

## **Abstracts**

**(virtual) International Symposium on Correlation, Polarization and Ionization  
in Atomic and Molecular Collisions**

**July 28-29, 2021**

## **Posters 1, July 28 6am-7am**

### **P1.1, *Invited*, On the electron impact single ionization of Hydrogen molecules by twisted electron**

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Since the first experiments in  $(e, 2e)$  by Amaldi et al. and Ehrhardt et al. Independently in 1969, many coincident experiments were performed on the atomic and molecular targets in various geometrical arrangements of the detected electrons. These studies help in the understanding of the structure of targets, electron-electron correlations, and reaction mechanisms involved in the ionization processes. Recently, it has been possible to generate a twisted electron beam characterized by a helical wave-front with a well-defined orbital angular momentum (OAM),  $m$ , along the propagation direction (Serbo V et al., 2015). There have been few theoretical studies on the scattering of the twisted electrons by microscopic targets. Till now, almost all of the coincident ionization processes (e.g.  $(e, 2e)$ ) have been performed for the plane wave electron beams (not possessing any angular momentum). The study of scattering/ionization processes with a twisted electron beam helps us to understand the interaction of electrons of non-zero OAM with atomic/molecular targets. In this communication, we present the calculations of the five-fold differential cross-section (5DCS) and triple differential cross-section (TDCS) for the  $(e, 2e)$  process on molecular hydrogen ( $H_2$ ) by the twisted electron beam. The formalism is developed within the first Born approximation using the plane wave and the twisted wave for the incident electron beam. We describe the plane wave, Heitler-London type wave function, Coulomb wave for the scattered electron, the  $H_2$  molecular state, and the ejected electron respectively. We compare the angular profiles of the 5DCS and TDCS for the different values of orbital angular momentum (OAM) number ( $m$ ) of the twisted electron beam with that of the plane wave beam. We also present the 5DCS for different molecular orientations and study the effect of  $m$  on the 5DCS. We will present our detailed findings on  $(e, 2e)$  processes at the time of the conference.

### **P1.2, *Invited*, Continuum-distorted-wave eikonal-initial-state description of the electron-impact ionization of $H_2O$ and aligned $H_2$ molecules**

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In the last few years, reaction microscopes have allowed for an unprecedented level of detail regarding the exploration of electron-impact ionization of atoms and molecules at the fully differential level. In this context, molecular targets, as simple as  $H_2$ , still provide a challenging testing ground for the state-of-the-art theoretical models, either based on numerically intensive or perturbative treatments. In this work, we present the fully differential cross sections (FDCS) obtained by implementing the continuum-distorted-wave (CDW) eikonal-initial-state (EIS) model, of ample use in the ion-atom context. Two molecular target systems are explicitly considered: non-oriented  $H_2O$  and aligned  $H_2$ . For the former, the final channel is described by using a single center description of the  $H_2O^+$  ion. For the latter, the multicenter nature of the molecular ion is explicitly taken into account. In both cases results obtained are contrasted against recent experimental data and reported theoretical calculations using the time-dependent close-coupling method and the distorted wave Born approximation. Present results suggest that, as in the ion-impact case, the CDW-EIS model is capable of providing a good description of the experimental FDCS and allows inferring valuable information on the physical mechanisms ruling the collision process.

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### P1.3, Invited, Formation of covalently bound C<sub>4</sub>H<sub>4</sub><sup>+</sup> upon electron-impact ionization of acetylene dimer

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We investigate the formation mechanisms of covalently bound C<sub>4</sub>H<sub>4</sub><sup>+</sup> cations from direct ionization of hydrogen bonding dimer of acetylene molecules through fragment ion and electron coincident momentum spectroscopy [1, 2] and quantum chemistry calculations. The measurements of momenta and energies of two outgoing electrons and one ion in triple-coincidence allow us to assign the ionization channels associated with different ionic fragments [3]. The measured binding energy spectra show that the formation of C<sub>4</sub>H<sub>4</sub><sup>+</sup> can be attributed to the ionization of the outermost 1 $\pi$ u orbital of acetylene dimer. The kinetic energy distributions of ionic fragments indicate that the C<sub>4</sub>H<sub>4</sub><sup>+</sup> ions originate from direct ionization of acetylene dimers while C<sub>4</sub>H<sub>5</sub><sup>+</sup> ions resulting from the fragmentation of larger clusters would obtain significantly larger momenta. The formation of C<sub>4</sub>H<sub>4</sub><sup>+</sup> through the evaporation mechanism in larger clusters is not identified in the present experiment. The calculated potential energy curves show a potential well for the electronic ground state of (C<sub>2</sub>H<sub>2</sub>)<sub>2</sub><sup>+</sup>, supporting that the ionization of (C<sub>2</sub>H<sub>2</sub>)<sub>2</sub> dimers can form stable C<sub>2</sub>H<sub>2</sub>·C<sub>2</sub>H<sub>2</sub><sup>+</sup> (1 $\pi$ u-1) cations. Further transition state analysis and ab initio molecular dynamics simulations reveal a detailed picture of the formation dynamics. Besides, we notice that for dimers once a covalent bond is formed between the two monomers, there is no further weakly bound moiety that can take away the internal energy. After ionization of (C<sub>2</sub>H<sub>2</sub>)<sub>2</sub>, the system undergoes a significant rearrangement of the structure involving, in particular, C–C bond formation and hydrogen migrations. It eventually evolved into different isomers of the stable C<sub>4</sub>H<sub>4</sub><sup>+</sup> cations that are methylenecyclopropene, cyclobutadiene, and 1,2,3-butatriene ion [4]. Detailed results on the ionization of acetylene dimer will be discussed at the conference.

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### P1.4, Invited, Cis → Trans Photoisomerisation of Azobenzene

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The cis → trans photo-isomerisation mechanism of azobenzene, after excitation to the n $\pi$ \* and  $\pi\pi$ \* states, is revisited using high-level ab initio surface hopping mixed quantum-classical dynamics in combination with multi-reference CASSCF electronic structure calculations. A reduction of photoisomerisation quantum yield of 0.10 on exciting to the higher energy  $\pi\pi$ \* state compared to the lower energy n $\pi$ \* state is obtained, in close agreement with the most recent experimental values [Ladányi et al., Photochem. Photobiol. Sci., 2017, 16, 1757–1761] which re-examined previous literature values which showed larger changes in quantum yield. By direct comparison of both excitations, we have found that the explanation for the decrease in quantum yield is not the same as for the reduction observed in the trans → cis photoisomerisation. In contrast to the trans → cis scenario, S<sub>1</sub> → S<sub>0</sub> decay does not occur at 'earlier' C–N–N–C angles along the central torsional coordinate after  $\pi\pi$ \* excitation, as in the cis → trans case the rotation about this coordinate occurs too rapidly. The wavelength dependency of the quantum yield is instead found to be due to a potential well on the S<sub>2</sub> surface, from which either cis or trans-azobenzene can be formed. While this well is accessible after both excitations, it is more easily accessed after  $\pi\pi$ \* excitation - an additional 15-17% of photochromes, which under n $\pi$ \* excitation would have exclusively formed the trans isomer, are trapped in this well after  $\pi\pi$ \* excitation. The probability of forming the cis isomer when leaving this well is also higher after  $\pi\pi$ \* excitation, increasing from 9% to 35%. The combination of these two factors results in the reduction of 0.10 of the quantum yield of photoisomerisation on  $\pi\pi$ \* excitation of cis-azobenzene, compared to n $\pi$ \* excitation.

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Nantes. M.V. acknowledges the Région des Pays de la Loire for financial support through the framework of the PULSAR programme.

