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Dr. Jeff Krause
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Basic Energy Sciences

Chemical Sciences, Geosciences and Biosciences Division
Atomic Molecular and Optical Sciences

Report from the past Budget Period (2010-2014)

II) Report from the past three years (2010-2013)

During the past three years, the group research work resulted in 43 publications (1 Scientific American, 1 Nature Photonics, 1 PNAS, 1 Nature, 11 Phys. Rev. Lett. and 1 Phys. Rev A Rapid Com.), 36 invited presentations at national and international conferences and workshops, 14 invited seminars and colloquia at national and international venues, and 57 contributed abstracts at national and international conferences. Furthermore, the PI was awarded the 2014 APS Davisson-Germer prize in Atomic or Surface Physics. The citation is: "*For pioneering experiments on the interaction of atoms, molecules, negative ions and clusters with ionizing vacuum ultraviolet and soft x-ray photons.*"

We present below projects completed and in progress during the past three years.

II.A. Multi-Photon Ionization of Molecules and Clusters using the LCLS

This part of our program consists of investigating the nature of the interaction between LCLS fs x-ray pulses and diatomic, polyatomic and C_{60} molecules.

1) Buckyball Explosion by Intense Femtosecond X-Ray Pulses: A Model System for Complex Molecules

- ✓ *B. F. Murphy, T. Osipov, L. Fang, Z. Jurek, S.-K. Son, M. Mucke, J. H. D. Eland, V. Zhaunerchyk, R. Feifel, L. Avaldi, P. Bolognesi, C. Bostedt, J. D. Bozek, J. Grilj, M. Guehr, L. J. Frasinski, J. Glownia, D. T. Ha, K. Hoffmann, E. Kukk, B. K. McFarland, C. Miron, E. Sistrunk, R. J. Squibb, K. Ueda, R. Santra and N. Berrah (Under review, Nature Communications)*

We have carried out an experimental and theoretical study of C_{60} molecules interacting with intense x-ray pulses from the LCLS, revealing the influence of processes not previously reported. Specifically, we demonstrate the effects of high per-atom x-ray absorption on the fragmentation dynamics of C_{60} molecules in the gas phase. This work presents an essential step for the rigorous, quantitative understanding of femtosecond molecular dynamics. Measurements guided the development of molecular dynamics simulations suitable for large molecules exposed to intense XFEL pulses. Experimental and simulation [21] data on C_{60} ion dynamics reveal that a complex variety of processes are present in these interactions. Our model demonstrates that full atomic fragmentation of C_{60} occurs at the highest fluences. We show that ionization suppression occurs for very short pulses. While an analogous effect is known for atoms [22] and small molecules [23], the mechanism for such a large molecule is more complex, as revealed by simulations. Furthermore, our experiment provides evidence that the charged particles produced by exposing an extended quantum system, C_{60}, to high-fluence x rays behave as if they were classical particles. At high fluence, the parent molecule explodes within few tens of fs, giving rise to fragment ions and highly charged state of C atom. In fact, we fully strip C of all of its 6 electrons as shown in Fig.1

We compare in Fig. 1 the experimental measurement and various modeling scenarios of the atomic ion yields following molecular fragmentation with long pulse durations (150 fs). Our final Molecular Dynamics (MD) model includes several independent phenomena: bonds between C atoms, bond breaking, molecular Auger decay and secondary ionization. The final model is compared with models ignoring one of these key ingredients. The discrepancies reveal the relative importance of each physical process implemented in the development of the model, leading to a final model that agrees very well with the data for both pulse durations. The first and second models represent two extreme cases: no chemical bonding and always-present bonding forces, respectively. Turning off the bonding force field and allowing the ions to interact with each other and with electrons only through simple Coulomb forces results in excessive pre-expansion, and an excess of C^{1+} (dark green bars) while suppressing higher charge states and eliminating all molecular ion fragments. Second, turning off the bond-breaking mechanism so that

ions experience the bonding field regardless of electronic configuration (but fragmentation can still happen due to the dominance of strong Coulomb repulsion over bonding forces). This scenario depletes the C^{1+} channel and results in excess of high charges (violet bars), as more energetic dissociation prevents recombination following the pulse. The model with no molecular Auger process produces similar results to the scenario without bond-breaking: insufficient C^{1+} and excess high charge states (cyan bars). Finally, the consequence of neglecting secondary ionizations further biases the ion yield toward higher charges (light green bars), because recombination processes, which occur mainly with slow secondary electrons, are suppressed. Theory support has been provided by Robin Santra's group, CFEL, DESY, Germany.

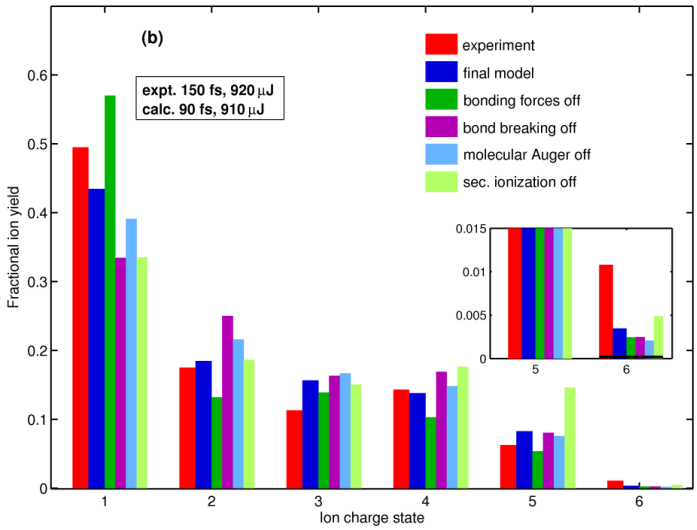

Figure 1. *Experimental data are compared to MD model calculations with individual model components turned off for 150 fs pulse duration. Broad bars for each ion charge state show experimental data (red) and the final model (dark blue). Narrow bars show MD neglecting bonding forces (dark green), MD neglecting bond breaking due to changes of the atomic electron configuration (violet), MD neglecting molecular Auger effect (light blue), and MD neglecting secondary ionization (light green). The C^{6+} yield is above the experimental detection limit (horizontal black line) (inset).*

2) Multiphoton Ionization as a Clock to Reveal Molecular Dynamics with Short, Intense X-ray FEL Pulses from the LCLS.

