MO 20: Atomic Physics, Molecular Physics, and Quantum Optics with X-ray FELs (joint session MO/A)

Time: Thursday 10:30–12:30 Location: S HS 002 Biologie

MO 20.1 Thu 10:30 S HS 002 Biologie

Nanodroplet production and characterization for single particle X-ray diffractive imaging — •Amine Gourram[1], Armando Estillore[1], Daniel Horke[1,3], and Jochen Küpper[1,2,3] — [1]Center for Free-Electron Laser Science, DESY, Hamburg, Germany — [2]Department of Physics, University of Hamburg, Hamburg, Germany — [3]The Hamburg Center for Ultrafast Imaging, University of Hamburg, Hamburg, Germany

X-ray diffractive imaging of single molecules or nanoparticles at free-electron lasers allows the extraction of structural information at sub-nanometer resolution [1]. However, this requires the efficient production and delivery of isolated samples into the x-ray beam. We present our proposed aerosol source for the efficient production of a high-density aerosol of sub-100˜nm nanoparticles, based on electrospray aerosolisation. The produced aerosol source will be characterized regarding its efficiency and density for different nanoparticle types and sizes using optical light scattering measurement [2] and differential particle mobility analysers.

[1] Seibert et al., Nature 470, 78-81 (2011) [2] Awel et al., Opt. Express 24, 6507-6521 (2016)

MO 20.2 Thu 10:45 S HS 002 Biologie

3D sensitive diffractive imaging of metal cluster shape transitions — •J. Jordan[1], S. Dold[2], I. Barke[3], P. Behrens[1], N. Bernhardt[1], J. Correa[4], S. Düsterer[4], B. Erk[4], L. Hecht[1], A. Heilrath[1], H. Hartmann[3], R. Irsig[3], N. Iwe[3], B. Kruse[3], B. Langbehn[1], B. Manschwetus[4], F. Martinez[3], K. Oldenburg[3], C. Passow[4], C. Peltz[3], F. Seel[1], R. Tanyag[5], R. Treusch[4], A. Ulmer[1], S. Walz[1], K.-H. Meiwes-Broer[3], T. Fennel[3,5], B. v. Issendorff[2], T. Möller[1], and D. Rupp[1,5] — [1]TU Berlin — [2]Univ. Freiburg — [3]Univ.Rostock — [4]FLASH@DESY — [5]MBI Berlin

With their ability to deliver ultra-short X-ray pulses of high brilliance, free-electron lasers (FELs) have opened up new possibilities for natural sciences. In cluster physics, FELs have been used to investigate fundamental light-matter interactions and create scattering images of single clusters in free flight for structure determination. In particular, gas phase metal clusters exhibit a large variety of shapes that are very sensitive to the growth conditions. Their shape can be altered by soft heating, leading to a reordering of the crystal lattice or melting of the surface. In order to image these changes and record their intrinsic timescale, we performed a pump-probe experiment at the FLASH FEL in Hamburg. Silver clusters were produced using a magnetron sputter source and subsequently heated with a picosecond-long, weak optical laser pulse. The temporal evolution of the shapes after excitation was traced by recording wide-angle scattering images that enable a 3D sensitive shape retrieval.

MO 20.3 Thu 11:00 S HS 002 Biologie

Neural Networks for Reconstruction of Nanoclusters from Soft X-Ray Scattering Images — •Thomas Stielow, Robin Schmidt, Thomas Fennel, and Stefan Scheel — Institut für Physik, Universität Rostock, Albert-Einstein-Straße 23, 18059 Rostock

Single-shot diffraction imaging by soft X-ray laser pulses is a valuable tool for structural analyses of unsupported and short-lived nanosystems, although inversion of the scattering patterns still prove challenging. Deep learning, on the other hand, is widely used in data sciences for the extraction of information from images and sees more and more application in various sciences. We demonstrate how neural networks can be utilized for full reconstructions of nanoclusters from single-shot wide angle scattering images. Our networks are trained solely on existing physical theories and can be applied to real-world experimental data without limitation to a specific setup due to its robustness. With deep learning, high quality real time evalutation for the next generation FEL systems can finally be implemented.

MO 20.4 Thu 11:15 S HS 002 Biologie

Controlling nanoparticles with external fields — •Jannik Lübke[1], Salah Awel[1,4], Armando Estillore[1], Nils Roth[1,2], Amit Samanta[1], Lena Worbs[1], Daniel Horke[1,4], and Jochen Küpper[1,2,3,4] — [1]Center for Free-Electron Laser Science (CFEL), Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany — [2]Department of Physics, Universität Hamburg, Germany — [3]Department of Chemistry, Universität Hamburg, Germany — [4]The Hamburg Center for Ultrafast Imaging (CUI), Universität Hamburg,

In single-particle coherent x-ray diffraction experiments, diffraction patterns are recorded from individual sample particles. To overcome the inherently small signal-to-noise ratio, large numbers of identical particles need to be controlled and guided subsequently into the small focus of free-electron lasers (FELs). We establish particle control for example *via* electrostatic deflection or optical guiding in tractor beams [1], ultimately aiming at delivering one nanoparticle at a time into successive FEL shots.