### **P1.5 Electron impact ionization of water molecule by twisted electron impact**

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The electron impact ionization process is of great importance in plasma physics, astrophysics, radiology, etc. Many theoretical and experimental methods have been developed to study the ionization of atomic and molecular targets. Water is the major component of living organisms. Thus, to investigate the ionization process by charged particles in biological systems, it is essential to study the ionization processes in water molecules by electron impact. The plane wave electron impact ionization of the water molecule is well documented in the literature ( Champion et al. (2001,2002,2006), Sahlaoui et al. (2011), etc. ). The discovery of twisted electron beams has provided a new aspect to the field of ionization. The study of scattering/ionization processes with a twisted electron beam helps us to understand the interaction of electrons of non-zero OAM with atomic/molecular targets. There have been few theoretical studies on the scattering of twisted electrons by microscopic targets. In this communication, we present the calculations of the triple differential cross-section (TDCS) for the (e, 2e) process on water molecule (H<sub>2</sub>O) by the twisted electron beam. The formalism is developed within the first Born approximation using the plane wave and the twisted wave for the incident electron beam. We describe the plane wave, Slater type wave function, Coulomb wave for the scattered electron, the molecular state of H<sub>2</sub>O, and the ejected electron respectively. We compare the angular profiles of the TDCS for the different values of orbital angular momentum (OAM) number (m) of the twisted electron beam with that of the plane wave beam. We have also studied the TDCS for the macroscopic molecular target to explore the effect of the opening angle ( $\theta_p$ ) of the twisted electron beam on the TDCS. We will present our detailed findings at the time of the conference.

### **P1.6 Numerical simulations of laser-assisted electron scattering in a He droplet**

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Monte Carlo simulations of laser-assisted electron scattering (LAES) are conducted for investigating the mechanism of high-energy photoelectron emission from a single atom or molecule doped in a superfluid He droplet by irradiation of femtosecond laser pulses. Results of numerical simulations are in good agreement with corresponding experimental results, showing that the high-energy electrons are generated through multiple-LAES processes between the photoelectron from the dopant and the surrounding He atoms.

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### **P1.7 Investigation of the high energy limit for the plane wave impulse approximation in atomic momentum spectroscopy**

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Intramolecular atomic motion can be directly observed by atomic momentum spectroscopy (AMS) that employs electron-atom Compton scattering. Since AMS cross section is connected with such motion by the plane wave impulse approximation

(PWIA), experimental confirmation of the PWIA high energy limit is essential for applying AMS as a molecular spectroscopic technique. In this study, we have observed dependence of the spectral shape of the AMS spectrum of H<sub>2</sub> on an incident electron energy (E<sub>0</sub>) ranging from 0.5 to 2.2 keV, because failure of the PWIA description appears as asymmetry of the spectrum. It is found that asymmetry of the AMS spectrum at 2.0 keV is minimal, indicating that the experiment reaches the PWIA high energy limit at around 2.0 keV. This is how we establish the AMS experimental condition to directly observe the intramolecular atomic motion for the H<sub>2</sub> molecule.

## **P1.8 Study of Electron-Impact Excitation of Highly Charged Tungsten Ions and the Polarization of their Subsequent Photon Emission**

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Spectroscopic studies of tungsten and its ions have become hot topic for researcher as the divertor region of the world's largest tokamak i.e. International Thermonuclear Experimental Reactor (ITER) [1]–[5] is planned to be made up of tungsten. Because of its exceptional chemical and physical properties it is preferred over the other materials. The ITER device will have a very high temperature gradient from divertor to core region and due to this temperature gradient the tungsten can be stripped to its distinct ionic states and can get further excited to several fine structure states and there after decay by photon emissions. To analyze spectroscopically the emitted lines and know about the details of the ITER plasma, the accurate and complete set of electron-impact excitation cross-section data are required in the wide range of incident electron energy. These results are the prime ingredient for the diagnostics of ITER plasma. Therefore, in the present work our aim is to study the electron-impact excitations of few highly charged tungsten ions and report their excitation cross sections as well as polarization of their subsequent decay photon emissions. Electron-impact excitation of tungsten ions ( ) has been studied using the fully relativistic distorted wave (RDW) [6] theory. The bound state wave functions of tungsten ions in their initial and final states are obtained in the multi-configuration Dirac-Fock approximation by using GRASP2K code [7]. To ensure the accuracy of the evaluated wave functions of the different tungsten ions, we have calculated the excitation energies and oscillator strengths for different transitions considered through GRASP2K code and compared with the available results [8]. Thereafter, the excitation cross-sections of selected electric dipole allowed transitions of these ions are calculated for the incident electron energies from the excitation threshold to 20 keV. Further, the calculated cross-section results are fitted with an analytical expression for direct applications in plasma modeling. In addition, using the density matrix theory [9], the linear polarization of the photons emitted from the excited tungsten ions when decay to their respective ground states is presented. References [1] Ikeda K., ITER on the road to fusion energy, Nucl. Fusion 50, 014002, 2010, doi: 10.1088/0029-5515/50/1/014002. [2] Shukla N., Das T., and Srivastava R., Electron impact N-shell excitation of Se-like to Ga-like tungsten ions and polarization of their subsequent emissions, J. Quant. Spectrosc. Radiat. Transf. 222–223, 247–256, 2019, doi: 10.1016/j.jqsrt.2018.10.031. [3] Shukla N. and Srivastava R., Electron-impact excitation of W<sup>40+</sup>-W<sup>43+</sup> ions: Cross-section and polarization, Int. J. Mod. Phys. B 34, 2050241, 2020, doi: 10.1142/S0217979220502410. [4] Shukla N., Priti, Sharma L., and Srivastava R., Electron-impact excitations of highly charged tungsten ions and polarization study of their successive photon decay, Eur. Phys. J. D 73, 109, 2019, doi: 10.1140/epjd/e2019-100010-9. [5] Shukla N. and Srivastava R., Study of electron impact fine-structure excitation and polarization of highly charged tungsten ions, J. Phys. Conf. Ser. 1412, 13–14, 2020, doi: 10.1088/1742-6596/1412/14/142008. [6] Sharma L., Surzhykov A., Srivastava R., and Fritzsche S., Electron-impact excitation of singly charged metal ions, Phys. Rev. A 83, 062701, 2011, doi: 10.1103/PhysRevA.83.062701. [7] Jönsson P., Gaigalas G., Bieroń J., Fischer C. F., and Grant I. P., New version: Grasp2K relativistic atomic structure package, Comput. Phys. Commun. 184, 2197–2203, 2013, doi: 10.1016/j.cpc.2013.02.016. [8] Kramida, A., Ralchenko, Yu., Reader J., NIST Atomic Spectra Database (version 5.8). Available: <https://physics.nist.gov/asd> [Thu Jun 03 2021]. National Institute of Standards and Technology, Gaithersburg, MD., , 2021. [9] Sharma L., Surzhykov A., Inal M. K., and Fritzsche S., Polarization transfer in the inner-shell photoionization of sodium like ions, Phys. Rev. A 81, 023419, 2010, doi: 10.1103/PhysRevA.81.023419.

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## **P1.9 Forward-backward asymmetry in electron-impact ionization of CO studied by (e, e+ion) spectroscopy**

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<sup>1</sup>IMRAM, Tohoku University

We have investigated the molecular-orientation dependence of electron-impact ionization of CO using scattered electron-fragment ion coincidence spectroscopy. The direction of the molecular-axis with respect to the momentum transfer vector has been determined from the angular correlation between the fragment ion and the scattered electron. The experimental results on the 3 doublet PI ionization reveal that at small momentum transfer, the scattering cross section is higher when the momentum transfer vector points toward the C atom along the molecular axis than when it is in the opposite direction. This forward-backward asymmetry is a nontrivial molecular orientation effect in charged-particle-induced ionization, which does not appear in photoionization.