- ✓ *L. Fang, T. Osipov, B. Murphy, F. Tarantelli, E. Kukk, J.P. Cryan, M. Glownia, P.H. Bucksbaum, R.N. Coffee, M. Chen, C. Buth, and N. Berrah, Phys. Rev. Lett.,* ***109****, 263001 (2012).*

We have used the intensity of the LCLS x-ray FEL as well as its time structure to probe molecular dynamics. We have used *multi-photon* ionization, and in particular, multiple Photoionizaton (P) and Auger decay (A) cycles as an "intrinsic" clock to probe the average time of the ionization and fragmentation dynamic of molecules under specific conditions. In other words, we can regard the multiple PA cycles as a pump-multiple probe scheme, by sequential absorption, within one single x-ray pulse. This scheme, which should be applicable for any system, was used in the case of N_2. We measured multiple-

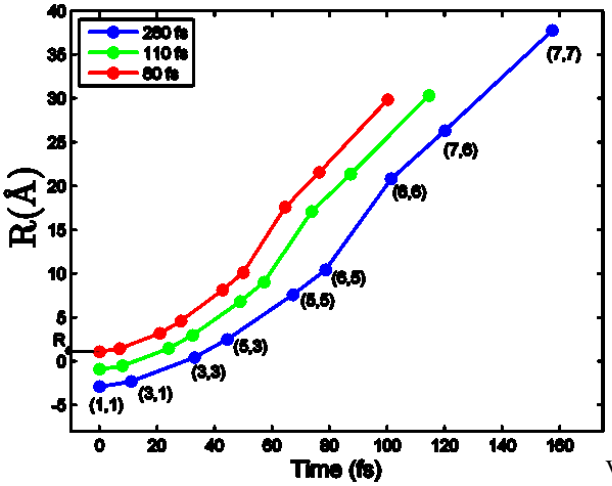

Fig. 2 *Extrated internuclear distance R as a function of time for different photoionization-dissociation pathways of N_2 at three different pulse durations. Each colored dot represents a photo-absorption events.*

(University of Perugia, Italy).

ionization leading to molecular fragmentation and fully stripped N atom, through multiple core-level photoabsorption and subsequent Auger decay processes induced by intense, short x-ray free electron laser pulses. The timing dynamics of the photoabsorption and dissociation processes is mapped onto the kinetic energy of the measured atomic fragment ions. The latter allowed us to obtain the average internuclear separation for every molecular photoionzation sequence step and to obtain the average time interval between the photoabsorption events. Using multiphoton ionization as the tool for the pump- multiple probe scheme, we demonstrated the modification of the ionization dynamics as we vary the x-ray laser pulse duration from 280, 110 and 80 fs. We find that the average time interval between photo-absorption events decrease, which means faster molecular dissociation, for shorter pulse duration as sown in Fig. 2. We also examined the ionization of the molecules throughout the spatial FEL beam profile. Theory support has been provided by F. Tarantelli

3) <u>Double Core-Hole Spectroscopy for Chemical Analysis using a Short and Intense X-Ray Femtosecond Laser.</u>

- ✓ *N. Berrah et al., Proc. Natl. Acad. Sci (PNAS),* ***108****, issue 41, 16912 (2011).*
- ✓ *P. Salen, P. van der Meulen, H.T. Schmidt, R.D. Thomas, M. Larsson, R. Feifel, L. Fang, B. Murphy, T. Osipov, N. Berrah, et al. Phys. Rev. Lett. Phys Rev. Lett.* ***108****, 153003 (2012)*
- ✓ *L.J. Frasinski, V. Zhaunerchyk, M. Mucke, R.J. Squipp, M. Siano, J.H.D. Eland, P. Linusson, P.v.d. Meulen, P. Salén, M. Larsson, T. Osipov, L. Fang, B.F. Murphy, N. Berrah, et al. Phys. Rev. Lett.* ***111,*** *073002 (2013).*

Twenty five years ago, Cederbaum *et al*. [24] predicted that double core hole (DCH) spectroscopy would provide a richer and more sensitive technique than inner-shell photoelectron spectroscopy (PES), amplifying and rendering observable subtle differences between similar chemical systems. More recently, Santra *et al.* [25] stipulated that when exposed to ultra-intense x-radiation sources such as FELs, the innermost electronic shell can efficiently be emptied, creating a transient hollow atom or molecule. They predicted that x-ray two-photon photoelectron spectroscopy (XTPPS) should enable measurements of DCH in molecules i.e., double core holes with both vacancies on a single site (ssDCH) and double core holes with a single vacancy on two different sites (tsDCH).

We tested experimentally the above predictions [25], using the LCLS intensity and short pulse duration, by carrying out measurements of DCH produced via sequential two-photon absorption. The production and decay of these states was characterized by using photoelectron spectroscopy, Auger electron spectroscopy, and mass spectrometry. The experimental results were interpreted with the help of *ab-initio* Green's function calculations of the energies of the DCH states and of the Auger decay energies. We were able to measure ssDCH [26] but the tsDCH allowing unambiguous chemical analysis, remained

difficult to measure because of overlapping spectral lines from single-photon absorption and excitation using conventional electron-time-of flight spectrometers.