[1] Eckerskorn et al., *Proc. SPIE* **9548**, 95480H1-95480H12, 2015

MO 20.5 Thu 11:30 S HS 002 Biologie

Detecting ultrafast hole dynamics in water using x-ray transient absorption — •Caroline Arnold[1,2,4], Ludger Inhester[1], Ralph Welsch[1,4], Linda Young[3], and Robin Santra[1,2,4] — [1]Deutsches Elektronensynchrotron DESY, Hamburg — [2]Universität Hamburg — [3]Argonne National Laboratory, USA — [4]Centre for Ultrafast Imaging, Hamburg

The dynamics that unfold in aqueous solutions on a molecular time scale are of direct relevance to biological and chemical processes. For example, radiation damage in biological tissues is caused by the photoionization of liquid water. The early steps of radiation damage can be understood by following the electron-hole pair dynamics with femtosecond time-resolution. While the hydrated electron has been addressed in experiments, the dynamics of the residual cation remains elusive. Today's XFEL sources allow to detect the hole by resonant x-ray absorption spectroscopy at the oxygen K-edge with femtosecond time resolution.

We present a theoretical, *ab initio* description of the hole dynamics in ionized water and the resulting x-ray absorption spectra. To this end, we consider excited-state molecular dynamics in liquid water following the removal of an electron from the valence band in a quantum-classical, QM/MM scheme including non-adiabatic transitions. We present first results on time-resolved x-ray absorption spectra in the first 100 femtoseconds following photoionization and discuss their use as a probe for hole dynamics.

MO 20.6 Thu 11:45 S HS 002 Biologie

X-ray emission spectroscopy using dispersive spectrometers at Synchrotron and X-ray FEL facilities — •Florian Otte[1,2], Christian Bressler[2], and Metin Tolan[1] — [1]Technische Universität Dortmund, Emil-Figge-Straße 50, 44227 Dortmund, Deutschland — [2]European XFEL GmbH, Holzkoppel 4, 22869 Schenefeld, Deutschland

Crystal spectrometers which enable the energy dispersive detection of X-ray fluorescence during irradiation with intense X-rays have found widespread distribution among X-ray facilities worldwide. Different designs and types exist, but all of them appeal through their ability to track electronic and magnetic properties of samples via characteristic features in X-ray emission signals during the experiment. Which electronic and magnetic properties are accessible specifically, is case and spectrometer dependent. We report on the use of an energy-dispersive von Hamos type spectrometer, which is being used at the FXE instrument at European XFEL GmbH on a regular basis in combination with additional complimentary experimental techniques such as X-ray diffraction for detection of K-edge emission lines on transition metal complexes. A smaller and highly mobile version of this spectrometer type has been successfully used at different beamlines (e.g. P01 at Petra III in Hamburg, Bl9 at DELTA in Dortmund). The highly flexible nature of this spectrometer type is rationalized with experimental results on transition metal complexes. Advantages and disadvantages in comparison with other available spectrometer types are discussed, with special consideration of applications at modern FELs.

MO 20.7 Thu 12:00 S HS 002 Biologie

Giant Enhancement of Molecular Ionization at High X-ray Intensity — •Ludger Inhester[1], Yajiang Hao[2], Sang-Kil Son[1], and Robin Santra[1,3] — [1]Center or Free-Electron Laser Science, DESY, Hamburg — [2]Department of Physics, University of Science and

Technology Beijing — [3]Department of Physics, Universität Hamburg

The ultraintense and ultrashort x-ray pulses provided by X-ray Free-Electron Lasers (XFELs) sequentially ionize molecular samples many times. We have developed an ab-initio electronic structure toolkit, XMOLECULE[1,2], that models this multiple ionization dynamics. Our calculations show that the rearrangement of charges between different parts of a molecule plays an important role for the ion yield distribution. In this context, we have recently discovered that under intense x-ray radiation the total charge yield of a molecule is enhanced compared to independent atoms[2,3].

We report here on new theoretical results for iodobenzene (C_6H_5I) that show an even stronger ionization enhancement than previously observed for iodomethane (CH_3I)[3]. This finding emphasizes the relevance of the charge-rearrangement-enhanced X-ray ionization of molecules (CREXIM) for the radiation damage in experiments with tightly focused XFEL beams.

[1] Struct. Dyn. 2, 041707 (2015). [2] Phys. Rev. A 94, 023422 (2016) [3] Nature 546, 129-132 (2017)

MO 20.8 Thu 12:15 S HS 002 Biologie

The Auger effect in dispersing and absorbing environments — •Janine Franz[1], Stefan Yoshi Buhmann[1,2], and Robert Bennett[1,2] — [1]Institute of Physics, University of Freiburg, Germany — [2]Freiburg Institute for Advanced Studies (FRIAS), Germany

The Auger effect is the radiationless decay of an inner-shell ionised atom. In this process, the atom relaxes by filling the inner vacancy with an outer shell electron, but instead of releasing the excess energy in form of a photon (spontaneous decay) the energy is reabsorbed by another electron belonging to the same atom. This effect finds many applications: for example in Auger electron spectroscopy, it is used to study material properties of surfaces.

It is well established that dielectric environments can have a significant impact on spontaneous decay (Purcell effect) [1] as well as interatomic energy transfer rates [2]. We present a general expression for the intra-atomic Auger process in the presence of dielectric environments that can be used both as a new starting point for ab initio quantum chemistry, or within the quantum-optical formalism of macroscopic quantum electrodynamics in order to circumvent complex numerics. Within our description, the decay rate can be given in analytical form for some simple environments. We compare Auger decay with a competing process known as interatomic Coulombic decay, focussing on their behaviour in the presence of surfaces.

[1] E. M. Purcell, Proc. Am. Phys. Soc. 69, 674 (1946).

[2] J. L. Hemmerich, R. Bennett and S. Y. Buhmann, Nature Commun. 9, 2934 (2018).