## Invited Talks 1, July 28 8am-10am

### **T1.1, 8am, Invited, Observation of laser-assisted (e, 2e) process of Ar in intense laser fields**

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<sup>3</sup>The University of Tokyo / Tokyo Metropolitan University / JST PRESTO

[Introduction] When an electron impact ionization occurs under the presence of a light field, the sum of the kinetic energies of the scattered electron and the ejected electron changes by multiples of the photon energy,  $n\hbar\omega$ , with  $n$  being an integer. This process is called laser-assisted (e, 2e) [LA(e, 2e)] [1] from which we can investigate how an atom or a molecule interacts with a light field because the scattered and the ejected electrons produced within the light field carry the information on the formation of the light-dressed states in the laser field. Höhr et al. [2] observed an LA(e, 2e) process of He in a nanosecond high-power laser field ( $\lambda = 1064$  nm,  $\tau = 7$  ns,  $3$  J / pulse,  $I = 4 \times 10^{12}$  W/cm<sup>2</sup>), but the number of photons,  $n$ , involved in the LA(e, 2e) processes was not identified. Because the effect of the formation of light-dressed states appearing on the triply-differential cross section varies depending on the number of photons  $n$  involved in the LA(e, 2e) process [3], experimental determination of an  $n$ -selective cross section of the LA(e, 2e) process has been highly awaited. In the present study, we perform measurements of an (e, 2e) process of Ar in an ultrashort near-infrared intense laser field ( $2 \times 10^{11}$  W/cm<sup>2</sup>, 1030 nm, 1.2 ps) using a home-built apparatus with which a scattered electron and an ejected electron from Ar are detected in coincidence, and observe LA(e, 2e) signals unambiguously at the total kinetic energy of the scattered and ejected electrons shifted by one photon energy ( $n = +1$ ) [4]. [Experiment] The output of a 100 kHz Yb:YAG laser system was focused on the scattering point ( $\lambda = 1030$  nm, 0.6 mJ/pulse,  $2 \times 10^{11}$  W/cm<sup>2</sup>, 1.2 ps). In addition, a part of the laser pulses were converted into UV pulses (0.1 pJ/pulse) and used for the generation of a pulsed electron beam by using a photocathode-type electron gun [5]. The generated electron pulses were accelerated to 1000 eV and focused on the argon gas flow. In order to record the (e, 2e) processes by detecting the fast scattered electrons (960 - 1010 eV) and the slow ejected electrons ( $< 10$  eV) in coincidence, we constructed an apparatus equipped with two angle-resolved time-of-flight (ARTOF) analyzers placed in the asymmetric configuration. [Results and Discussion] In the sum energy spectra of scattered and ejected electron signals, two peaks appear at 984.2 and 970.8 eV that correspond to the electron impact ionization from the Ar 3p (15.76 and 15.94 eV) and 3s (29.24 eV) orbitals, respectively. In addition, a peak structure shows up in the signal intensity at 985.4 eV, that is, the kinetic energy shifted by 1.2 eV from the (e, 2e) peak for the Ar 3p orbital. This peak structure appearing in the (e, 2e) signals can be assigned to the LA(e, 2e) process with  $n = +1$ . The intensity of the LA(e, 2e) signal is estimated numerically using the formula derived by Cavaliere et al. [6], in which the triply-differential cross section of the LA(e, 2e) processes was calculated from the field-free triply-differential cross section. The intensity of the experimental LA(e, 2e) spectrum is found to be approximately twice as large as that of the theoretical spectrum. The larger intensity of the recorded LA(e, 2e) signals than the theoretical estimate can be attributed to the interaction between an Ar and the laser field, which is neglected in the theoretical simulation. As shown in this study, the measurement of a triply-differential cross section of LA(e, 2e) process provide us with valuable data by which we can discuss how the formation of the light-dressed states deforms orbitals of multielectron atomic and molecular systems interacting with a light field. [References] [1] A. Makhoute et al. *Atoms* 7, 40 (2019). [2] C. Höhr et al. *Phys. Rev. Lett.* 94, 153201 (2005). [3] C. J. Joachain et al. *Phys. Rev. Lett.* 61, 165 (1988). [4] T. Hiroi et al., Submitted. [5] R. Kanya et al. *Phys. Rev. Lett.* 105, 123202 (2010). [6] P. Cavaliere et al. *J. Phys. B.* 13, 4495 (1980).

### **T1.2, 8:30am, Invited, Laser-assisted elastic electron scattering by Xe in the quasi-Sturmian-Floquet approach.**

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Laser-assisted elastic electron scattering by Xe in the quasi-Sturmian-Floquet approach.

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### **T1.3, 9am, Invited, On the quest for projectile coherence - solving the C6+ mystery**

Markus S. Schöffler<sup>1</sup>, Lothar Ph. H. Schmidt<sup>1</sup>, Jonas Rist<sup>1</sup>, Max Kircher<sup>1</sup>, Alaine Mery<sup>2</sup>, Jimmy Rangama<sup>2</sup>, S. Grundmann<sup>1</sup>, I. Vela Perez<sup>1</sup>, D. Tsitsonis<sup>1</sup>, D. Trabert<sup>1</sup>, S. Eckart<sup>1</sup>, G. Kastirke<sup>1</sup>, K. Fehre<sup>1</sup>, T. Jahnke<sup>1</sup>, R. Dörner<sup>1</sup>, R. Moshhammer<sup>3</sup>, J. Ullrich<sup>4</sup>, D. Fischer<sup>5</sup>, M. Schulz<sup>5</sup>, A. Cassimi<sup>2</sup>

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20 years ago, single ionization of Helium induced by 100 MeV/u C6+ projectiles was investigated in a kinematically complete experiment. The experimental results, were in strong contrast to state of the art theories at this time and even most recent calculations. While the electron momentum distribution should exhibit two distinct lobes, the so-called binary- and recoil-lobe, the node between them was mostly filled. This launched controversial discussions, which are still ongoing today. The most heavily debated explanations are a) experimental issues/limited resolution and b) transversal coherence of the projectile, introduced by Schulz and coworkers. In order to solve the "C6+-mystery", we used a state-of-the-art COLTRIMS (COLd Target Recoil Ion Momentum Spectroscopy) Reaction-Microscope and redid the initial experiment in Cave D4 of GANIL. As insufficient momentum resolution might have been an issue in the original experiment, ion arm of the spectrometer was build in a time- and space-focussing geometry in order to reduce the diminishing influence of the extended target size. The electron arm was build in a time-focussing geometry. On both ends of the spectrometer, hexagonal delay-line-detectors were used, which have an overall non-linearity <100  $\mu\text{m}$ . Also the gas jet was precooled to 80 K and for both, electrons and ions, separate calibrations, using an additional 25 keV ion source were used. With this we achieved a He+ momentum resolution of  $\Delta p < 0.1$  au was achieved. The electron arm of the spectrometer was calibrated via autoionizing states of a Neon, which create numerous energetically sharp isotropically emitted electrons. Results of the experiment will be presented and discussed.

Acknowledgements: The research leading to these results has received funding from the European Union's HORIZON2020 Program under grant agreement n°654002. We thank the GANIL staff for running the accelerators, especially A. Cassimi, A. Mery and J. Rangama for their outstanding support.



## **T1.4, 9:30am, Invited, Filming molecular movies with machine-learning-based high harmonic spectroscopy**

Pengfei Lan<sup>1</sup>

<sup>1</sup>Huazhong University of Science and Technology

Resolving molecular dynamics in time and space, i.e., making a “molecular movie”, has been long desired goal in ultrafast optics. As an emerging tool, high-harmonic spectroscopy (HHS) enables accessing molecular dynamics on femtosecond to attosecond time scales. However, decoding information from the harmonic signals is usually very challenging. Here we show that this obstacle can be effectively overcome by exploiting machine learning in HHS. We have experimentally demonstrated an angular high-harmonic spectroscopy method to probe the rotation dynamics of molecular rotational wave packet in real time. By using a global optimization algorithm, we can retrieve a movie of molecular rotation from the HHG spectra. After that, we have also demonstrated how to retrieve the charge migration process in N<sub>2</sub> and CO<sub>2</sub>.

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## Invited Talks 2, July 28 10:15am-12:15pm

### **T2.1, 10:15am, Invited, Scattering processes with twisted particles carrying orbital angular momentum**

Dmitry Karlovets<sup>1</sup>

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Twisted photons with orbital angular momentum with respect to a propagation axis have been generated in recent years with the energies up to a few keV along with the moderately relativistic vortex electrons (up to 300 keV) and cold neutrons (a few meV). These wave packets interact differently with atoms, targets, nuclei, electromagnetic fields and media due to a different set of quantum numbers and due to their finite spatial coherence with a doughnut-like spatial profile. Remarkably, the differences of the corresponding scattering cross sections from those obtained within a standard plane-wave approximation can often be seen with a naked eye already in the Born approximation for realistic parameters. I review basic properties of the twisted wave packets and the quantum theory of scattering beyond a plane-wave approximation. I show how one can take into account the transverse coherence length of the projectile -- be it a photon, an atom, an electron, or a neutron -- and how such observables as a number of scattering events and an effective cross section are altered due to the finite coherence and/or due to the angular momentum of the projectile. As a specific example, I analyze elastic scattering of the vortex electrons by hydrogen atoms, Schwinger scattering of the twisted neutrons by nuclei, and the resonant scattering of optical twisted photons by relativistic atoms or ions. The latter process has a cross section that is many orders of magnitude bigger than that of the inverse Compton scattering and, therefore, it can be efficiently used for generating twisted photons in the X-ray and gamma ranges. Thus, twisted particles emerge as a new tool not only for atomic physics and quantum optics, but also for high-energy physics and nuclear physics.