Our improvement in carrying out XTPPS experiments allowed us however to report for the first time the direct observation of tsDCH in CO, produced via sequential two-photon absorption, by carrying out measurements with the full FEL intensity, then carrying out the same measurement with attenuated intensity. We then subtracted the two spectra leading to very clear signatures of tsDCH but also ssDCH [27] as shown in Fig. 3. Our measurements agree very well with theoretical modeling for the CO molecule [27]. We also carried out experiments on N_2O and CO_2 to assess the validity of the method, ie signature of the chemical environment using XTPPS measurement, by comparing our previous results in N_2 with N_2O and also comparing our findings in CO with CO_2 [28]. Typical single core hole ionization cannot differentiate between CO and CO_2 or between N_2 and N_2O but our DCH methodology was indeed successful [28] in separating the different chemical environments. Note however that synchrotron radiation experiments with high detection efficiency magnetic bottle spectrometers have also been able to separate the chemical environment for similar molecules via single photon absorption [29,30]. Thus, double K-hole is achieved via electron correlation processes (albeit with very small cross section) while our measurements are due to a non-linear process, ie.,two photons ionizing two K-shell electrons.

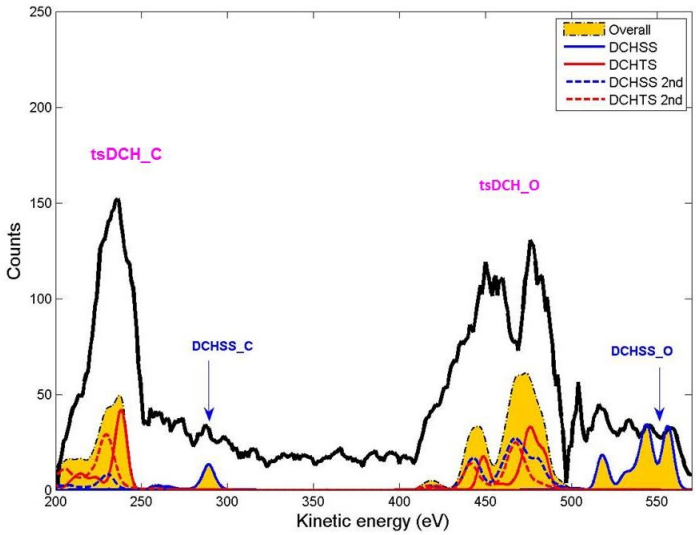

Fig. 3*. Measured Auger spectra (black curve) compared to theoretical DCH Auger spectra. Theoretical Auger spectra: overall calculation (yellow shaded area);ssDCH (solid blue curve) tsDCH (solid red curve); ssDCH secondary processes dashed blue curve);tsDCH secondary processes (dashed red curve).*

In order to apply the XTPPS method effectively to larger molecules, we decided to use a magnetic bottle spectrometer whose detection efficiency is high compared to an e-TOF and which could also allow the use of a statistical method for analyzing the data. Our recent work demonstrated the capacity of a correlation method called "partial covariance mapping" (similar to coincidences technique which can't be used due to the low repetition rate of the LCLS) to probe the electron dynamics of Ne atoms, as the test-case, exposed to intense 8 fs pulses of 1062 eV photons [31]. A complete picture of ionization processes competing in hollow atom formation and decay is visualized with unprecedented ease and the map reveals hitherto unobserved nonlinear sequences of photoionization and Auger events. The technique is particularly well suited to the high counting rate inherent in FEL experiments. Theory support has been given M. Tashiro and M. Ehara, Institute for Molecular Science, Okazaki, Japan.

4) Multiphoton L-Shell Ionization of H_2S using Intense LCLS X-ray Pulses

- ✓ *B. F. Murphy, L. Fang, M.-H. Chen, J. D. Bozek, E. Kukk, E. P. Kanter, M. Messerschmidt, T. Osipov, and N. Berrah, Phys. Rev. A* ***86****, 053423 (2012).*

Sequential multiphoton *L*-shell ionization of hydrogen sulfide exposed to intense femtosecond pulses of 1.25-keV x rays has been observed via photoelectron, Auger electron, and ion time-of-flight

spectroscopies. In the most intense part of the x-ray focal volume, an average molecule can absorb more than five photons, producing multiple *L*-shell ionization followed by the Auger process. Fig. 4 shows time of flight spectra depicting the charge state distribution from S^{1+} to S^{14+} as a function of fluence. Monte Carlo simulations based on relativistic Dirac-Hartree-Slater calculations of Auger decay rates in S with single and double *L*-shell vacancies accurately model the observed spectra. While single-vacancy-only calculations are surprisingly accurate even at the high x-ray intensity used in the experiment, calculations including double-vacancy states improve on yield estimates of highly charged sulfur ions. For 280-fs pulse duration and ~10^{17} W/cm^{-2} focal intensity, the yield of S^{13+} is ~1% of the S^{3+} yield, in good agreement with simulations. An overabundance of S^{12+}, and S^{14+} observed in the experimental ion spectra is not predicted by either single-vacancy or double-vacancy calculations. We do not however observe S^{15+}, which would have been the non-linear signature of the absorption of 2 photons by one electron. Theory support has been provided by M. H. Chen from LLNL.

