PI), College of Arts & Sciences Teaching and Research Award (ASTRA), *Travel Support to Attend SPARC Workshop in Paris*, awarded \$500 for Spring 2007.

**A. H. Wuosmaa** (PI), DOE, Office of Nuclear Physics, *Study of Exotic Light Nuclei with Few Nucleon Transfer Reactions*, awarded \$440,000 over three-year period 5/15/07-5/14/10.

**A. H. Wuosmaa**, (PI), DOE, National Nuclear Security Administration, *Instrumentation of the HELIOS Silicon Detector Array*, requested \$460,000, pending.

**A. H. Wuosmaa** (PI), *Study of Excited States in  $^{10}\text{C}$  from the  $^3\text{He}(^{10}\text{B},t)^{10}\text{C}$  Reaction*, ATLAS Facility Argonne National Laboratory Program Advisory Committee, 5 days of ATLAS Accelerator Beam Time, awarded.

**A. H. Wuosmaa**, (PI), *Study of  $^{13}\text{O}$* , ATLAS Facility Argonne National Laboratory Program Advisory Committee, 6 days of ATLAS Accelerator Beam Time, declined.



## 11 SCHOLARLY ACTIVITY

**N. Berrah**, member, ALS, LBNL, UC, Berkeley, Science Advisory Committee (SAC), 2007-2010.

**N. Berrah**, member, SSRL, SLAC, Stanford University, Science Advisory Committee (SAC), 2006-2009.

**N. Berrah**, co-team leader with Lou Dimauro for Atomic and Molecular Science at the femtosecond Linac Coherent Light Source (LCLS) at SLAC, Stanford, CA, 2004-present.

**N. Berrah**, co-Chair with Artie Bienenstock, *Strengthening the Physics Enterprise in Universities and National Laboratories through Gender Equity*, CSWP, APS, May 7-9, 2007.

**N. Berrah**, co-Chair, International Conference on Photonic, Electronics and Atomic Collisions, ICPEAC09.

**N. Berrah**, member, Committee of the Status of Women in Physics, CSWP, 2006-2008.

**N. Berrah**, chair, Davisson-Germer Prize, American Physical Society, 2006-2007.

**N. Berrah**, member, Executive Committee of the Division of Atomic Molecular and Optical Physics (DAMOP) of the American Physical Society, 2005-2008.

**N. Berrah**, member, the Executive Committee of the APS Topical Group on Few-Body Physics (GFB).

**N. Berrah**, member, Basic Energy Science Advisory Committee (BESAC) for the Office of Science, U. S. Department of Energy, 2002-2011.

**N. Berrah**, member, committee of the International Conference in X-Ray and Inner-Shell Processes, 2005-2008.

**S. G. Chung**, refereed 2 papers for Physics Lett. A.

**T. W. Gorczyca**, reviewed 3 manuscripts for Physical Review Letters, 1 manuscript for Physical Review A, and 2 manuscripts for Astrophysical Journal.

**C. Henderson**, refereed 9 papers for i) Proceedings, Physics Education Research Conference; ii) The Physics Teacher; iii) Journal of Research in Science Teaching; iv) American Journal of Physics; v) American Journal of Physics, Physics Education Research Section; vi) Physical Review - Special Topics: Physics Education Research.

**C. Henderson**, chair, American Association of Physics Teachers Committee for *Research in Physics Education*.

**C. Henderson**, second vice president (to advance to president) for the Michigan chapter of the American Association of Physics Teachers.

**C. Henderson**, member, *Physics Education Research Leadership and Organizing Council*.

**C. Henderson**, co-editor, Proceedings of the annual *Physics Education Research Conference*.

**C. Henderson**, external evaluator, *Physics and Astronomy New Faculty Workshop*.

**E. Y. Kamber**, reviewed 3 papers for Journal of Physics B, 1 paper for Physical Review A, and 3 papers for Journal of Physics: Conference Series.

**E. Y. Kamber**, member of the Executive Committee for the International Conference on Photonic, Electronic, and Atomic Collisions (ICPEAC), July 2007-2009.

**A. R. McGurn**, reviewed 1 grant for Research Corporation, 2 grants for Research Grants Council of Hong Kong, 10 grants for Civilian Research and Development Fund, Georgian proposals, 20 grants for Civilian Research and Development Fund, 2006 Physics Panel, wrote 3 reviews for Physical Review E, 3 for Journal of Physics D, 1 for Journal of the Optical Society of America B, 1 for Physical Review A, 2 for Physical Review Letters, 3 for Journal of Physics: Condensed Matter, 2 for Journal of Optics A: Pure and Applied, 1 for Applied Physics Letters, 2 for Applied Optics, 1 for Journal of Electromagnetic Waves and Applications, 1 for Journal of Applied Physics, 1 for Optics Express.