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### **T2.2, 10:45am, Invited, The phase of continuum transitions**

Anne Harth<sup>1</sup>, Divya Bharti<sup>1</sup>, Hemkumar Srinivas<sup>1</sup>, Farshad Shobeiry<sup>1</sup>, Rober Moshhammer<sup>1</sup>, Thomas Pfeifer<sup>1</sup>, Nicolas Douguet<sup>2</sup>, Kathryn Hamilton<sup>3</sup>, Klaus Bartschat<sup>3</sup>

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Ultrafast electron dynamics in atomic and molecular systems are often triggered by light fields that drive transitions between electronic states. It depends on the system and the frequency of the field if bound-bound (bb), bound-continuum (bc) or continuum-continuum (cc) transitions are addressed. The photoionization process is basically a bc transition. Recently, relative photoionization time delays in the order of attosecond could be measured [1] with the help of a method called “reconstruction of attosecond beating by interference of two-photon transitions” (RABBITT) [2,3]. The measurement of photoionization time delays via RABBITT requires at least one or more additional cc transitions [4]. In this talk I will introduce a three-sideband RABBITT scheme [5] that has the potential to isolate the phase of cc transition from bc contributions and from laser parameters in photoionization experiments. This method will be analyzed in detailed for atomic hydrogen [6]. I will further present our first experimental data using an argon target, which is easier to handle experimentally but much more challenging for theory, due to the multi-electron nature and the active 3p electron having a non-vanishing orbital angular momentum. [1] K. Kluender, J. M. Dahlstroem, M. Gisselbrecht, T. Fordell, M. Swoboda, D. Guenot, P. Johansson, J. Caillat, J. Mauritsson, A. Maquet, R. Taieb, and A. L’Huillier, Phys. Rev. Lett. 106, 143002 (2011) [2] P. M. Paul, E. S. Toma, P. Breger, G. Mullot, F. Auge, P. Balcou, H. G. Muller, and P. Agostini, Science 292, 1689 (2001) [3] H. Muller, Appl. Phys. B 74 (2002) S17 [4] J. Dahlstroem, D. Guenot, K. Kluender, M. Gisselbrecht, J. Mauritsson, A. L’Huillier, A. Maquet, and R. Taieb, Chem. Phys. 414, 53 (2013) [5] A. Harth, N. Douguet, K. Bartschat, R. Moshhammer, and T. Pfeifer, Phys. Rev. A 99, 023410 (2019) [6] D. Bharti, D. Atri-Schuller, G. Menning, K.R. Hamilton, R. Moshhammer, T. Pfeifer, N. Douguet, K. Bartschat, and A. Harth Phys. Rev A 103, 022834 (2021)

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### **T2.3, 11:15am, *Invited*, A polarization control study in two-color single ionization of water molecule**

Lara Martini<sup>1</sup>, Diego I R Boll<sup>1</sup>, Alicia Palacios<sup>2</sup>, Omar A Fojón<sup>1</sup>

In this work we study the polarization control in two-color water molecule ionization. We investigate, by means of second-order time dependent perturbation theory [1], the dependencies with polarization in a commonly employed pump-probe scheme: an extreme ultraviolet (XUV) ultra-short pulse ionized the target emitting a photoelectron with a smooth energy distribution, then the photoelectron can exchange extra photons with an infrared (IR) laser producing sidebands in the energy spectrum. The sideband intensities present an oscillatory behavior with a maximum when the polarization of the XUV and IR fields are collinear and a minimum when the fields have perpendicular polarization. Recently, the same behavior was reported in above threshold laser assisted ionization of water molecules [2]. These experiments were performed at photoelectron energies for which the soft-photon approximation (SPA) exhibits discrepancies with the measurements [2]. With our method and employing two basis sets for water molecules [3], we improve the description of the experiments and we unveil that the discrepancies presented by the SPA might be associated to the coulombic nature of the scattering process for continuum-continuum transitions. [1] Boll D I R et al 2020 Phys. Rev. A 101 013428. [2] Leitner T et al 2015 Phys. Rev. A 91 063411. [3] Martini L et al 2019 J. Phys. B: At. Mol. Opt. Phys. 52 105204.

Acknowledgements: The authors acknowledge the financial support of the Agencia Nacional de Promoción Científica y Tecnológica, Project PICT No. 01912 (2015-3392), from the Consejo Nacional de Investigaciones Científicas y Técnicas de la República Argentina, Project PIP No. 0784 (11220090101026) and from the Ministerio de Economía y Competitividad in Spain, Projects No. PID2019-105458RB-I00 and No. FIS2017-92382-EXP.

### **T2.4, 11:45am, *Invited*, Quantum Control of entangled photon pair emission in electron-ion collisions by laser-synthesized photoelectron wave packets**

Esteban Goetz<sup>1</sup>, Klaus Bartschat

<sup>1</sup>Department of Physics and Astronomy, Drake University

We theoretically investigate the coherent control of correlated two-electron dynamics and quantum light emission in multichannel electron-atom and electron-ion collisions. The projectile electron is defined by a laser-synthesized photoelectron wave packet. The coherence of the latter is engineered by promoting interfering multi-photon ionization pathways in the parent atom. We show that the coherence of the incident electron wave packet can be engineered to control the collision dynamics and the rearrangement channel, as well as underlying processes within each channel, such as entangled photon-pair production after electron impact. In particular, we demonstrate coherent control over the polarization and angular distributions of entangled photon-pairs emitted after inelastic scattering and dielectronic recombination by modulating the spectral coherence of the incident electron based on interferometric multi-photon ionization of its parent atom. Quantum control of the correlated electron-ion collision dynamics and photon-pair emission upon radiative decay is achieved by exploiting matter-wave coherences of the incident electron wave packet to manipulate interferences between quantum pathways contributing to the same final photon modes and projectile-target states, i.e., the composite system formed by the target and the scattered or trapped incident electron wave packet.

Acknowledgements: This work was supported by the United States National Science Foundation under grant No. PHY-1803844.

## **Posters 2, July 28 4pm-5pm**

### **P2.1, *Invited*, Photoionization of polarized lithium atoms out of an all-optical atom trap**

Daniel Fischer<sup>1</sup>

<sup>1</sup>Missouri University of Science and Technology

Photo-electron angular and energy distributions provide insights into the dynamics of photoionization processes. The information is particularly detailed, if the target is prepared in an excited and polarized eigenstate before it is exposed to the ionizing radiation. Here we report on an experiment, where lithium atoms are resonantly excited to the polarized  $2p(m = +1)$  state in an all-optical atom trap, before they are ionized in a femtosecond laser field of an optical parametric chirped pulse amplifier (OPCPA) with a tunable center wavelength. The momenta of emitted electrons and ions are analyzed in a COLTRIMS spectrometer with excellent resolution. In several series of experiments, symmetry breaks in multiphoton ionization processes depending on the relative polarization of atoms and laser field are observed. The measurements give direct access to the quantum-mechanical details of the systems including the complex phase information of the electronic final state. Besides their fundamental relevance, the studies provide tools to control the details of the fragmentation processes.

Acknowledgements: The experimental material presented here is based upon work supported by the National Science Foundation under Grant No. PHY-1554776

### **P2.2, *Invited*, Generalized Sturmians functions in prolate spheroidal coordinates for continuum states**

Ana Laura Frapiccini<sup>1</sup>, Dario Mitnik<sup>2</sup>, F A Lopez<sup>2</sup>, Ugo Ancarani<sup>3</sup>

<sup>1</sup>IFISUR - CONICET

<sup>2</sup>UBA - CONICET

<sup>3</sup>Université de Lorraine

We propose and implement a spectral approach to describe continuum states of diatomic systems. The method is based on Generalized Sturmian Functions in prolate spheroidal coordinates. With the one-electron dihydrogen cation as an example, we demonstrate the numerical efficiency by calculating photoionization cross sections.

