Final Technical Report for Grant No. DE-FG02-07ER46357

Auburn University, Auburn, Alabama 36849

Title: Detailed Investigations of Interactions between Ionizing Radiation and Neutral Gases

Principle Investigator: Allen Landers, Department of Physics

Report Date: March 31, 2014

Period covered: February 1, 2007 through January 31, 2010

Description of Accomplishments

We are investigating phenomena that stem from the many body dynamics associated with ionization of an atom or molecule by photon or charged particle. Our program is funded through the Department of Energy EPSCoR Laboratory Partnership Award in collaboration with Lawrence Berkeley National Laboratory. We are using variations on the well established COLTRIMS technique to measure ions and electrons ejected during these interactions. Photoionization measurements take place at the Advanced Light Source at LBNL as part of the ALS-COLTRIMS collaboration with the groups of Reinhard Dörner at Frankfurt and Ali Belkacem at LBNL. Additional experiments on charged particle impact are conducted locally at Auburn University where we are studying the dissociative molecular dynamics following interactions with either ions or electrons over a velocity range of 1 to 12 atomic units.

Results through 2010

1. Angular correlation of electrons emitted via the double Auger decay of *K*-shell ionized neon

The primary result from work we published in 2009 (pub. 5) indicated a breakdown in the 2-step picture of photoelectron emission followed by Auger decay for the small amount of phase space where the two are emitted in the same direction from the neon atom. To further investigate this phenomenon, we have now performed a similar measurement but restricted (*a posteriori*) the decay path to be a *double*-Auger to the Ne^{3+} state (Fig. 1 left). We used circularly polarized light from the ALS at LBNL to remove any lab-frame orientation of the photoelectron in the plane perpendicular to the photon propagation axis. This in turn allowed us to cleanly measure the momenta of *all three* continuum electrons (2 measured, 1 calculated by momentum conservation with the ion) for a kinematically complete measurement. By restricting the energy sum of two of the electrons, we were able to isolate the double-Auger channel (Fig. 1 right).

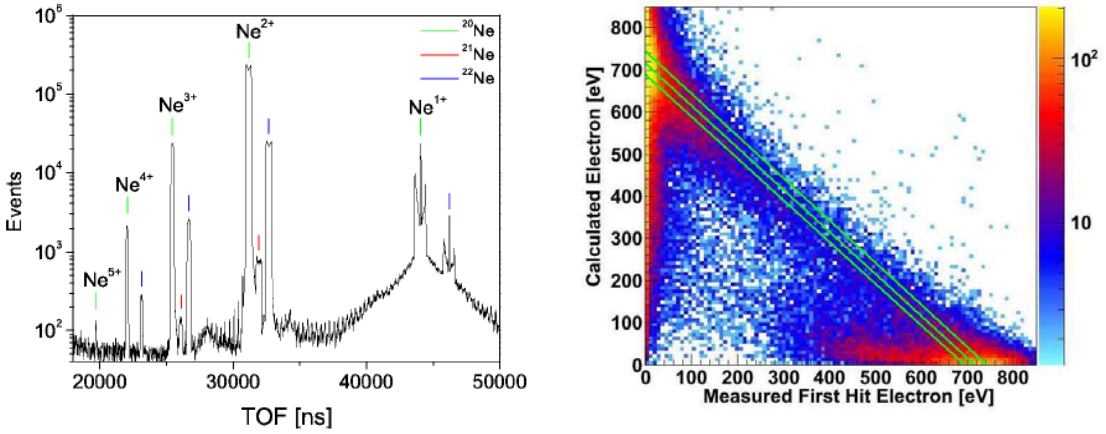

Figure 1 (Left): Neon ion time of flight spectrum following K-Shell photo-ionization just above threshold. The Ne^{3+} channel contributes about 6% to the total number of events

and is only accessible through double-Auger. **(Right):** Energy correlation between the measured first hit and calculated electron. The diagonal line corresponds to the constant energy sum for the double Auger channel. The variation in resolution as a function of energy is apparent.

The isolated double-Auger channel resembles strongly the single-photon double-photoionization of helium. Figure 2 shows the energy sharing between the two double-Auger electrons. There is a much higher probability for asymmetric sharing than

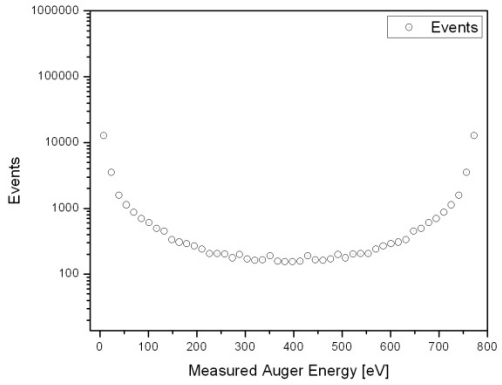

Figure 2: Energy sharing between the two double-Auger electrons. Note strong propensity for asymmetric energy sharing, which is similar to the well known single photon double ionization result.

symmetric sharing. This is consistent with double photoionization result, where the "shake" and "knock-out" processes are often used to model the asymmetric and symmetric energy sharing cases respectively. Figure 3 shows the angular correlation between the Augers for different energy sharing, where 0° is defined by the momentum vector of the fast electron. For extremely low energies where the photoelectron is indistinguishable from the low-energy Auger, we observe a distribution consistent with the single Auger case with the forbidden region. For symmetric and asymmetric cases that don't overlap with the photoelectron energy, we observe roughly isotropic ("shake") and ~130° peaked ("knockout") distributions.

