A 22: Atomic Clusters (joint session A/MO)

Time: Thursday 11:00–13:00 Location: F107

Invited Talk A 22.1 Thu 11:00 F107

Efficient and accurate simulation of wide-angle single-shot scattering — •Paul Tuemmler, Björn Kruse, Christian Peltz, and Thomas Fennel — Institute for Physics, University of Rostock, Albert-Einstein-Str. 23-24, D-18059 Rostock, Germany

In recent years coherent diffractive imaging has been established as a powerful method for the structural investigation of unsupported nanoparticles. A large number of studies have been successfully performed in the small angle regime, where the recorded scattering image is directly connected to the target's density projection along the optical axis. An established technique to invert the scattering image is the well-known phase retrieval algorithm. Single-shot 3d information only becomes available when scattering signal can be recorded at wide scattering angles, which typically requires wavelengths of several object diameters. However, in this scattering regime a direct inversion via phase retrieval is no longer possible and iterative forward fitting schemes have to applied. These schemes require many iterations and therefore heavily rely on an efficient method to calculate scattering images. Unfortunately, optical parameters in the long wavelength regime are typically quite far from vacuum parameters, such that absorption and multiple scattering effects become important. So far, available methods either lack the necessary accuracy (e.g. MSFT methods) or the numerical efficiency (e.g. FDTD).

Here we present a rigorous split step method that retains the efficiency of multislice methods, while yielding accuracy comparable to Mie and FDTD methods.

A 22.2 Thu 11:30 F107

3D Femtosecond Snapshots of Silver Nanoclusters — •Alessandro Colombo for the FLASH-SilverClusters-Collaboration — Laboratory for Solid State Physics, ETH Zurich, 8093 Zurich, Switzerland

Thanks to X-ray Free-Electron Lasers, Coherent Diffraction Imaging (CDI) allows femtosecond snapshots of matter at the nanoscale. When the diffracted light is recorded up to a sufficiently wide scattering angle, a single two-dimensional diffraction pattern carries 3D structural information on the sample. However, the non-trivial mathematical link between the sample's 3D shape and the 2D diffraction pattern renders 3D single-shot CDI a scientific challenge. Here we present a reconstruction method [1] that unveils the intriguing three-dimensional architectures of free-flying silver nanoclusters, retrieved from single wide-angle scattering images acquired at the soft X-ray Free-Electron Laser FLASH in Hamburg. The retrieved shapes of the silver clusters show satisfactory reliability and consistency, also revealing new structural motifs. Thanks to its great versatility, the method is then further extended to nanocrystals agglomerates, allowing for the first time a direct 3D insight into their growth process and surprising structures. This work represents a strong proof of concept for this imaging approach, raising the bar of the capabilities of 3D coherent diffraction imaging from single shot.

[1] Colombo, A. , et al. arXiv:2208.04044 (2022).

A 22.3 Thu 11:45 F107

Quenching of photon emission in heterogeneous noble gas clusters — •Lutz Marder, Catmarna Küstner-Wetekam, Nils Kiefer, Dana Bloss, André Knie, Arno Ehresmann, and Andreas Hans — Institut für Physik und CINSaT, Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany

Noble gas clusters represent prototype systems suited for the investigation of fundamental atomic and molecular processes. The Van-der-Waals bonds enable new relaxation pathways not available in isolated systems. Many of these have been studied during the recent years, often using coincidence measurement techniques.

We present our state-of-the-art experiment where both electrons and photons were detected in coincidence, which allows for investigation of multi-particle decay pathways after ionization with synchrotron radiation. The results show that the addition of a heavier noble gas to clusters of a lighter noble gas strongly alters the emission by the opening of faster ionizing decay channels compared to the radiative decay.

A 22.4 Thu 12:00 F107

Electron-Photon Coincidence Measurements at Synchrotron Facilities with Arbitrary Filling Pattern — •Johannes Viehmann, Andreas Hans, Christian Ozga, and Arno Ehresmann — Institut für Physik und CINSaT, Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany

Coincidence measurements are an important experimental tool in atomic or molecular physics. Our group has used electron-photon coincidence measurements to investigate rare gas clusters after synchrotron irradiation. The clusters exhibit a plethora of local and non-local electronic relaxation processes after core hole excitation. Most of these pathways produce free electrons and/ or photons. In order to distinguish signals of certain pathways from the general background, coincidence measurements are very useful.