Acknowledgements: D. M. wishes to acknowledge financial support from Agencia Nacional de Promocion Cientifica y Tecnologica (PICT-2017-2945), Consejo Nacional de Investigaciones Cientificas y Tecnicas (PIP 11220130100607CO) and Universidad de Buenos Aires (UBACyT 20020170100727BA)

### **P2.3, *Invited*, Appearance of coherence in initially non-coherent systems**

Raul O. Barrachina<sup>1</sup>, Tamara A. Guarda<sup>1</sup>, Francisco Navarrete<sup>2</sup>, Marcelo F. Ciappina<sup>3</sup>

<sup>1</sup>Bariloche Atomic Centre, National Atomic Energy Commission, 8400 Bariloche, Argentina

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<sup>3</sup>Guangdong Technion - Israel Institute of Technology, Shantou, Guangdong 515063, China

The appearance of coherence in initially non-coherent systems is one of the most interesting and least understood effects of Quantum Physics. Just as the coherence length of a particle beam increases as the particles move away from their source, there are also effects that can alter this trend. In this work we present a simple and analytical description of this process, showing its usefulness in the interpretation and qualitative analysis of scattering processes.

## **P2.4, Invited, Scaling rules for the ionization of biomolecules**

Alejandra Mendez<sup>1</sup>, Claudia Montanari<sup>1</sup>, Jorge Miraglia<sup>1</sup>

<sup>1</sup>Instituto de Astronomía y Física del Espacio, CONICET-UBA

The ionization of biomolecules by multicharged ions is a challenging task with critical implications. Many comprehensible yet straightforward ab initio models have been presented over the years to compute the ionization for several DNA and RNA bases. In a recent work [Mendez et al. JPB 53 (2020) 055201], we combined continuum distorted wave with eikonal initial state (CDW) calculations with a simple molecular stoichiometric model (SSM) to determine the ionization cross sections of over a hundred biologically relevant collisional systems. Further examination of our theoretical results led us to propose three scaling rules [Mendez et al. JPB 53 (2020) 11752021]. The first law considers the nature of the projectile by reducing the cross-section with the ion charge,  $Z^\alpha$ , as a function of the reduced impact energy  $E/Z^{2-\alpha}$ , with  $\alpha = 1.2$ . The second rule accounts for the molecular structure of the target scaling the ionization with an optimal number of active electrons per molecule,  $n_e$ . The third scaling considers the entire collisional system, and the cross-sections become independent of both the target and ion. The implementation of this general rule on CDW-SSM calculations and available experimental data proved to be valid within 35% in a wide energy range.

## **P2.5 Sub-cycle interference phenomena induced by strong and ultrashort laser pulses**

Abdelmalek Taoutioui<sup>1</sup>, Károly Tókési<sup>1</sup>

<sup>1</sup>Institute for Nuclear Research (ATOMKI), Debrecen, Hungary.

Photoelectron holography is a promising technique for the dynamical imaging of ultrafast phenomena in atomic and molecular systems such as chemical reactions. This latter is based on the deep understanding of the sub-cycle quantum interference occurring in strong-field tunnel ionization regime. We present a theoretical investigation of the holographic interference patterns in the two-dimensional photoelectron momentum distribution (PMD) for single-cycle, two-cycle, and three-cycle pulses by solving numerically the time-dependent Schrödinger equation. In addition, the photoelectron energy-angle resolved spectra and the photoelectron energy spectra as a function of the carrier-envelope phase will be presented as well.

Acknowledgements: This work was supported by the Bilateral relationships between Morocco and Hungary in science and technology (S&T) under the project number 2018-2.1.10-TET-MC-2018-00008.

## Posters 3, July 28 5pm-6pm

### **P3.1, Invited, Ultrafast structural dynamics of laser-induced nanoplasma probed by time-resolved X-ray diffraction**

Akinobu Niozu<sup>1</sup>

<sup>1</sup>Hiroshima University

Ultrafast structural dynamics of nanoplasmas induced by intense laser irradiation have been studied by time-resolved diffraction measurements using X-ray free-electron lasers (XFELs). Recent experimental results have suggested that the disordering in nanoplasma proceeds from the surface towards the inner core with a speed compatible with the plasma sound speed, and the crystalline order in nanoplasmas survives within a few hundred femtoseconds after the laser excitation. Here we report that the time scale of structural disordering in the nanoplasma strongly depends on the pump near-infrared (NIR) laser intensity. The NIR intensity-dependence was interpreted in terms of plasma parameters deduced from ion time-of-flight spectra of NIR-laser-induced nanoplasmas, suggesting that the time scale of crystalline disordering scales with the inverse of the plasma sound speed.

Acknowledgements: This work was done in collaboration with Yoshiaki Kumagai, Hironobu Fukuzawa, Naomichi Yokono, Daehyun You, Shu Saito, Yu Luo, Edwin Kukk, Claudio Cirelli, Jonas Rist, Isabel Vela-Perez, Takashi Kameshima, Yasumasa Joti, Koji Motomura, Tadashi Togashi, Shigeki Owada, Tetsuo Katayama, Kensuke Tono, Makina Yabashi, Linda Young, Kazuhiro Matsuda, Christoph Bostedt, Kiyoshi Ueda, and Kiyonobu Nagaya. The experiments were performed at SACLA with the approval of JASRI and the program review committee (No. 2018B8063). This study was supported by the Japan Society for the Promotion of Science (JSPS) KAKENHI Grant Nos. JP15K17487 and JP16K05016, by JSPS Grant-in-Aid for JSPS Fellows No. JP19J14969, and by Research Program for Next Generation Young Scientists of "Dynamic Alliance for Open Innovation Bridging Human, Environment and Materials" in "Network Joint Research Center for Materials and Devices".

### **P3.2, Invited, Benchmark differential cross section ratios for excitation of the $4p^{\{6\}} \rightarrow 4p^{\{5\}5s,5s'}$ [K]<sub>J</sub> transition in krypton**

Ahmad Sakaamini<sup>1</sup>, Murtadha Khakoo<sup>1</sup>, Jean B. Faure<sup>1</sup>

<sup>1</sup>California State University, Fullerton

It seems reasonable to assume that  $\beta$ -alanine molecules linked into a cluster present greater sensitivity than the isolated molecules to key kinetic events, such as binding, insertion and dimerization, similarly to those observed in peptides [2]. The evolution of the isolated  $\beta$ -alanine molecules into neutral clusters has been studied theoretically for  $(\beta\text{-ala})_n$ , where  $n \leq 5$  [3]. The analysis of intermolecular interactions was essential to understand the structure, stability and chemical rearrangements of these clusters and therefore to explain the experimentally measured peaks for protonated intact clusters. Furthermore, the most intense experimental peaks coming from fragmentation of dimers and trimers were analyzed using potential energy surface (PES) and also MD simulations. This study showed the energetically favorable peptide bond formations after singly ion impact for the protonated  $\beta$ -alanine molecules embedded into clusters [4].

Acknowledgements: The US National Science Foundation for funding Dr. Ahmad Sakaamini's Postdoctoral Fellowship, the guidance and supervision of Dr. Murtadha Khakoo of California State University-Fullerton, where the experimental results were obtained, and the B-spline R-matrix results from Drs. Oleg Zatsarinny and Klaus Bartschat of Drake University, USA.

### **P3.3 XPS and Auger processes in 2D materials**

Juana L. Gervsoni<sup>1</sup>, Silvina Segui<sup>2</sup>

<sup>1</sup>CNEA-CONICET, Argentina

<sup>2</sup>CONICET

In this work, we analyze the process of excitation of plasmons during the emission of electrons in the proximity of two-dimensional (2D) material surfaces. We detail the effects due to the interaction between an electron and a stationary positive ion (or atomic hole) in the vicinity of the metal surface. We use the dielectric response of the material and the specular reflection model for the case of flat surfaces. In particular, we study how the interaction of the electron-hole pair can influence the loss of energy of the emerging electron. The method described here is useful to understand the excitation spectra of electrons in 2-dimensional materials, (different from those of the same volumetric material).