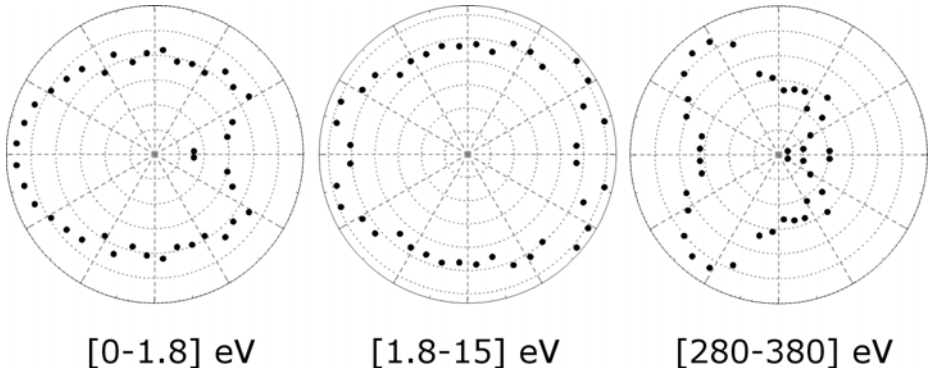

Figure 3: Distribution of the angle between double-Auger electrons as a function of the energy of one Auger. The left plot covers the same energy range as the photo-electron, so the low-energy Auger and photo-electron are indistinguishable. The middle plot

covers an energy range just above the photoelectron energy where the two Auger electrons share energy asymmetrically. The right plot covers an energy range where the sharing is more symmetric.

We are currently analyzing this data further to explore the 3-electron coincidence to see if we can better understand the breakdown of the 2-step picture of Auger decay. For example: we can restrict the double-Auger to symmetric energy sharing where both Auger electrons have hundreds of eV energy. Is there a correlation between the Auger momentum sum for this case and the photoelectron momentum? This and other questions are being explored.

2. Formation and characterization of helium Rydberg atoms

One of the calibration techniques we use for COLTRIMS at the ALS is to singly photoionize helium gas slightly above threshold. During one such calibration run, we found an unexpected image on the helium ion detector shown in the left panel Figure 5. The expected features are the horizontal stripe and small spot just above it that

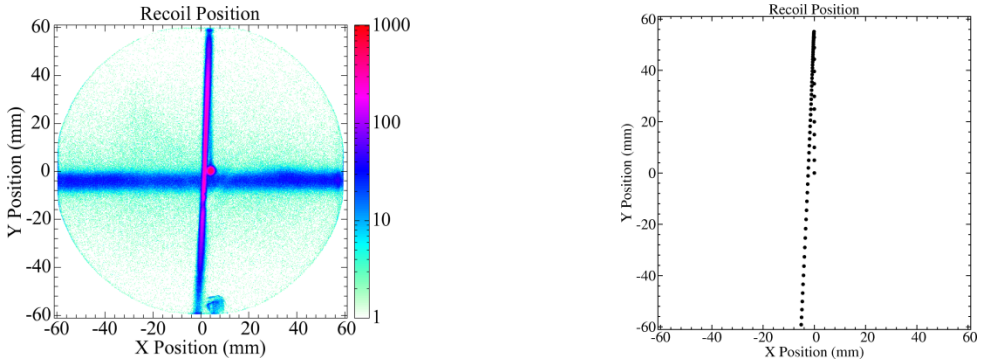

Figure 5 (Left): Helium ion detector showing vertical curved stripe produced from field-ionized Rydberg atoms.
(Right): SIMION calculation reproducing the detector image.

correspond to photon interaction with background gas and ionization of the helium jet by harmonic contamination. The unexpected feature is the stripe that rises vertically from the jet spot and then comes back down with a slight curve to the left. After further analysis and extensive simulation (see Fig. 5 right), we have concluded that we were producing helium Rydberg atoms.

The photon energy was tuned slightly below threshold and therefore excited the atoms in the jet to Rydberg states. These then traveled vertically at the jet velocity until they left the spectrometer. Because the spectrometer had a voltage bias relative to the

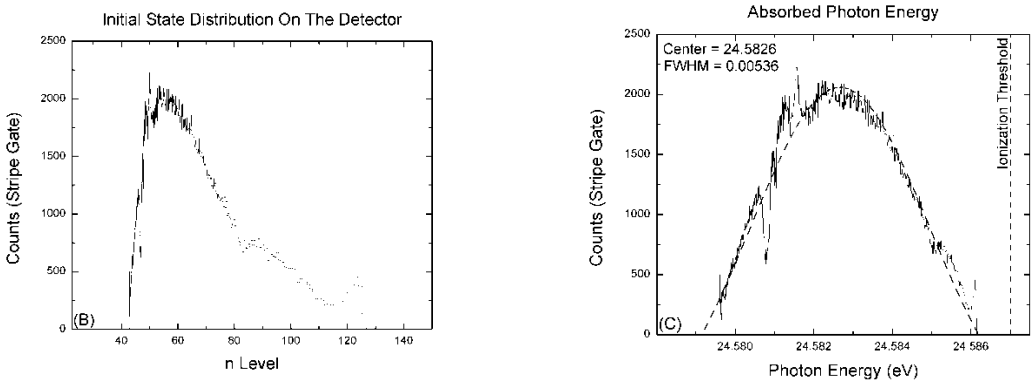

Figure 2 (Left): Distribution of principle quantum number of field-ionized helium Rydberg atoms.
(Right): Energy distribution of absorbed photons derived from data in left panel. The structures on the left side of the peak are experimental artifacts that are well understood. The 5.36 meV width is consistent with the monochrometer-defined resolution of the photon beam.

grounded jet-catcher tube, they were field ionized just outside the spectrometer and then directed back into the spectrometer by the same voltage bias. Different *n* levels were ionized at different points along the path as the electric field increased, which lead to different ion trajectories and corresponding hit positions on the detector. After careful modeling of the spectrometer, we have been able to extract the populated *n* levels based on the hit positions on the detector. This distribution is shown in the left panel of Figure 6. Converting to binding energy and adding the helium ionization potential (Fig. 6 right) yields a distribution consistent with the expected photon distribution from the monochrometer.