So far, the combination of coincidence techniques with synchrotron radiation has mainly been restricted to the single bunch operation mode of the synchrotron facility due to difficulties in data acquisition. Here, we present a solution to combine coincidence measurements with multi-bunch operation modes and an example of using such technique to study rare gas clusters.

A 22.5 Thu 12:15 F107

Quantum nanofriction in trapped ion chains with a topological defect — •Lars Timm[1], Luca A. Rüffert[2], Hendrik Weimer[1,3], Luis Santos[1], and Tanja E. Mehlstäubler[2,4] — [1]Institut für Theoretische Physik, Appelstr. 2, 30167 Hannover — [2]Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig — [3]Institut für Theoretische Physik, Hardenbergstr. 36, 10623 Berlin — [4]Institut für Quantenoptik, Welfengarten 1, 30167 Hannover

After an introduction into the fundamental properties of the Frenkel-Kontorova model, one of the paradigmatic models of nanofriction, I will present the observation of a sliding to pinned transition with the help of a topological defect inside a two-dimensional self-assembled ion crystal. Subsequently, I shortly introduce one major consequence of this so-called Aubry transition, i.e. the localization of energy in the pinned phase of the defect. In the main part of my talk I discuss the quantized version of the Frenkel-Kontorova model and the consequences for the Aubry transition inside an ion crystal. As for that matter, we make use of a simple single particle formalism treating the defect as a quasiparticle, which captures the important dynamics of the defect close to the Aubry transition. This convenient approach gives access to its quantum properties revealing its quantum tunneling on a micron length-scale in a range of trap configurations and lets us identify a transition into a quasi-classical regime away from the transition point. Lastly, we give estimates for the temperature requirements and strategies to observe these effects in an experiment.

A 22.6 Thu 12:30 F107

Experimental studies on Interatomic Coulombic Decay after inner-shell ionization of heterogeneous rare gas clusters — •Catmarna Küstner-Wetekam[1], Lutz Marder[1], Dana Bloss[1], Nils Kiefer[1], Uwe Hergenhahn[2], Arno Ehresmann[1], Přemysl Kolorenč[3], and Andreas Hans[1] — [1]Institut für Physik und CINSaT, Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany — [3]Institute of Theoretical Physics, Charles University, V Holesovickach 2, 180 00 Prague, Czech Republic

Non-local decay mechanisms play an important role in the relaxation of electronic vacancies in dense media such as biological samples. To explore these mechanisms in a less complex environment, rare gas clusters can be used as a prototype system for experiments. The use of multi-coincidence spectroscopy enables the detection of core-level Interatomic Coulombic Decay (ICD), which is a comparatively weak process in relation to the local Auger decay followed by Radiative Charge Transfer (RCT). Here, we present the observation of changes in ICD efficiency when going from homogeneous Ar and Kr clusters to heterogeneous ArKr clusters and thereby introducing a different environment to the excited atom in the respective cluster.

A 22.7 Thu 12:45 F107

Electron-photon-coincidence investigations on neighbor induced photoelectron recapture in argon clusters — •Nils Kiefer, Carolin Honisch, Catmarna Küstner-Wetekam, Niklas Golchert, Arno Ehresmann, and Andreas Hans — 1Institute of Physics, University of Kassel, Kassel, Germany

Noble gas clusters are an ideal prototype system for fundamental research on atomic and molecular processes. The Van-der-Waals-bound atoms create an environment, which enables further decay pathways and scattering effects. These have been studied already with high resolution electron spectroscopy and multi-electron-coincidence spectroscopy. With use of a state-of-the-art experimental set-up, which allows coincident electron and photon detection, radiative and electronic processes after excitation of clusters with synchrotron radiation can be directly observed. Here, we present the results of electron-photon-coincidence measurements of a recent experiment on argon clusters. Here a slow photoelectron after 2p ionization is expected to be scattered on neighboring atoms in a "Bremsstrahlung"-like process. Thus, the scatted electron can be recaptured to the Ion and further decay in a resonant Auger-like process.