Acknowledgements: We are grateful for financial support to CONICET (research project PIP11220170100353) and National University of Cuyo (research project 06/C550). Z.L.M.acknowledges support from the Natural Sciences and Engineering Research Council of Canada (RGPIN-2016-03689).

### **P3.4 Emergence of light-induced states in the few-photon ionization of atomic helium**

Aaron Bondy, Severin Meister, Robert Moshhammer, Nicolas Douguet, Klaus Bartschat

In this joint experimental and theoretical work [1], photoelectron emission from excited states of laser-dressed atomic helium is analyzed. The experiment is carried out at DESY in Hamburg using the FLASH2 free-electron laser with analysis at the reaction microscope (REMI) end station [2]. The helium atom is subject to (temporally) overlapping extreme ultraviolet (XUV) and an infrared (IR) pulses, with either parallel or orthogonal relative polarization. The XUV pulse is scanned over excited states of helium. Electric dipole-allowed nP states corresponding to single XUV photon excitation always lead to ionization; however, dipole-forbidden transitions to light-induced states (LIS), such as nS and nD states, corresponding to multiphoton (XUV  $\pm$  nIR) excitation, are observed only during temporal overlap. Studying photoelectron angular distributions (PADs) in the case where the ionization pathway of a LIS is difficult to resolve energetically allows for an unambiguous determination of the dominant LIS. Relative orientation of the two lasers is employed to study its effect on PADs and to control the suppression of certain ionization pathways. Numerical solutions of the time-dependent Schrödinger equation support the experimental findings in this project. [1] S. Meister et al., Phys. Rev. A 102 (2020) 062809; Phys. Rev. A 103 (2021) in press. [2] S. Meister et al., Applied Sciences 10 (2020) 2953. [1] S. Meister et al., Phys. Rev. A 102 (2020) 062809; Phys. Rev. A 103 (2021) in press. [2] S. Meister et al., Applied Sciences 10 (2020) 2953.

Acknowledgements: XSEDE, NSF, NSERC

### **P3.5 Development of a general protocol for observing atomic momentum distributions in molecules using electron-atom Compton scattering**

Yuichi Tachibana<sup>1</sup>, Yuuki Onitsuka<sup>1</sup>, Hirohiko Kono<sup>1</sup>, Masahiko Takahashi<sup>1</sup>

<sup>1</sup>Tohoku university

We demonstrate that atomic motion in a molecule can directly be observed by means of electron-atom Compton scattering experiments or atomic momentum spectroscopy. This is realized by developing a protocol to extract intramolecular atomic momentum distributions from raw experimental data, which also includes contributions of molecular translational motion and instrumental response function. The protocol is based on convolution theorem and its efficiency is shown by applying it to experimental data on hydrogen molecules. The extracted momentum distribution of the H-atom in the hydrogen molecule is in satisfactory agreement with an associated one that has been calculated by using rovibrational wave functions predicted by quantum chemistry theory. This indicates not only the validity of our proposed protocol but also feasibility of use of AMS as a completely new molecular spectroscopy technique.

## **Invited Talks 3, July 29 6am-8am**

### **T3.1, 6am, *Invited*, Compton double ionization of helium: experiment, theory, results**

V. Yu. Popov<sup>1</sup>, Max Kircher<sup>2</sup>, Reinhard Doerner<sup>2</sup>, Ochbadrakh Chuluunbaatar<sup>3</sup>, Salim Houamer<sup>4</sup>, Igor P. Volobuev<sup>1</sup>

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In the report, recent results of a large international team of theorists and experimenters on the Compton double ionization (CDI) of the helium atom with the use of the COLTRIMS (COLD Target Recoil Ion Momentum Spectroscopy) technique are presented. In these experiments, only the momentum of the helium atom nucleus and that of one of the electrons (the slow one) are measured in coincidence. As a result, the total differential cross section is integrated over the momentum of the final photon for the initial photon energy of 40 keV. In order to increase the experimental yield, various single scattering cross sections are also measured. The experiment is compared with the theory within the so called  $A^2$  approximation. Various models of the initial and final states of the atom are used, including states with strong electron correlations. Unfortunately, in the presented experiments it is impossible to exclude the scattering of the final photon into the forward cone, where exchange processes make a large contribution, and where both electrons have relatively low energies. In such a situation, it is impossible to realize the kinematics with a large difference in the energies of the electrons, which takes place in the so-called (e, 3e) impact electron reactions used as a method for studying electron correlations in a target. Nevertheless, even in this implementation, single differential cross sections show an obvious dependence on the character of a pair of initial and final (double continuum) wave functions

### **T3.2, 6:30am, *Invited*, A Sturmian approach to study ionization of molecules by photon or electron impact**

Lorenzo Ugo Ancarani<sup>1</sup>

<sup>1</sup>Universite de Lorraine and CNRS, Metz, France

We have developed a Sturmian approach to describe ionization processes of small molecules by photon or electron impact. In this spectral method, two-body Generalized Sturmian Functions are built appropriately as to represent the continuum states of the electrons ejected with a given energy and to possess the adequate Coulomb asymptotic behavior. This tool has been applied to several processes. We have calculated differential cross sections for the single ionization by electron impact of a variety of small polyatomic molecules, and in different kinematical and geometrical configurations. Single photoionization has also been investigated; for diatomic molecules we have recently implemented the method as to use prolate spheroidal coordinates. Describing double continuum states is more challenging as it requires to include properly the electron-electron interaction. Building on the success for the atomic three-body case, we have performed calculations of angular distributions for the photodouble ionization of water molecules under different excess energy and energy sharing regimes. In all considered processes and molecules, the calculated cross sections are compared with available measurements. A satisfactory global agreement is observed.

Acknowledgments: The material presented here results from the work of many collaborators, in particular from Metz and from the Argentinian groups in Bahia Blanca, Bariloche and Buenos Aires.



### **T3.3, 7am, Invited, Investigating dissociation dynamics of small molecules using COLTRIMS Reaction Microscopes and XFELs**

Till Jahnke<sup>1</sup>

<sup>1</sup>European XFEL, Schenefeld, Germany

Since early 2019 a dedicated COLTRIMS Reaction microscope is in operation at the SASE3 branch of the European XFEL. THE SQS-REMI combines the outstanding properties of XFEL light pulses with the capabilities of coincident electron and ion momentum detection. The talk will provide several examples of investigations on small to mid-sized molecules depicting their break-up dynamics, either employing Coulomb explosion imaging and/or photoelectron diffraction imaging.

### **T3.4, 7:30am, Invited, Femtosecond Dynamics in Biomolecules Probed with Soft X-ray Spectroscopy**

Zhong Yin<sup>1</sup>, Yi-Ping Chang<sup>2</sup>, Tadas Balciunas<sup>2</sup>, Yashoj Shakya<sup>3</sup>, Giuseppe Fazio<sup>1</sup>, Ludger Inhester<sup>4</sup>, Robin Santra<sup>3</sup>, Jean Pierre Wolf<sup>2</sup>, Hans Jakob Wörner<sup>1</sup>

<sup>1</sup>ETH Zürich

<sup>2</sup>Université de Genève

<sup>3</sup>DESY & Universität Hamburg

<sup>4</sup>DESY

Photoinduced excitation and ionization of matter are essential for a wide range of bio-chemical phenomena. In many cases, multiphoton ionization can lead to ultrafast structural dynamics, which constitutes an experimental challenge to follow in real-time, due to the lack of sufficient time resolution. Here, we present experimental evidence of coupled electron-nuclear dynamics in a solvated biomolecule utilizing a water window high-harmonic-generation source coupled with a sub- $\mu\text{m}$  thin flat jet. Theoretical simulations support the observation of valence-hole-induced structural dynamics.