While no new science resulted directly from this measurement and analysis, it has nonetheless been useful. We are now designing of a new type of COLTRIMS experiment that will allow us to study near threshold effects. By tuning the synchrotron energy to near (just above, just below, or straddling) the double ionization threshold, we can study in detail ionization-excitation by measuring *in coincidence* the photoelectron momentum and Rydberg state of the singly charged helium ion.

Results through 2009

1. Breakdown of the Two-step Model in Core-level Photoionization of Neon.

We recently published results in Physical Review Letters [pub 2] that demonstrate for the first time the ability to simultaneously measure the full momentum vectors of both a low energy (~1 eV) photoelectron and an energetic (~800 eV) Auger electron over 4π solid angle following core-level photoionization by a single photon. This ability to directly measure the angular relationship between the two particles in the Ne^{2+} continuum revealed an interesting effect. Specifically, the photoelectron flux along the direction of the subsequent Auger electron is not diverted, as one might expect in a two-step description of photoionization followed by Auger decay. Rather, the photoelectron flux appears to simply be lost along the small fraction of solid angle near the Auger emission direction.

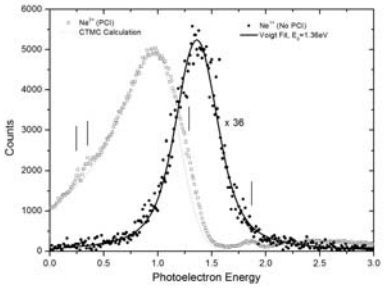

Figure 1: Photoelectron energies. The closed circles (●) of the right hand peak are photoelectrons measured in coincidence with Ne^+ ions and corresponding to direct photoionization with no PCI. The solid line is a Voigt fit. The open squares (□) of the left hand peak are photoelectrons measured in coincidence with Ne^{2+} ions and corresponding to photoionization followed by an Auger decay. The dashed line is the CTMC calculation by Robicheaux. The short vertical markers indicate recapture-remission lines.

Presented here are two figures from the article that demonstrate the power of the technique as well as the effect described above. Figure 1 shows the distribution of electrons for two final charge states of Ne. In the case of Ne+, the photo electrons emerge with energies given by the photon energy minus the ionization potential, and are spread by the width of the Ne(1s) hole and the experimental resolution. The electrons that correspond to the doubly charged final state of the ion have been shifted in energy by the potential change from 1/r to 2/r upon Auger decay. One can also see the small bumps and shoulders (marked with vertical lines) that arise from recapture of the photoelectron when the potential changes followed by re-emission at discreet energies.

The primary result from this work is shown in Figure 2, which shows the relative angle between Auger and photo electrons. Within the two step model, the initial photoelectron flux is diverted away from the Auger emission direction, as is demonstrated in the calculation by Robicheaux. However, in the measurement, we find that the photoelectrons emitted along the Auger direction are not diverted, but rather, they don't come out at all. This is a strong indication that initial state correlation plays a critical role in this photoionization/Auger process and the 2-step picture of the emission of one electron preceding that of the other doesn't fit for the small amount of phase space where the two are emitted in the same direction. Additional curves include the calculation folded with multiple factors of the experimental resolution to test if the difference is an instrumental effect.

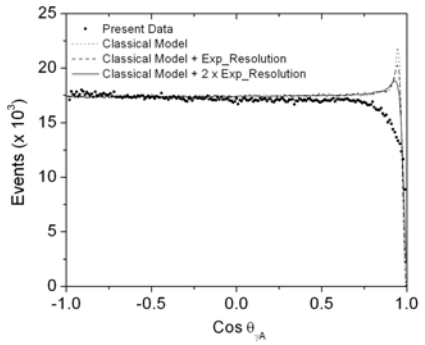

Figure 2: Distribution in cosine of the angle between the Auger electron and photoelectron. Closed circles (•) represent experiment data. Dashed and solid lines correspond to a two-step CTMC calculation (Robicheaux), including cases where the experiment resolution and twice the experiment resolution have been folded into the calculation. The calculation clearly shows a redistribution of photoelectron flux, while it can be seen from the data the flux is actually lost.

2. Double Auger Decay of Neon Following by Core-level Photoionization

There is a small probability (~6%) that the $Ne(1s^{-1})^+$ hole state will decay via double Auger electron emission. In this decay channel, the final state includes the photoelectron, two Auger electrons and the residual Ne^{3+} ion. We have recently performed an experiment to measure the angular correlation between the three continuum electrons. This measurement might allow, for example, a study of how the relationship between the photoelectron momentum and the momentum sum of the two Augers as function of the energy sharing between the two electrons, which would lead to significant further insight into the roles of initial- and final-state correlation in core-photoionization. Data are currently being analyzed and we anticipate results soon.

Specifically, we have measured three electrons e^- and a recoiling Ne^{3+} ion in coincidence following the core-photoionization of neon. Recognizing that the two-step interpretation is at heart of this investigation, we still use this model to describe the process:

$$Ne + h\nu\ (870\text{-}890eV) \rightarrow Ne(1s^{-1})^+ + e^-_{photo}\ \text{(photoelectron emission)}$$

$$Ne(1s^{-1})^+ + e^-_{photo} \rightarrow Ne(1s^{-1})^{3+} + e^-_{photo} + e^-_{Auger} + e^-_{Auger}\ \text{(Double Auger decay)}$$

The aim is to explore the entangled angular distribution of the three emitted electrons with respect to one another. Such a simultaneous vector momentum measurement of three continuum electrons will likely enable a deeper understanding of the relaxation processes in excited atoms. Described below is the physics we plan to investigate as analysis of the data progresses.