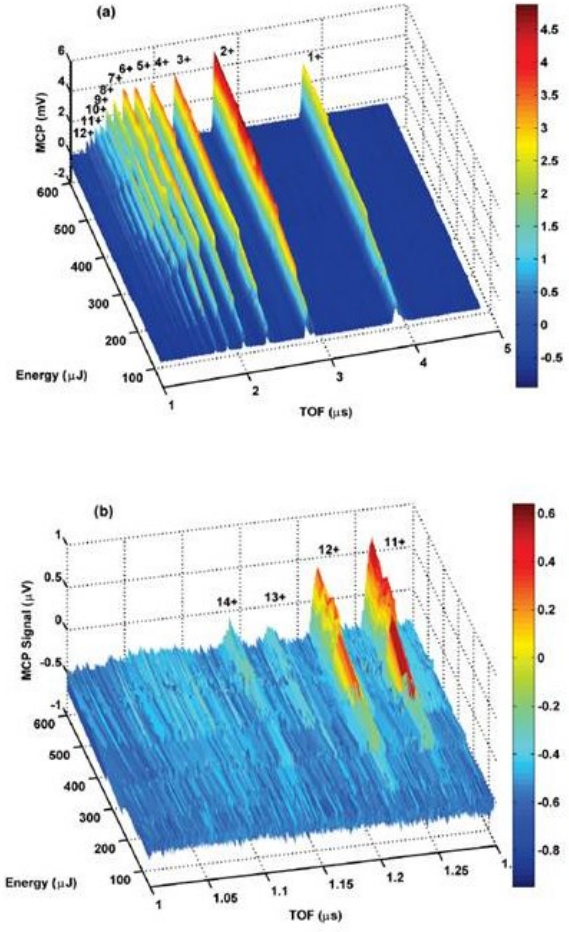

Fig. 4 *Ion time-of-flight MCP signal from H_2S versus transmission-corrected x-ray pulse energy. (a) Ion charge states from S^{1+} to S^{14+} are observed, with higher charge states appearing as the x-ray intensity increases. (b) For x-ray pulse energies over 500 μJ, S^{11-14+} ions are observed.*

5. Sequential Multiple Ionization and Fragmentation of SF_6 Induced by an Intense Free Electron Laser

✓ *T. Osipov, L. Fang, B. Murphy, F. Tarantelli, E.R. Hosler, E. Kukk, J. D. Bozek, C. Bostedt, E. P. Kanter and N. Berrah, J. Phys. B: At. Mol. Opt. Phys.* ***46*** *, 164032 (2013)*

We have also investigated multiphoton ionization of a polyatomic molecule, SF_6, and its subsequent fragmentation under intense x-ray FEL pulses. In this case, we observed highly-charged molecular and atomic ions which were absent in previous single-photon absorption experiments with synchrotron light source. We have observed fully stripped fluorine ions resulting from sequential multiphoton ionization processes with intermediate 1s electron excitation. We measured the average momentum and kinetic energy of each fragment which points toward many-body fragmentation pathways of the molecular SF_6 ions. We observed non-monotonic dependence of the kinetic energy on F charge states indicating multiphoton ionization of isolated atomic neutral fluorine or fluorine ions resultant from bond cleavages. Our results imply that the fragmentation of highly-charged molecular ions is produced at a later time during a single FEL pulse. Theory support has been provided by F. Tarantelli (University of Perugia, Italy).

II.B. Study of Correlated Processes in Select Anions using the ALS

This part of our program consisted of investigating the interaction of anions with vuv-x-ray photons via *single-photon absorption* from the ALS synchrotron radiation facility. Anions are strongly correlated

systems presenting differences both qualitatively and quantitatively compared to neutral and positive ions. The difference in behavior arises from the different binding potential in negative ions which results in dramatic differences, such as resonance structures in the electronic structure and photodetachment dynamics. We have observed in previous inner-shell photodetachment cross sections of atomic anions Feshbach or shape resonances [32-38] in He^-[32], Li^-[33], B^-[34], B_2^-&B_3^-, [35] Fe^- [36], C^- [37] and C_{60}^- [38]. However, an extended system like C_{60}^- shows unexpectedly similar ionization cross section landscape compared to its neutral counterpart, C_{60}, albeit demonstrating a large enhancement of the cross section as described in select highlights below. The measurements were carried out using the Ion-Photon-Beamline (IPB) at ALS beamline 10.0.1 where the ions and photons are merged collinearly. We measure the positive ion channel resulting from two electrons ionization (photoionization and Auger decay).

1) **<u>Single-Photon Multiple Detachment in Fullerene Negative Ions: Absolute Ionization Cross Sections and the Role of the Extra Electron</u>**

✓ *R. C. Bilodeau, N. D. Gibson, C. W. Walter, D. A. Esteves-Macaluso, S. Schippers, A. Muller, R. A. Phaneuf, A. Aguilar, M. Hoener, J. M. Rost, and N. Berrah, Phys. Rev. Lett.* ***111****,043003 (2013*)

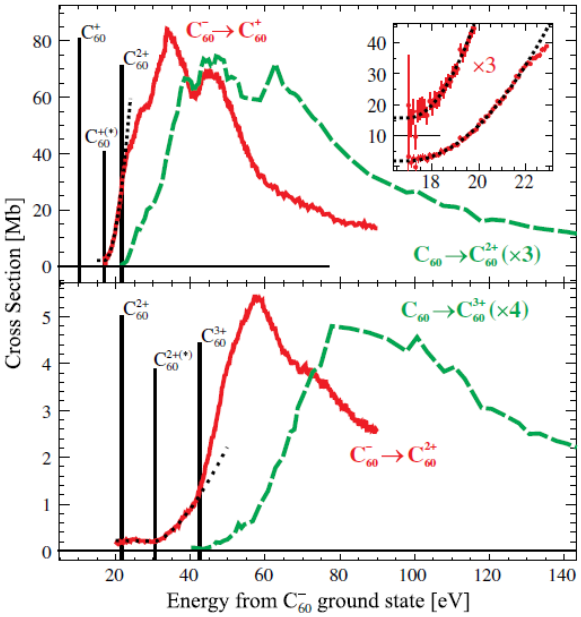

Fig.5 *Measured absolute cross-section from the removal of 2 (top) or 3 (bottom) electrons from C_{60} Anion (solid lines) compared to neutral C_{60} (dashed lines).*