## **Invited Talks 4, July 29 8:15am-10:15am**

### **T4.1, 8:15am, *Invited*, Studying Attosecond Electron Dynamics with X-ray Free Electron Lasers**

James Cryan<sup>1</sup>

<sup>1</sup>SLAC National Accelerator Laboratory

Electron motion is a key ingredient of all chemical reactions. The natural timescale for such electronic motion is set by the electron's binding energy to be in the range of tens to hundreds of attoseconds. Consequently, the study of ultrafast electronic phenomena requires the generation of laser pulses shorter than 1 fs, and of sufficient intensity to interact with their target with high probability. Free Electron Lasers (FELs), such as the Linac Coherent Light Source (LCLS), offer interesting opportunities to achieve these conditions, allowing for the probing of electrons on this natural time scale, elucidating the earliest processes involved in chemical change. In this talk, I will present our first results showing isolated attosecond soft X-ray pulses from the FEL. Such high power pulses open the door for nonlinear spectroscopies such as pump/probe spectroscopy, and X-ray wave mixing. We have demonstrated the preparation of a coherent electronic wavepacket by driving stimulated X-ray Raman scattering in gas phase molecules. Combing attosecond X-ray pulses with an external laser field we are able to time-resolve the photoemission dynamics of core-level electrons in molecules, and observe coherent electron motion in core-excited molecules.

Acknowledgements: This work was supported by the AMOS program within the Chemical Sciences, Geosciences, and Biosciences Division of the Office of Basic Energy Sciences, Office of Science, U.S. Department of Energy. Use of the Linac Coherent Light Source (LCLS), SLAC National Accelerator Laboratory, is supported by the U.S. Department of Energy (DOE), Office of Science, Office of Basic Energy Sciences (BES) under Contract No. DE-AC02-76SF00515.

### **T4.2, 8:45am, *Invited*, Circular Dichroism in Atomic Resonance-Enhanced Few-Photon Ionization**

Santwana Dubey<sup>1</sup>

<sup>1</sup>University of Central Florida

Symmetry breaking due to chirality is a ubiquitous phenomenon in nature, ranging from particle physics to biochemistry. This talk presents recent investigations on few-photon ionization of polarized atoms with circularly polarized light – one of the simplest conceivable chiral systems. Lithium atoms are prepared in the polarized 2p ( $m_l = +1$ ) state and subjected to circularly polarized femtosecond light pulses at center wavelengths between 665 and 920 nm. Strong asymmetries are found in the ionization cross-section for the electric field co- or counter-rotating with the initial electronic current density and quantitatively analyzed in terms of “circular dichroism” (CD). While the intensity dependence of the measured CD values is rather weak throughout the investigated regime, a very strong sensitivity on the center wavelength of the incoming radiation is observed. For a field frequency near the excitation energy of the oriented initial state, the photoelectron energies are significantly affected by the helicity-dependent Autler-Townes splitting. While the co-rotating situation prevails for most wavelengths, the counter-rotating geometry is strongly favored around 800 nm due to the 2p-3s resonant transition, which can only be driven by counter-rotating fields. These observations provide insights into the helicity dependence of light-atom interactions, and on the possible control of emission of spin-polarized electrons in atomic few-photon ionization by polarization-selective couplings to resonant atomic states.

Acknowledgements: The experimental material presented here is based upon work supported by the National Science Foundation (NSF) under Grant No. PHY-1554776. The theoretical part of this work was funded by the NSF under Grants No. PHY-2012078 (T.M. and N.D.) and No. PHY-1803844 (K.B.), and by the XSEDE supercomputer allocation Grant No. PHY-090031. The calculations were carried out on Comet at the San Diego Supercomputer Center and Bridges-2 (via a trial allocation) at the Pittsburgh Supercomputing Center.

### **T4.3, 9:15am, Invited, Asymmetric electron emission in non-linear processes in the X-ray regime**

Arturo Sopena<sup>1</sup>, Alicia Palacios<sup>1</sup>, Fabrice Catoire<sup>2</sup>, Henri Bachau<sup>2</sup>, Fernando Martín<sup>3</sup>

<sup>1</sup>Universidad Autónoma de Madrid / Centre des Lasers Intenses et Applications

<sup>2</sup>Centre des Lasers Intenses et Applications

<sup>3</sup>Universidad Autónoma de Madrid / IMDEA / IFIMAC

The rise of free-electron lasers (XFELs) throughout the world over the last two decades has opened the door to extending X-rays to study non-linear processes in the attosecond domain. At these short wavelengths the commonly used dipole approximation breaks down and non-dipole effects need to be considered. In this talk, I will be presenting results from our theoretical simulations on a novel scheme of stimulated Compton scattering (SCS) on the hydrogen molecule using a highly intense ultrashort X-ray pulse with frequencies ranging from 0.5 to 1.6 keV. It is found that the coherent contributions of dipole and non-dipole effects lead to a symmetry breaking in the photoelectron emission, which strongly depends on the X-ray wavelength and the molecular orientation. This is a pure non-linear effect captured in the low-energy lying electrons emitted after absorption and subsequent stimulated emission of photons within the energy bandwidth of the pulse. Additionally, I will be presenting results on SCS using two ultrashort pulses with different photon energies and propagation directions. In this kind of two-color scheme, the relative propagation angle modulates the non-dipole response of the system which, in turn, affects the asymmetry in the photoelectron emission.

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## Posters 4, July 29 11am-12pm

### **P4.1, Invited, Few-femtosecond dynamics of CO<sub>2</sub> super-excited states**

Rocío Borrego-Varillas<sup>1</sup>, Matteo Lucchini<sup>2</sup>, Mario Murari<sup>2</sup>, Thomas Schnappinger<sup>3</sup>, Regina de Vivie-Riedle<sup>3</sup>, Mauro Nisoli<sup>4</sup>

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Relaxation of low lying Rydberg states ( $n < 5$ ) is known to occur on time scales ranging from 20 fs to 20 ps. If the excitation photon energy is high enough, a wave packet can be created in a superexcited state (i.e., a neutral excited state with internal energy higher than the ionization energy). Up to date, the relaxation dynamics of these superexcited states are poorly understood due to the lack of proper experimental and theoretical tools. Here we employ VUV photoelectron spectroscopy with sub-15 fs temporal resolution and quantum mechanical simulations to study the ultrafast dynamics of the super-excited states in carbon dioxide (CO<sub>2</sub>). We use few-femtoseconds pulses at 17 eV produced by high-order harmonic generation in combination with a time-delay compensated monochromator (TDCM) to selectively populate the excited states of CO<sub>2</sub> below the first excited state of the molecular cation and 12-fs infrared pulses to subsequently probe the dynamics. Our results show sub-50 fs dynamics originating from a complex mechanism, where the lower vibrational levels of the super-excited state couple to a repulsive state. We resolve, for the first time, the ultrafast oscillations coming from the vibrational structure of a super-excited state which show a period as fast as 24 fs.

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### **P4.2, Invited, Electron loss to the continuum in collisions of uranium ions with nitrogen targets**

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Calculations of doubly differential cross sections for projectile ionization in fast collisions of Li- and Be-like uranium ions with a N<sub>2</sub> target are performed. These cross sections can be efficiently studied experimentally by measurements of the electron-loss-to-continuum cusp, observed as coincidence events between the ejected electron and the ionized projectile. The cusp electrons detected in the laboratory frame at small degrees with respect to the projectile beam and with velocities comparable to the projectile velocity originate from the electrons ejected into the projectile continuum. The measured energy distribution provides insight into the ionization mechanisms beyond investigation of absolute ionization cross sections without need for selecting arguable cuts of the continuum electron phase space for comparison of experiment and theory. Our results obtained within the first order of the relativistic perturbation theory [1] are compared with the recent measurements of the electron-loss-to-continuum cusp [2, 3] and good agreement is found. The role of relativistic and nonperturbative effects is also explored within a complementary approach [4, 5]. References [1] A. I. Bondarev et al., *Atoms* 8, 89 (2020). [2] P. -M. Hillenbrand et al., *Phys. Rev. A* 90, 042713 (2014). [3] P. -M. Hillenbrand et al., *Phys. Rev. A*, accepted (2021). [4] A. I. Bondarev et al., *Phys. Rev. A* 95, 052709 (2017). [5] A. I. Bondarev et al., *Eur. Phys. J. D* 73, 46 (2019).