Goal 1: Investigation of the correlated Auger-electron emission. We are exploring, for example, the simultaneous angular and energy correlation between the two Auger electrons to deepen our understanding of this highly-correlated decay pathway. We suspect that the double-Auger decay is in many ways similar to the well documented direct double photoionization (one photon in, two electrons out) of say,

helium. For roughly equal energy sharing, there might a strong correlation between the two Auger electrons as in a knock-out type mechanism; and for strongly asymmetric energy sharing, there might be little or no correlation between the two electrons as in a shake-off type mechanism.

Goal 2: Understanding the role of initial and final state correlation in core-level photoionization. As discussed above, one primary motivation of the experiment is to shed further light on the breakdown of the two-step model in describing photo-ionization and (possibly) successive Auger-decay. A strong initial-state effect might be observed in the correlation between the sum momentum of the two Augers and the photoelectron. It might be that such an effect is observed to vary with different energy sharing between the Augers.

3. Investigating Asymmetries in the $HD^+(1s\sigma)$ Branching Ratio through Collisions with Electrons

We have built an electron-molecule collision experiment that uses a pulsed COLTRIMS technique that allows for momentum imaging of molecule fragments after dissociative ionization by electrons with energies from 10eV to 2000 eV. Preliminary experiments focus on isotope effects in the dissociative ionization of HD based on prior work by Ben-Itzhak and coworkers for ion impact [ref 1]. A beam from a pulsed electron gun passes through a diffuse target, followed by a synchronized electric field pulse which extracts the ions to a multi-channel plate detector with delay-line anode.

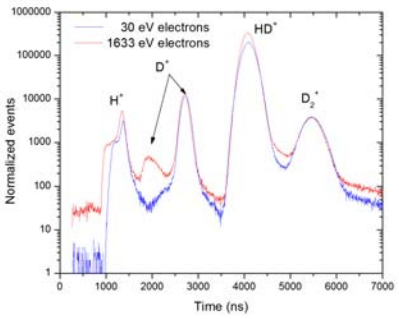

Figure 3: Typical time of flight spectrum showing flight times for ions created by electron impact on HD. The blue and red curves correspond to 30 eV and 1633 eV electron impact energies respectively.

Figure 3 shows data from initial measurements. The shoulder to the left of the H^+ peak arises from fast protons from H_2O contaminant as well as dissociation of HD^{2+} and D_2^{2+}. The secondary D^+ peak arises from energetic dissocation events that are inaccessible for the low energy impact case. Currently we are unable to clearly isolate the dissociative channel of interest due to background effects from water and contaminant H_2 and D_2 in the target gas. We have begun work on a new apparatus that incorporates a localized gas jet for a target, which will allow for full momentum imaging of the molecule fragments and a substantially better separation from background. In the meantime the present apparatus is being rebuilt to accommodate a larger detector and a spectrometer designed for fragment-fragment coincidences in multiply ionizing electron-molecule collitions.

4. Orientation Dependence in the Double Ionization of HD Molecules by Fast Ions

We are currently studying the level of orientation isotropy in the dissociative double ionization of HD molecules by fast ions as a function of projectile velocity. The light ions used to doubly ionize ground state HD molecules originate at the Auburn University Accelerator, which is capable of producing ions with velocities ranging from 1 to 13 atomic units.

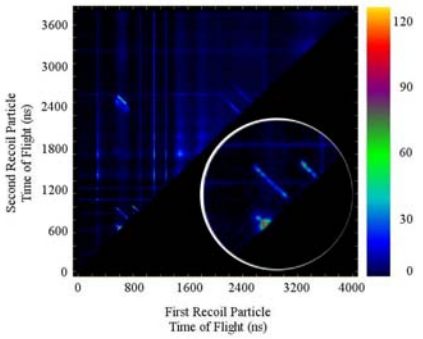

Figure 4: Fragment coincidence spectrum. The enlarged view shows the three species in the equilibrium target gas: HD, H_2 and D_2. This spectrum also shows coincidences from background gases H_2O, N_2 and O_2.

Previous studies have shown that the fragmentation of neutral hydrogen molecules by ion impact sometimes exhibit angular dependencies akin to Young's double slit experiment. These quantum mechanical effects have been observed in capture or transfer ionization [ref 2] as well as in double ionization [ref 3]. A similar experiment on the ground-state dissociation following single ionization [ref 4] showed no such angular dependence. In each case, results were consistent with a simple two-center model that predicts the angular distribution:

$$d\sigma(\theta) = d\sigma_a\left[1+\cos\left(q_z R\cos(\theta)\right)\right]$$

Where R is the internuclear position vector, θ is the angle between the molecular axis and the ion beam direction, and qz is the longitudinal momentum transfer. The latter is well approximated by the energy transfer divided by the incident projectile velocity $q_Z \cong Q/v_p$. Because of the velocity dependence of this model, we are investigating the molecule orientation isotropy for a variety of ion velocities. Preliminary results presented here are for 3 MeV He^{2+} ions with a velocity of 5.5 au. This initial projectile was chosen for convenience and because the results from [ref 3] are for F^{8+} ions with a similar velocity (6.3 au).

Figure 4 shows a typical time of flight correlation plot which demonstrates our success in producing our own HD by mixing H_2 and D_2 with a catalyst. Current results are statistics limited, but we anticipate momentum spectra and molecule angular distributions soon.