We have measured the *singe-photon* multiple ionization of fullerene anions and we compared our data to ionization of neutral fullerene. The measured absolute valence photodetachment cross sections of C_{60}^- were found to be 2 and 2.5 times larger than those for neutral C_{60} and appear to be compressed and shifted in photon energy as compared to neutral C_{60} ionization as shown in Fig. 5. Our analysis reveals that the additional electron in C_{60} primarily produces screening which is responsible for the modification of the spectrum. Both screening effects, the shift and the compression, can be quantitatively accounted for by a linear transformation of the energy axis. Applying the transformation allowed us to map the neutral and negative ion cross sections onto each other, pointing out to the *unexpected* close relationship of correlated electron dynamics in neutral and negatively charged extended systems such as C_{60} molecule. In contrast, dynamics of neutral and negatively charged atoms or small molecules are typically *not* closely related. They have so far always shown drastic dissimilarities [32-37]. Theory support has been given by J-M. Rost (Dresden, Germany).

2) **Inner-Shell Photodetachment from Ru^-**

✓ *I. Dumitriu, R. C. Bilodeau, T. W. Gorczyca, C. W. Walter, N. D. Gibson, Z. D. Pesic, D. Rolles and N. Berrah, Phys. Rev. A.* ***82****, 043434 (2010).*

In contrast to the previous highlight, the photodetachment of atomic Ru^- presents resonance structure as do most small anion systems [32-38]. Inner-shell photodetachment from Ru^- was studied near and above the 4*p* excitation region, 29-to-91-eV photon energy range, using a merged ion-photon-beam technique. The absolute photodetachment cross sections of Ru^- ($[Kr]4d^7 5s^2$) leading to Ru^+, Ru^{2+}, and Ru^{3+} ion production were measured. In the near-threshold region, a Wigner *s*-wave law, including estimated post-

collision interaction effects, locates the $4p_{3/2}$ detachment threshold between 40.10 and 40.27 eV. Additionally, the Ru^{2+} product spectrum provides evidence for simultaneous two-electron photodetachment (likely to the Ru^{+} $4p^5 4d^6 5s^2$ state) located near 49 eV. Resonance effects are observed due to interference between transitions of the $4p$ electrons to the quasi-bound $4p^5 4d^8 5s^2$ states and the $4d \rightarrow \varepsilon f$ continuum. Despite the large number of possible terms resulting from the Ru^{-} $4d$ open shell, the cross section obtained from a 51-state *LS*-coupled *R*-matrix calculation agrees qualitatively well with the experimental data. Theory support has been given by T. Gorczyca (WMU).

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Personnel

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2. Dr. Hui Xiong (LCLS program) -Postdoctoral fellow

C. Technical Support Staff

Mr. Michael Rosman - Computer Technician
Mr. Alan Chasse - Instrument Maker
Dr. David Perry -Assistant technical Staff

D. Students

PhD., Soroush Khosravi Dehaghi, graduation fall 2016. All other students graduated and I plan to hire two more graduate and one undergraduate student fall of 2014

Biographical Sketches

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Assistant Professor, Physics Department, Western Michigan University, August 1991.
Assistant Scientist, Physics Division, Argonne National Laboratory, October 1989-1991.
Postdoctoral appointee, Physics Division, Argonne National Laboratory, May 1987-October 1989.

AWARDS:

1. Davisson-Germer Prize, American Physical Society, 2014.
2. Western Michigan University, Arts and Science College, Global Engagement award, 2012.
3. Western Michigan University (WMU) Dean's Faculty Research Appreciation Award, 2007, 2008.
4. David. S. Shirley Award for "Outstanding Scientific Achievements at the Advanced Light Source", Lawrence Berkeley National Laboratory, 2002.
5. WMU Distinguished Faculty Scholar Award, 2000.
6. Fellow, American Physical Society, 1999.
7. WMU President's Award for Excellence in Research, 1996.
8. WMU Dean's Award for Excellence in Research, 1995, 1997.
9. Humboldt Fellowship, Alexander von Humboldt Foundation , 1992-1993.
10. Graduate Fellowship, Physics Department, University of Virginia, 1985-1986.

11. Scholarship, University of Orsay, Paris, France, 1979-1980.
12. Scholarship, Ministere de L'Enseignement Superieure et de la Recherche Scientifique, Algeria, 1981-1985.
13. Baccalaureate exam with Honors, 1975.

MAJOR PROFESSIONAL ACTIVITIES:

1. Member, APS Nominating Committee, 2013-2015.
2. Member, Executive Committee, Division of Laser Science (DLS), APS, 2010-2013.
3. Member, Science Advisory Committee, Advanced Light Source (ALS), LBNL, 2007-2014.
4. Member, Users Executive Committee, Linac Coherent Light Source (LCLS), 2012-2015.
5. Member, Basic Energy Sciences Advisory Committee (BESAC), Office of Science, DOE, 2002-2012.
6. Member, Review Committee for the Physics Department, Uppsala University, Sweden, June 2011.
7. Member, DAMOP, Nominating Committee, 2008-2010.
8. Discussion Leader/Writer, DOE workshop "New Era of Science: Solving Science and Energy Grand Challenges with Next-Generation Photon Sources" Oct.2008. Report published, National Academy Press.
9. Member, Science Advisory Committee, SSRL, SLAC National Accelerator Laboratory, 2006-2009.
10. Co-team leader for Atomic and Molecular Science, LCLS, SLAC, 2004-2009.
11. Chair, Davisson-Germer Prize Committee, American Physical Society, 2007.
12. Member, Executive Committee, DAMOP, American Physical Society, 2005-2008.
13. Member, Executive Committee, APS Topical Group on Few-Body Physics, 2006.
14. Member, Forum on International Physics (FIP), APS, 2006-2007.
15. Member, Science Advisory Committee for the LCLS, 4th Generation Light Source, SLAC,2003-2005.
16. Member, CAMOS, National Research Council, 2000-2002.
17. Chair, Users Executive Committee, Advanced Light Source (ALS), LBNL, 2000.
18. Member, Subcommittee to Review 4th Generation Light Sources, BESAC, Department of Energy, 1999.
19. Member, I. I. Rabi Prize Committee, American Physical Society, 1998-2000.
20. Member, Committee on International Scientific Affairs (CISA), APS, 1994-1997
21. Member, Executive Committee, Division of Atomic Molecular and Optical Physics, APS, 1995-1998.
22. Chair, Participation Research Team (PRT) of AMO ALS, 1995-2004.
23. Member, Proposal Study Panel, ALS, LBNL, 1995-2000.

Recent Publication from DOE Sponsored Research (2010-2013)

1. L. Fang, D. Rolles, A. Rudenko, V. Petrovich, C. Bostedt, J. D. Bozek, P. Buckbaum and N, Berrah "Probing ultrafast electronic and molecular dynamics with free electron lasers" *J. Phys. B: At. Mol. Opt. Phys.* **47** 124006 (2014) doi:10.1088/0953-4075/47/12/124006).
2. N. Berrah, L. Fang, T. Osipov, B. Murphy, C. Bostedt and J.D. Bozek, "Multiphoton Ionization and Fragmentation of Molecules with the LCLS X-Ray FEL" J. Elec. Spect and Rela. Phen, **196**, 34-37 (2014).
   N. Berrah and P. H. Bucksbaum, "The Ultimate X-ray Machine" Scientific American, **310**, 64, January 2014.
3. R. C. Bilodeau, N. D. Gibson, C. W. Walter, D. A. Esteves-Macaluso, S. Schippers, A. Muller, R. A. Phaneuf, A. Aguilar, M. Hoener, J. M. Rost, and N. Berrah, "Single-Photon Multiple-Detachment in Fullerene Negative Ions: Absolute Ionization Cross Sections and the Role of the Extra Electro, Phys. Rev. Lett. **111**,043003 (2013)
4. L.J. Frasinski, V. Zhaunerchyk, M. Mucke, R.J. Squipp, M. Siano, J.H.D. Eland, P. Linusson, P.v.d. Meulen, P. Salén, R.D. Thomas, M. Larsson, L. Foucar, J. Ullrich, K. Motomura, S. Mondal, K. Ueda, T. Osipov, L. Fang, B.F. Murphy, N. Berrah, C. Bostedt, J.D. Bozek, S. Schorb, M. Messerschmidt, .M. Glownia, J.P. Cryan, R.N. Coffee, O. Takahashi, S. Wada, M.N. Piancastelli, R. Richter, K.C. Prince, and R. Feifel Phys. Rev. Lett. **111**, 073002 (2013).
5. B.K. McFarland, N. Berrah ,C. Bostedt, J. Bozek, P. H. Bucksbaum, J. C. Castagna, R. N. Coffee, J. P. Cryan, L. Fang, J. P. Farrell, R. Feifel, K. J. Gaffney, J. M. Glownia, T. J. Martinez, S. Miyabe,M. Mucke, B. Murphy, A. Natan, T. Osipov , V. S. Petrović, S. Schorb, Th.Schultz, L. S. Spector, M. Swiggers, F. Tarantelli, I. Tenney, S. Wang, J. L. White, W. White, and M Gühr, "Experimental strategies for optical pump – soft x-ray probe experiments at the LCLS" (Journal of Physics-Conference Series in 2014 (in press).
6. V. Zhaunerchyk, M. Mucke, P. Salén, P.v.d. Meulen, M. Kaminska, R.J. Squipp, L.J. Frasinski, M. Siano, J.H.D. Eland, P. Linusson, R.D. Thomas, M. Larsson, L. Foucar, J. Ullrich, K. Motomura, S. Mondal, K. Ueda, T. Osipov, L. Fang, B.F. Murphy, N. Berrah, C. Bostedt, J.D. Bozek, S. Schorb, M. Messerschmidt, J.M. Glownia, J.P. Cryan, R.N. Coffee, O. Takahashi, S. Wada, M.N. Piancastelli, R. Richter, K.C. Prince, and R. Feifel J. Phys. B: At. Mol. Opt. Phys**. 46**, 164034 (2013).
7. C. Bostedt, J. D. Bozek, P. H. Bucksbaum, R. N. Coffee, J. B. Hastings, Z. Huang, R. W. Lee, S. Schorb, J. N. Corlett, P. Denes, P. Emma, R. W. Falcone, R. W. Schoenlein, G. Doumy, E. P. Kanter, B. Kraessig, S. Southworth, L. Young, L. Fang, M. Hoener, N. Berrah, C. Roedig, and L. F. DiMauro, J. Phys. B: At. Mol. Opt. Phys. **46**, 164003 (2013).
8. T Osipov, L Fang, B Murphy, F Tarantelli, E R Hosler, E Kukk, J D Bozek, C Bostedt, E P Kanter and N Berrah, " Multiphoton ionization and fragmentation of SF_6 induced by intense free electron laser pulses", J. Phys. B: At. Mol. Opt. Phys. **46** , 164032 (2013).
9. M Larsson, P Salén, P van der Meulen, H T Schmidt, R D Thomas, R Feifel, M N Piancastelli, L Fang, B Murphy, T Osipov, N Berrah, E Kukk, K Ueda, J D Bozek, C Bostedt, S Wada, R Richter, V Feyer and K C Prince "Double core-hole formation in small molecules at the LCLS free electron laser" J. Phys. B: At. Mol. Opt. Phys. **46**, 164030 (2013).
10. J.C. Castagna, B. Murphy, J. Bozek, and N. Berrah,"X-ray split and delay for soft x-rays at LCLS". Journal of Physics:Conference Series 425 152021, (2013).
11. L. Fang, T. Osipov, B. Murphy, F. Tarantelli, E. Kukk, J.P. Cryan, M. Glownia, P.H. Bucksbaum, R.N. Coffee, M. Chen, C. Buth, and N. Berrah, "Multiphoton Ionization as a Clock to Reveal Molecular Dynamics with Intense Short X-ray Free Electron Laser Pulses", Phys. Rev. Lett., **109**, 263001 (2012).