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#### **P4.3, Invited, Photoionization and fragmentation of cyclic dipeptide. An insight on the “origin of life”**

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Shedding light on the mechanisms of production of prebiotic building blocks is of paramount importance to understand the abiotic synthesis of relevant biologically active compounds and therefore the “origin of life”. To the purpose a combined experimental and theoretical study of the photofragmentation of cyclo-Alanine-Alanine, c-AlaAla, one of the 2,5-Diketopiperazines (DKPs) has been carried out. Photoelectron-Photoion coincidence measurements (PEPICO) in the VUV energy range, performed at the CIPO beamline of Elettra synchrotron [1], allow to follow the formation of the different fragment ions depending on the internal energy, i.e (binding energy – ionization energy) available to the molecule. Ab initio molecular dynamics (MD) simulations and calculations of the potential energy surface (PES) of the fragmentations paths [2] guide the interpretation of the experimental results, as well as disclosing the mechanisms behind the experimental observations. The results show that the interaction of VUV radiation with c-AlaAla produces reactive oxa-zolidinone intermediates. The theoretical simulations show how the interaction of these intermediates with other neutral and charged fragments released in the molecular decomposition of the c-AlaAla leads either to the reconstruction of the cyclic dipeptide or to the formation of longer linear peptide chains [3]. These results may explain how cyclic dipeptides could have on one hand survived hostile chemical environments and on the other provided the seed for amino acid polymerization.[1] P. Bolognesi et al. Phys. Chem. Chem. Phys. 17, 24063 (2015). [2] S. Maclot et al. Phys. Rev. Lett. 117, 073201 (2016) [3] A. Biscans, Life, 8 (2018)

#### **P4.4, Invited, Polypeptide Formation in Clusters of Beta-Alanine Amino Acids by Single Ion Impact**

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The chemical behavior and biological activity of biomolecules in molecular cluster are driven by weak intermolecular interactions [1]. Chemical reactions can be induced with external energy for instance, highly charged ions (HCI), in principle producing different secondary events: emission of electrons, doubly charged reactive species, radicals etc. In this context, understanding of the behavior of amino acids after interaction with alpha particles can give additional information to the formation of biologically active species in the outer space such as the origin of life.

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#### **P4.5, Invited, The contribution to opacity from transitions between multiply-excited states in moderately charged tin ions for EUV nanolithography**

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Extreme ultraviolet (EUV) radiation emanating from laser-driven tin ( $Z = 50$ ) plasmas is now used to print nanometre-scale patterns on silicon wafers to make integrated circuits. This process is known as EUV lithography. In industrial machines, these plasmas are generated by irradiating tin microdroplets with high-intensity CO<sub>2</sub> laser pulses (laser wavelength = 10.6 microns). For many years, it was believed that bound-bound transitions originating from singly-excited states in the open 4d subshell ions Sn<sup>11+</sup> - Sn<sup>14+</sup> were responsible for intense EUV emission observed from these plasmas. Recently, we have shown that these transitions make only a minor contribution to EUV emission. Rather, it is transitions from complex, multiply-excited states that dominate EUV emission from these plasmas. In this poster, I will give an overview of our recent work investigating the contribution to EUV emission from transitions from multiply-excited states in tin plasmas.

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#### **P5.6, Invited, Competitive Dehydrogenation and Backbone Fragmentation of Super-Hydrogenated Polycyclic Aromatic Hydrocarbons: A Laboratory Study**

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Super-hydrogenated Polycyclic Aromatic Hydrocarbons (PAHs) have been suggested to catalyze the formation of H<sub>2</sub> in certain regions of space, but it remains unclear under which circumstances this mechanism is viable given the reduced carbon backbone stability of super-hydrogenated PAHs. We have assessed the photo-stability of super-hydrogenated PAHs using the Photo-Electron Photo-Ion Coincidence technique.

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## **P5.7 Electron impact fine-structure excitation of Kr<sup>+</sup> and polarization study of its subsequent photon emissions**

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The theoretical calculation of electron impact excitation (EIE) cross-section of several transitions of Kr<sup>+</sup> ion is considered, which is of special importance in various plasma modeling based applications, such as electric propulsion devices viz. Hall effect thrusters and ion engines etc. The electron impact excitation of singly ionized krypton is performed from its ground state 4p<sup>5</sup> ( $J=3/2$ ) to the different fine structure levels of 4p45s, 4p45p, 4p46s, 4p46p, 4p44d and 4p45d configurations. A fully relativistic distorted wave method is used for the calculation of excitation cross-section of Kr<sup>+</sup> ion [1]. The required ground and excited bound state wave functions of Kr<sup>+</sup> ion are expressed as multi-configuration Dirac-Fock wave functions which we obtain using the GRASP2K code [2]. The electron impact excitation cross-sections calculation is performed for 114 transitions from the ground state to the various fine structure levels with varying electron energies from threshold to 1 KeV. Further, the related EIE rate coefficients for all the transitions are calculated using the obtained cross-sections. In addition, the calculation is performed for the linear polarization of the radiation emitted through the dipole allowed decay transitions from the electron impact excited Kr<sup>+</sup> ion [3]. The subsequent photon emission gives the information of population of various magnetic excited sub-states which is also an important diagnostic tool to study the different laboratory and astrophysical plasmas. References: [1] S Gupta, L Sharma, R Srivastava, Electron-impact excitation of Xe<sup>+</sup> and polarization of its subsequent emissions. *J Quant Spectrosc Radiat Transf*, 219:7–22, 2018. [2] Per Jonsson, X He, C Froese Fischer, and I P Grant, The grasp2K relativistic atomic structure package. *Comput. Phys. Commun.*, 177(7):597-622, 2007. [3] Dipti and Rajesh Srivastava, Electron-impact excitation rate-coefficients and polarization of subsequent emission for Ar<sup>+</sup> ion. *J. Quant. Spectrosc. Radiat. Transfer*, 176: 12-23, 2016.

## **P5.8 Energy levels and collision strengths of He-like Copper**

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The need for more accurate atomic data becomes greater than before with the ongoing ITER project [1]. Therefore, in recent years, there have been extensive spectroscopic studies, both experimental and theoretical, of helium isoelectronic sequence [2]. Such an analysis requires information for a wide range of atomic parameters, including energy levels and collision strengths. Our aim was to provide a set of accurate energy levels calculations among the lowest 71 levels arising of 1s 2 and 1snl ( $n \leq 6, l \leq (n - 1)$ ) configurations of He-like Cu and carried out through the relativistic configuration interaction (RCI) method implemented in the Flexible Atomic Code (FAC) [3]. We have also considered relativistic effects by incorporating quantum electrodynamics (QED) and Breit corrections. Therefore, we present results for the electron impact excitation (EIE) concerning the 4 excited states of He-like Cu. These results were obtained using the relativistic distorted wave method (DW) implemented in the code FAC (Flexible Atomic Code) [3]. A detailed comparison of the target structure has been made to assess the uncertainty on collision strengths from the target levels. Detailed comparisons for the collision strengths are made with the results of previous calculations, which will pose insight on the uncertainty in their usage by astrophysical and fusion modeling. The present results show good agreement and some significant differences are found to occur.

## **P5.9 Evolution of the (e,2e) Differential Cross Section of Xenon from Coplanar to the Perpendicular Plane at Intermediate Energies**

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Electron impact ionisation of atomic and molecular species is important in many physical processes such as in the behaviour of stellar atmospheres [1]. The (e,2e) process provides the most precise experimental data for the study of ionisation by

electron impact [2]. In these experiments an incident electron of well-defined momentum collides with a target atom or molecule and produces scattered and ejected electrons that are measured in coincidence. Theoretical models are now successful at characterising the  $(e,2e)$  differential cross section (DCS) of light atoms but do not agree well with data for heavier atoms or complex molecules [3, 4]. When the momentum of the incident electron is moved out of the scattering plane the experiment provides a more sensitive test of scattering theories, as multiple scattering events must then occur for momentum and energy to be conserved. The computer controlled and computer optimised  $(e,2e)$  spectrometer in Manchester has been used to make measurements of the  $(e,2e)$  differential cross section with low impact energy for the first five noble gases in a perpendicular geometry [5]. This study found significant differences in the DCS for xenon compared with all other noble gases. A further investigation found that at more intermediate energies the DCS for Xe diverged away from the trend set by the lighter noble gases [6]. New experimental work has now measured the symmetric DCS of Xe at incident energies of 60, 80, and 100 eV above the ionisation potential from a coplanar geometry to the perpendicular plane. The results from these studies is presented here.

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