Results through 2008

ALS-1: **Breakdown of the Two-step Model in Core-level Photoionization of Neon.**

For a single multi-level atom such as neon, the photoionization process is yet to be understood in full detail. In particular, just above the core photoionization threshold two interesting phenomena can occur: (1) the three body post-collision interaction (PCI) between the photoelectron, residual ion and subsequent Auger electron; and (2) the possible recapture of the photoelectron. Both processes are associated with the change in potential caused by the fast Auger decay of the core-excited Ne^{*+} that occurs after photoionization. Shortly after emerging from the atom, the outgoing photoelectron is subject to a change in potential associated with the change of parent ion from Ne^{*+} to Ne^{2+}. Within the sudden approximation, the loss in energy (in atomic units) of the photoelectron is simply the change in potential energy given by 1/r, where r is the distance traveled from the ion before Auger decay occurs. If this energy loss is less than the original continuum energy, then the electron simply remains in the continuum with reduced kinetic energy (process 1). In this case, all three bodies can exchange momentum and energy. If, however, the energy loss is greater than the photoelectron's initial energy, the electron can be recaptured into Rydberg state orbiting the Ne^{2+} core (process 2).

At the LBNL-ALS in Berkeley, California, we have used the COLTRIMS technique to investigate in detail both processes (1) and (2) above along with the associated fundamental physics. We have measured the full momentum vectors of both the slow photoelectron and the recoiling neon ion in coincidence. For case (1), the momentum of the faster Auger electron has been determined by conservation laws, giving us the full momentum vectors three-body continuum state in coincidence.

A CTMC calculation by Robicheaux is used to model the interaction between the photoelectron and Auger electron. Because the De Broglie wavelengths differ by a factor of 23, their interaction in the continuum should be well approximated classically. Each event in the calculation consisted of the emission from the origin of a 1.36 eV electron followed by the emission of an 800 eV Auger electron in a random direction after a random time delay with and exponential distribution determined by the Auger lifetime. For the calculations, we assume no correlation between the original outgoing directions of the two electrons. Once both electrons are launched, he solves the classical time dependent equation of motion to determine the final momenta of the two electrons. Thus, the full electron-electron interaction in the field of the ion is incorporated in this classical calculation. The three components of each electron's momentum were stored in list mode, which allowed for the same sorting analysis of the CTMC data as was used in the analysis of the experimental data. This allowed for a realistic modeling of the experimental resolution.

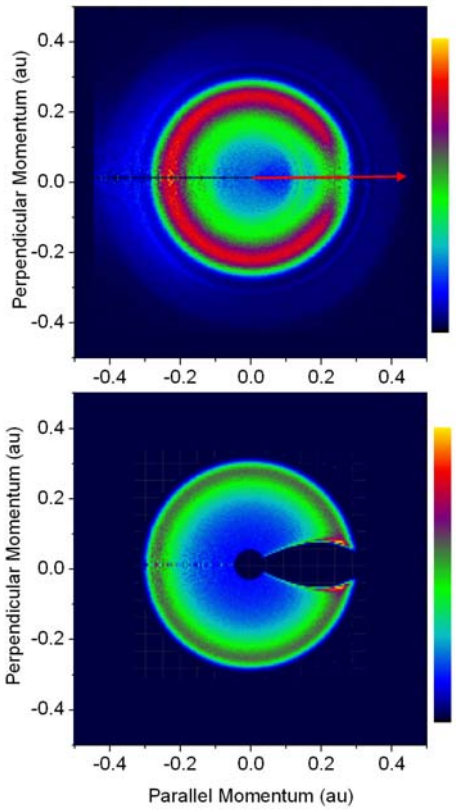

Figure 1: Momentum image of the photoelectron in a frame defined with axes parallel and perpendicular to the Auger emission direction (indicated by the red arrow). The color scale is linear and represents the number of events. The top panel shows the experimental result for low energy electrons in coincidence with the Auger electron. The isotropic discreet rings correspond to a separate recapture/re-emission process. The lower panel shows 2-step CTMC result (Robicheaux) in the same format. Note: The pileup along the edge of the opening of the "C" is not present in the experimental data.

The primary result that has stemmed from this work is the following: Within the two step model, the initial photoelectron flux is diverted away from the Auger emission direction, as can be seen in the calculation Robicheaux in the lower panel of Fig 1. However, in the measurement, we find that the photoelectrons emitted along the Auger direction are not diverted, but rather, they don't come out at all. This is a strong indication that initial state correlation plays a critical role in this photoionization/Auger process and the 2-step picture of the emission of one electron preceding that of the other doesn't fit for the small amount of phase space where the two are emitted in the same direction.

This effect can be seen more clearly in Figure 2, where the cosine of the relative angle between the emission directions of the photo- and Auger- electron is plotted. Here isotropy corresponds to a flat distribution. Here we show the data and CTMC calculation as a function of the cosine of the angle between the two electrons. The CTMC calculation is shown in three curves. The first is the model alone, and the other two correspond to including the 1x and 2x momentum resolution of the experiment in the initial conditions of the CTMC calculation. The calculated pile up of flux is not an effect of the classical treatment of the final state correlation. Such a redistribution rather than suppression of flux is a consequence of the two-step assumption.