12. B. F. Murphy, L. Fang, M.-H. Chen, J. D. Bozek, E. Kukk, E. P. Kanter, M. Messerschmidt, T. Osipov, and N. Berrah," Multiphoton L-Shell Ionization of H_2S using Intense X-ray Pulses from the LCLS Free Electron Laser" Phys. Rev. A **86**, 053423 (2012).

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14. R.C. Bilodeau, N.D. Gibson, C.W. Walter, A. Aguilar, N. Berrah, "Inner-shell photodetachment: Shape and Feshbach resonances of anions", Journal of Electron Spectroscopy and Related Phenomena **185** 219– 225 (2012).
15. V. S. Petrović, M. Siano, J.L. White, N. Berrah, C. Bostedt, J. D. Bozek, D. Broege, M. Chalfin, R. N. Coffee, J. Cryan, L. Fang, J. P. Farrell, L. J Frasinski, J. M. Glownia, M. Gühr, M. Hoener, D.M. P. Holland, J. Kim, J. P. Marangos[3], T. Martinez, B. K. McFarland, R. S. Minns, S. Miyabe, S. Schorb, R. J. Sension, L. S. Spector, R. Squibb, H. Tao, J. G. Underwood, and P. H. Bucksbaum "Transient X-ray fragmentation: Probing a prototypical photoinduced ring opening", Phys. Rev. Lett. Phys. Rev. Lett. **108**, 253006, (2012).
16. Christian Buth, Ji-Cai Liu, Mau Hsiung Chen, L. Fang, M. Hoener, N. Berrah, "Ultrafast absorption of intense x rays by nitrogen molecules", J. Chem. Phys.**136**, 214310 (2012).
17. P. Salen, P. van der Meulen, H.T. Schmidt, R.D. Thomas, M. Larsson, R. Feifel, M.N. Piancastelli, L. Fang, B. Murphy, T. Osipov, N. Berrah, E. Kukk, K. Ueda, J.D. Bozek, C. Bostedt, S. Wada, R. Richter, V. Feyer and K.C. Prince, "X-ray FEL-induced Two-Site Double Core-Hole Formation for Chemical Analysis", Phys. Rev. Lett. PRL **108**, 153003 (2012).
18. H. Thomas, A. Helal, K. Hoffmann, N. Kandadai, J. Keto, J. Andreasson, B. Iwan, M. Seibert, N. Timneanu, J. Hajdu, M. Adolph, T. Gorkhover, D. Rupp, S. Schorb, T. Möller, G. Doumy, L.F. DiMauro, M. Hoener, B. Murphy, N. Berrah, M. Messerschmidt, J. Bozek, C. Bostedt and T. Ditmire, "Explosions of Xe-clusters in ultra-intense femtosecond x-ray pulses from the LCLS Free Electron Laser", Phys. Rev. Lett. **108**, 133401 (2012).
19. James P. Cryan, J. M. Glownia, Andreasson, A. Belkacem, N. Berrah, C. I. Blaga, C. Bostedt, J. Bozek, N. A. Cherepkov, L. F. DiMauro, L. Fang, O. Gessner, M. Guehr, J. Hajdu, M. P. Hertlein, M. Hoener, O. Kornilovy, J. P. Marangos, A. M. March, B. K. McFarland, H. Merdji, M. Messerschmidt, V. Petrovic, C. Raman, D. Ray, D. Reis, S. K. Semenov, M. Trigo, J. L. White, W. White, L. Young,P. H. Bucksbaum, and R. N. Coffee, **"**Molecular frame Auger electron energy spectrum from N_2" J. Phys. B: At. Mol. Opt. Phys. **45**, 055601 (2012).
20. T.Y. Osipov, L. Fang, B.F. Murphy, M. Hoener, and N. Berrah, "X-Ray FEL Induced Double Core-Hole and High Charge State Production", Journal of Physics: Conference Series **388,** 012030, (2012).
21. L. Fang, T. Osipov, B. Murphy,et al. and N. Berrah, Multiple ionization and double core-hole production in molecules using the LCLS x-ray FEL", Journal of Physics: Conference Series **388,** 032028, (2012).
22. T. Osipov, D. Rolles, C. Bostedt, J-C. Castagna, R. Hartman, J. D. Bozek, I. Schlichting, L. Struder, J. Ullrich and N. Berrah, "Next generation endstation for concurrent measurements of charged products and photons in LCLS FEL experiments" Journal of Physics: Conference Series **388,** 142025 (2012).
23. P. Salen, P. van der Meulen, R. D. Thomas, H. T. Smith, M. Larsson, R. Feifel, L. Fang, T. Osipov, B. Murphy, N. Berrah, et al. "X-ray FEL-induced double core hole formation in ployatomic molecules, J. Phys.: Conf. Ser. **388**, 022083 (2012).
24. B.F. Murphy, L. Fang, T.Y. Osipov, M. Hoener, and N. Berrah, "Intense X-ray FEL-Molecule Physics: Highly Charged Ions" the American Institute of Physics (AIP) Conference Proceedings of ICAPiP, **1438**, 249 (2012).
25. Philip H. Bucksbaum, Ryan Coffee, and Nora Berrah, "The First Atomic and Molecular Experiments at the Linac Coherent Light Source X-Ray Free Electron Laser" Book Chapter, Elsevier Inc., Advances in Atomic, Molecular, and Optical Physics, **60**, p. 240 (2011).