**P. V. Pancella**, sat on the panel reviewing proposals to the NSF Course, Curriculum, and Laboratory Improvement (CCLI) program, February 2007.

**J. A. Tanis**, refereed 2 papers for Physical Review Letters, 3 papers for Physical Review A, 1 paper for Nuclear Instruments and Methods in Physics Research, 1 paper for Journal of Physics: Conference Series, and 1 National Science Foundation proposal.

**J. A. Tanis**, member of the International Advisory Committee, 20<sup>th</sup> International Symposium on Ion-Atom Collisions (XX ISIAC), Agios Nikolaos, Crete, Greece, 2005-07.

**J. A. Tanis**, member of the International Scientific Committee for the International Conference on X-ray and Inner Shell Processes, June 2002 – August 2008.

**J. A. Tanis**, Member of the Executive Committee for the International Conference on Photonic, Electronic, and Atomic Collisions (ICPEAC), July 2003 – July 2011.

**J. A. Tanis**, ICPEAC 2009 Conference Chair (with N. Berrah, T. Gorczyca, and E. Kamber) for the XXVI International Conference on Photonic, Electronic, and Atomic Collisions (ICPEAC), to be held in Kalamazoo, July 22-28, 2009. This conference is the largest and most prestigious international conference on atomic collision physics attracting ~500 participants and ~200 accompanying persons.

**Alan Wuosmaa**, reviewed 4 articles for *Physical Review C*, and two articles for *Physics Letters B*.

**Alan Wuosmaa**, reviewed one DOE Outstanding Junior Investigator grant proposal, one NSF Career grant proposal, two DOE Phase I SBIR/STTR grant proposals, and one DOE Phase II SBIR/STTR grant proposal.

**Alan Wuosmaa** served on the Review Panel of DOE visiting committee for the Texas A&M University Cyclotron upgrade project.

**Alan Wuosmaa**, served on one National Science Foundation Grant Review Panel.

## 12 PERSONNEL

### Faculty

Berrah, Nora  
Burns, Clement  
Chung, Sung  
Famiano, Michael  
Gorczyca, Thomas  
Halderson, Dean  
Hardie, Gerald (Assistant  
Chair)  
Henderson, Charles  
Isola, Drew (Teacher in  
Residence)  
Kaldon, Philip (Part Time)  
Kamber, Emanuel  
Kayani, Asghar  
Korista, Kirk  
McGurn, Arthur  
Pancella, Paul (Chair)  
Paulius, Lisa  
Rosenthal, Alvin  
Schuster, David  
Tanis, John  
Wuosmaa, Alan

### Faculty Emeriti

Bernstein, Eugene  
Derby, Stanley  
Kaul, Dean  
Soga, Michitoshi  
Poel, Robert  
Shamu, Robert

### Adjunct Faculty

Stolterfoht, Nikolaus

### Staff

Cochran, Kerry  
Gaudio, Benjamin  
Kern, Allan  
Krum, Lori  
Scherzer, Bob  
Welch, Rick

### Post-Docs

Bilodeau, René  
Fu, Jun  
Nikolić, Dragan  
Pesic, Zoran  
Rolles, Daniel  
Said, Ayman

### Graduate Students

Abdel Naby, Shahin  
Abunima, Alaa  
Adams, Dan  
Al-Amar, Mohammad  
Al Faify, Salem  
Ayyad, Asmá  
Baran, Jamie  
Cassidy, David  
Cipri, Robert  
Das, Susanta  
Dassanayake, Buddhika  
Dumitriu, Ileana  
Durren, Michael  
El Kafrawy, Tamer  
Ganapathy, Subramanian  
Garratt, Elias  
Ghannam, Talal  
Giacherio, Brenna

### Graduate Students (cont.)

Goodman, Nicholas  
Grineviciute, Janina  
Hasoglu, Muhammet Fatih  
Hoekstra, Paul  
Kodikara, Ravin  
Kodituwakku, Nalaka  
Li, Shujun  
Lighthall, Jonathan  
Marley, Scott  
Moore, Andrew  
Nandasiri, Manjula  
Rai, Buddhi  
Vyas, Anjali  
Wang, Lihua  
Wang, Xue  
Wei, Haipeng  
Winkworth, Melike  
Zhang, Huaizhen  
Zhang, Yingfa