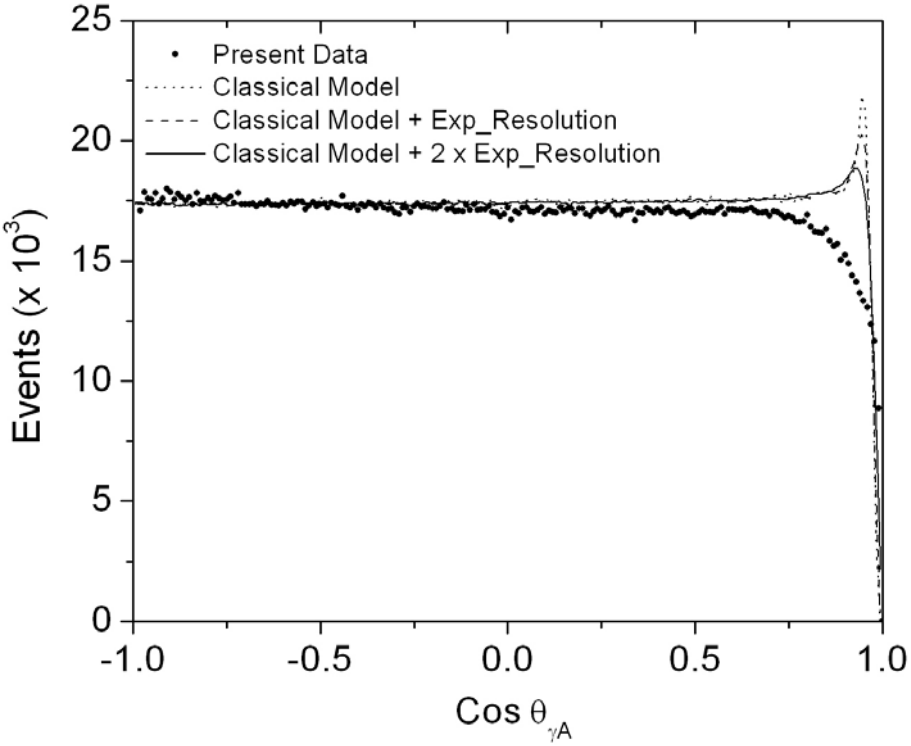

Figure 2: Distribution in cosine of the angle between the Auger electron and photoelectron. Closed circles (•) represent experiment data. Dashed and solid lines correspond to a two-step CTMC calculation (Robicheaux), including cases where the experiment resolution and twice the experiment resolution have been folded into the calculation. The calculation clearly shows a redistribution of photoelectron flux, while it can be seen from the data the flux is actually lost.

Future Plans

There is a small probability (~6%) that the $Ne(1s^{-1})^{+}$ hole state will decay via double Auger electron emission. In this decay channel, the final state includes the photoelectron, two Auger electrons and the residual Ne^{3+} ion. This relaxation pathway has been investigated previously through use of a magnetic bottle spectroscopy technique [3]. However, to date no measurement exists of the angular correlation between the three continuum electrons. Such a measurement would allow, for example, a study of how the relationship between the photoelectron momentum and the momentum sum of the two Augers as function of the energy sharing between the two electrons, which would lead to significant further insight into the roles of initial- and final-state correlation in core-photoionization.

We plan to pursue a coincidence momentum imaging experiment, measuring three electrons e^{-} and a recoiling Ne^{3+} ion in coincidence following the core-photoionization of neon. Recognizing that the two-step interpenetration is at heart of this investigation, we still use this model to describe the process:

$$Ne + h\nu\ (870\text{-}890eV) \rightarrow Ne(1s^{-1})^{+} + e^{-}_{photo} \text{ (photoelectron emission)}$$

$$Ne(1s^{-1})^{+} + e^{-}_{photo} \rightarrow Ne(1s^{-1})^{3+} + e^{-}_{photo} + e^{-}_{Auger} + e^{-}_{Auger} \text{ (Double Auger decay)}$$

The aim is to explore the entangled angular distribution of the three emitted electrons with respect one another. Such a simultaneous vector momentum measurement of three continuum electrons will enable a deeper understanding of the relaxation processes in excited atoms. We plan to pursue these measurements in the spring 2009 two-bunch mode operation at the Advanced Light Source at LBNL.

Goal 1: Investigation of the correlated Auger-electron emission. We will be able to explore, for example, the simultaneous angular and energy correlation between the two Auger electrons to deepen our understanding of this highly-correlated decay pathway. We suspect that the double-Auger decay is in many ways similar to the well documented direct double photoionization (one photon in, two electrons out) of say, helium. For roughly equal energy sharing, there might a strong correlation between the two Auger electrons as in a knock-out type mechanism; and for strongly asymmetric energy sharing, there might be little or no correlation between the two electrons as in a shake-off type mechanism.

Goal 2: Understanding the role of initial and final state correlation in core-level photoionization. As discussed above, one primary motivation of the experiment is to shed further light on the breakdown of the two-step model in describing photo-ionization and (successive?) Auger-decay. A strong initial-state effect might be observed in the correlation between sum momentum of the two Augers and the photoelectron. It might be that such an effect is observed to vary with different energy sharing between the Augers.

[1] A. Russek and W. Mehlhorn, *J. Phys. B* **19** 911 (1986), and references therein.
[2] T. W. Gorczyca, O. Zatsarinny, H.-L. Zhou, S. T. Manson, Z. Fel and A. Z. Msezane, *Phys Rev A* **68**, 050703(R) (2003).
[3] Y Hikosaka, T Aoto, P Lablanquie, F Penent, E Shigemasa and K Ito, *J. Phys. B* **39** 2006 3457-64).

ALS-2: Other Photoionization measurements

In addition to the work discussed above where Auburn has taken the lead role, we e continue to participate in other experiments at the ALS as part of the COLTRIMS collaboration. These experiments include measurements of interference and entanglement in H_2, core-hole localization in N_2, fragmentation pathways in acetylene and correlation in bonding electrons in C_2H_4. Results from these investigations are included in the publications list below.

<u>Recent Advances at Auburn University: Ionization of Molecules through Collisions with Ions and Electrons</u>

The materials and supplies costs accrued during this grant period have gone largely to the development of the apparatus used in the local experiments at Auburn

University. In addition to the science that will be explored, these fundamental collision measurements provide an excellent opportunity for student involvement with the technical aspects of experimental research.