26. N. Berrah, R.C. Bilodeau, I. Dumitriu, D. Toffoli, and R. R. Lucchese, "Shape and Feshbach Resonances in Inner-Shell Photodetachment of Negative Ions, J. Elect. Spectr. and Relat. Phen., Kai Siegbahn Memorial Volume **183** pp 64-69. (2011)
27. L. Fang, M. Hoener, N. Berrah, "Ultra intense x-ray induced non-linear processes in Molecular nitrogen", J. of Physics, **288,** 012019 (2011)
28. N. Berrah, L. Fang, T. Osipov, B. Murphy, E. Kukk, K. Ueda, R. Feifel, P. van der Meulen, P. Salen, H. Schmidt, R. Thomas, M. Larsson, R. Richter, K. C. Prince, J. D. Bozek, C. Bostedt, S. Wada, M. Piancastelli, M. Tashiro, M. Ehara, "Double Core-Hole Spectroscopy for Chemical Analysis with an Intense X-Ray Femtosecond Laser" Proc. Natl. Acad. Sci. USA(PNAS), **108**, issue 41, 16912 (2011).
29. E. P. Kanter, B. Krassig, Y. Li, A. M. March, N. Rohringer, R. Santra, S. H. Southworth,L. F. DiMauro, G. Doumy, C. A. Roedig, N. Berrah, L. Fang, M. Hoener, P. H. Bucksbaum, S. Ghimire, D. A. Reis, J. D. Bozek, C. Bostedt, M. Messerschmidt, L. Young, "Modifying Auger Decay with Femtosecond X-ray Pulses" Phys. Rev. Lett. **107**, 233001 (2011).
30. G. Doumy, C. Roedig, S.-K. Son, C. I. Blaga, A. D. DiChiara, R. Santra, N. Berrah, C. Bostedt, J. D. Bozek, P. H. Bucksbaum, J. P. Cryan, L. Fang, S. Ghimire, J. M. Glownia, M. Hoener, E. P. Kanter, B. Krässig, M. Kuebel, M. Messerschmidt, G. G. Paulus, D. A. Reis, N. Rohringer, L. Young, P. Agostini, and L. F. DiMauro, "Nonlinear Atomic Response to Intense Ultrashort X Rays", Phys. Rev. Lett. **106**, 083002 (2011).
31. O. Gessner, O. Kornilov, M. Hoener, L. Fang, and N. Berrah, "Intense Femtosecond X-ray Photoionization Studies of Nitrogen - How Molecules interact with Light from the LCLS" in Ultrafast Phenomena XVII, M. Chergui, D. M. Jonas, E. Riedle, R. W. Schoenlein, A. J. Taylor, Eds.,Oxford University Press, 47 (2011).
32. I. Dumitriu, R. C. Bilodeau, T. W. Gorczyca, C. W. Walter, N. D. Gibson, Z. D. Pesic, D. Rolles and N. Berrah, "Inner-shell photodetachment from Ru^{-}", Phys. Rev. A. **82**, 043434 (2010).
33. J. M. Glownia, J. Cryan, J. Andreasson, A. Belkacem, N. Berrah, C. I. Blaga, C. Bostedt, J. Bozek, L. F. DiMauro, L. Fang, J. Frisch, O. Gessner, M. Gühr , J. Hajdu, M. P. Hertlein, M. Hoener, G. Huang,O. Kornilov,J. P. Marangos, A. M. March, B. K. McFarland, H. Merdji, V. S. Petrovic,C. Raman, D. Ray,D. A. Reis, M. Trigo, J. L. White, W. White, R. Wilcox, L. Young, R. N. Coffee, and P. H. Bucksbaum, "Time-Resolved Pump-Probe Experiments at the LCLS" Optics Express, Vol. 18, Issue 17, pp. 17620-17630 (2010).
34. J. P. Cryan, J. M. Glownia, J. Andreasson, A. Belkacem, N. Berrah, C. I. Blaga, C. Bostedt, J. Bozek, C. Buth, L. F. DiMauro, L. Fang, O. Gessner, M. Guehr, J. Hajdu, M. P. Hertlein, M. Hoener, O.Kornilov, J. P. Marangos,11 A. M. March,12, B. K. McFarland, H. Merdji, V. Petrovic, C. Raman, D. Ray, D. Reis, F. Tarantelli, M. Trigo, J. White, W. White, L. Young, P. H. Bucksbaum,and R. N. Coffee, "Auger electron angular distribution of double core hole states in the molecular reference frame", Phys. Rev. Lett; **105**, 083004 (2010).
35. L. Fang, M. Hoener, O. Gessner, F. Tarantelli, S.T. Pratt, O. Kornilov, C. Buth, M. Guehr, E.P. Kanter, C. Bostedt, J.D. Bozek, P.H. Bucksbaum, M.Chen, R. Coffee, J. Cryan, M. Glownia, E. Kukk, S.R. Leone, and N. Berrah, "Double core hole production in N_2: Beating the Auger clock", Phys. Rev. Lett **105,** 083005 (2010).
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