Auburn-1: Modified COLTRIMS to Measure Electron Interactions with Molecules

One of the main challenges associated with applying imaging techniques to measurements of low-energy electron processes is that the typical fields involved strongly influence the incident electron's trajectory. To approach this problem, we have built a modified COLTRIMS apparatus to measure electron collisions with atoms and molecules that uses both pulsed incident electrons and pulsed electric fields. A beam from a pulsed electron gun passes through a diffuse target, followed by a synchronized electric field pulse which extracts the ions to a multi-channel plate detector with delay-line anode. By measuring positions and times of the extracted ions, information similar to that of more traditional RIMS methods can be obtained. For example, knowledge of charge state distributions, ion energy/momentum and molecule orientation become accessible.

We are currently measuring the H+/D+ ratio for ground state dissociation of HD initiated by electron impact. Initial results for energetic electrons (1.6 keV) indicate a strong asymmetry that is in disagreement with a Franck-Condon overlap model. There are two possibilities: 1) the model is inappropriate because the electron energy is too low to ensure a vertical transition or 2) the experiment is wrong. We plan to repeat this benchmark measurement to check for the consistency of the experiment and the validity of the model in this regime. We will then measure the same system for lower electron impact energies from near threshold (~20eV) up to 2 keV.

Future plans for this experiment include upgrading the ion imaging detector from 40mm to 80mm. This will give better momentum resolution and allow for 4π solid angle for more energetic dissociate processes. We will then pursue measurements of dissociative ionization of simple molecules.

Auburn-2: Ion-molecule interactions at the Auburn University accelerator

At the Auburn University accelerator we have established a COLTRIMS system that includes a supersonic gas jet, an ion momentum imaging detector as well as an electron time-of-arrival detector. Using the electron as a time marker, we are able to study dissociative ionization of small molecules with full 3-d momentum imaging of the molecule fragments. Experiments are in progress.

Initial experiments will be the measurement of the orientation dependence of HD molecules relative to the incoming projectile direction. We use HD so that we can cleanly separate both ions in TOF in order to get a full 4π momentum sphere for both ions. In order to produce sufficient HD to drive a gas jet, we've brewed our own using H_2, D_2 and a catalyst. We are currently analyzing dissociative ionization of CH_4 for calibration. Initial measurements of the orientation dependence of HD have begun and will continue for a variety of ion energies (0.3 to 2 MeV/u) and charge states (1 to 7).

Refereed Papers Supported from this Funding

- **Auger decay of $1\sigma_g$ and $1\sigma_u$ hole states of N_2 molecule: II. Young type interference of Auger electrons and its dendence on internuclear distance** N. A. Cherepkov, S. K. Semenov, M. S. Schöffler, J. Titze, N. Petridis, T. Jahnke, K. Cole, L. Ph. H. Schmidt, A. Czasch, D. Akoury, O. Jagutzki, J. B. Williams, T. Osipov, S. Lee,M. H. Prior, A. Belkacem, A. L. Landers, H. Schmidt-Böcking, R. Dörner and Th. Weber, *Phys. Rev. A* **82**, 023420 (2010).
- **Auger decay of $1\sigma_g$ and $1\sigma_u$ hole states of the N_2 molecule: Disentangling decay routes from coincidence measurements** S. K. Semenov, M. S. Schöffler, J. Titze, N. Petridis, T. Jahnke, K. Cole, L. Ph. H. Schmidt, A. Czasch, D. Akoury, O. Jagutzki, J. B. Williams, T. Osipov, S. Lee, M. H. Prior, A. Belkacem, A. L. Landers, H. Schmidt-Böcking, Th. Weber, N. A. Cherepkov, and R. Dörner, *Phys. Rev. A* **81**, 043426 (2010).
- **Carbon K-shell photoionization of fixed-in-space C_2H_4** T. Osipov, M. Stener, A. Belkacem, M. Schöffler, Th. Weber, L. Schmidt, A. Landers, M. H. Prior, R. Dörner, and C. L. Cocke, *Phys. Rev. A* **81**, 033429 (2010) .
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- **Separation of Auger transitions into different repulsive states after *K*-shell photoionization of N_2 molecules** N. A. Cherepkov, S. K. Semenov, M. S. Schöffler, J. Titze, N. Petridis, T. Jahnke, K. Cole, L. Ph. H. Schmidt, A. Czasch, D. Akoury, O. Jagutzki, J. B. Williams, T. Osipov, S. Lee,M. H. Prior, A. Belkacem, A. L. Landers, H. Schmidt-Böcking, R. Dörner and Th. Weber, *Phys. Rev. A* **80**, 051404(R) (2009).
- **Photo and Auger Electron Angular Distributions of Fixed-in-Space CO_2** F.P. Sturm, M. Schöffler, S. Lee, T. Osipov, N. Neumann, H.-K. Kim, S. Kirschner, B. Rudek, J.B. Williams, J.D. Daughhetee, C.L. Cocke, K. Ueda, A.L. Landers, Th. Weber, M.H. Prior, A. Belkacem, and R. Dörner, *Phys. Rev. A* **80**, 032506 (2009).
- **Angular Correlation between Photo- and Auger electrons from K-Shell Ionization of Neon** A.L. Landers, F. Robicheaux, T. Jahnke, M. Schöffler, T. Osipov, J. Titze, S.Y. Lee, H. Adaniya, M. Hertlein, P. Ranitovic, I. Bocharova, D. Akoury, A. Bhandary, Th. Weber, M.H. Prior, C.L. Cocke, R. Dörner, and A. Belkacem, *Phys. Rev. Lett*. **102**, 223001 (2009).
- **Ultrafast Probing of Core Hole Localization in N_2** M. S. Schöffler, J. Titze, N. Petridis, T. Jahnke, K. Cole, L. Ph. H. Schmidt, A. Czasch, D. Akoury, O. Jagutzki, J. B. Williams, N. A. Cherepkov, S. K. Semenov, C. W. McCurdy, T. N. Rescigno, C. L. Cocke, T. Osipov, S. Lee, M. H. Prior, A. Belkacem, A. L. Landers, H. Schmidt-Böcking, Th. Weber, and R. Dörner, Science, **320**, 920 (2008).

- **Photo-double-ionization of H2: Two-center interference and its dependence on the internuclear distance** M. S. Schöffler, K. Kreidi, D. Akoury, T. Jahnke, A. Staudte, N. Neumann, J. Titze, L. Ph. H. Schmidt, A. Czasch, O. Jagutzki, R. A. Costa Fraga, R. E. Grisenti, M. Smolarski, P. Ranitovic, C. L. Cocke, T. Osipov, H. Adaniya, S. Lee, J. C. Thompson, M. H. Prior, A. Belkacem, Th. Weber, A. Landers, H. Schmidt-Böcking, and R. Dörner, Phys. Rev. A **78**, 013414 (2008).
- **Fragmentation pathways for selected electronic states of the acetylene dication** T Osipov, T N Rescigno, T Weber, S Miyabe, T Jahnke, A S Alnaser, M P Hertlein, O Jagutzki, L Ph H Schmidt, M Schöffler, L Foucar, S Schössler, T Havermeier, M Odenweller, S Voss, B Feinberg, A L Landers, M H Prior, R Dörner, C L Cocke and A Belkacem, J Phys B, **41** (2008).
- **Interference in the collective electron momentum in double photoionization of H_2** Kreidi K, Akoury D, Jahnke T, Weber T, Staudte A, Schoffler M, Neumann N, Titze J, Schmidt LPH, Czasch A, Jagutzki O, Costa Fraga RA, Grisenti RE, Smolarski M, Ranitovic P, Cocke CL, Osipov T, Adaniya H, Thompson JC, Prior MH, Belkacem A, Landers AL, Schmidt-Bocking H, and Dorner R., Phys. Rev. Lett., **100**, 133005 (2008).
- **A two-electron double slit experiment: interference and entanglement in photo double ionization of H_2** D. Akoury, K. Kreidi, T. Jahnke, Th. Weber, A. Staudte, M. Schöffler, N. Neumann, J. Titze, L. Ph. H. Schmidt, A. Czasch, O. Jagutzki1, R.A. Costa Fraga1, R. Grisenti, R. Diez Muino, N. Cherepkov, S. Semenov, P. Ranitovic, C.L. Cocke, T. Osipov, H. Adaniya, M.H. Prior, A. Belkacem, A. Landers, H. Schmidt-B¨ Böcking, and R. Dörner, Science, **318**, 949 (2007).
- **Single Photon-Induced Symmetry Breaking of H_2 Dissociation** F. Martín, J. Fernández, T. Havermeier, L. Foucar, Th. Weber, K. Kreidi, M. Schöffler, L. Schmidt, T. Jahnke, O. Jagutzki, A. Czasch, E. P. Benis, T. Osipov, A. L. Landers, A. Belkacem, M. H. Prior, H. Schmidt-Böcking, C. L. Cocke, R. Dörner, *Science* **315**, 629 (2007).

Personnel

Principle Investigator:

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Senior Personnel:

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Joshua Williams : PhD (currently postdoc)
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Ali Moradmand: PhD (Currently postdoc)
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Current and Pending Support

(See GPG Section II.C.2.h for guidance on information to include on this form.)

The following information should be provided for each investigator and other senior personnel. Failure to provide this information may delay consideration of this proposal.

Investigator: Allen Landers

Other agencies (including NSF) to which this proposal has been/will be submitted.

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title: Imaging Multi-particle Atomic and Molecule Dynamics

Source of Support: Department of Energy
Total Award Amount: $ 360,000 Total Award Period Covered: 07/01/11 - 06/30/14
Location of Project: Auburn, AL
Person-Months Per Year Committed to the Project. Cal:0.00 Acad: 0.00 Sumr: 1.00

Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title: Robotics and Engineering Education Fostering the Conceptual Understanding of Science (The RE2-FoCUS Initiative)

Source of Support: Math and Science Partnership, Department of Education
Total Award Amount: $ 633,321 Total Award Period Covered: 10/01/12 - 09/30/15
Location of Project: Auburn, AL
Person-Months Per Year Committed to the Project. Cal:0.00 Acad: 0.00 Sumr: 1.00

Support: ☒ Current ☒ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title: STEM-IQ: Science, Technology, Engineering and Mathematics Inquiry- Enhancing Science Education in Southeast Alabama

Source of Support: National Science Foundation
Total Award Amount: $ 742,711 Total Award Period Covered: 04/01/14 - 03/31/19
Location of Project: Auburn, AL
Person-Months Per Year Committed to the Project. Cal:0.00 Acad: 0.00 Sumr: 1.00

Support: ☐ Current ☒ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title: Electron-driven Correlated Dynamics of Complex Systems

Source of Support: National Science Foundation
Total Award Amount: $ 248,276 Total Award Period Covered: 05/01/14 - 04/30/17
Location of Project: Auburn, AL
Person-Months Per Year Committed to the Project. Cal:0.00 Acad: 0.00 Sumr: 1.00

Support: ☐ Current ☐ Pending ☐ Submission Planned in Near Future ☐ *Transfer of Support
Project/Proposal Title:

Source of Support:
Total Award Amount: $ Total Award Period Covered:
Location of Project:
Person-Months Per Year Committed to the Project. Cal: Acad: Summ:

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