A 25: Poster – Cluster and Nanoparticles (joint session MO/A)

Time: Wednesday 17:00–19:00 Location: Philo 1. OG

A 25.1 Wed 17:00 Philo 1. OG

Penning ionization and direct photoionization of Mg and Na doped in helium nanodroplets — •Rajni Rajni[1], Narcis-Silviu Blaj[1], Asbjorn Ornemark Lagdsmand[1], Marcel Mudrich[1], Ltaief L. Ben[2], Niklas Scheel[2], and Henrik Pedersen[2] — [1]Institute of Physics, University of Kassel, D-34132 Kassel, Germany — [2]Department of Physics and Astronomy, Aarhus University, 8000 Aarhus C, Denmark

We investigate the direct photoionization and Penning ionization of alkali (Na) and alkaline-earth metals (Mg) embedded in superfluid helium nanodroplets under irradiation with extreme ultraviolet (XUV) synchrotron radiation that resonantly excites the He droplets. Helium is a well-suited system for studying indirect ionization processes due to the simple electronic structure of He, well-resolved electron spectra, weak interaction with embedded species, efficient pick up of molecules and controlled aggregation inside the nanodroplets. We measured spectra of all electrons and of electrons recorded in coincidence with specific ions for He nanodroplets doped with Mg and Na atoms. For Na, the Penning ionization electron spectrum is well resolved but shifted due to attractive interaction of the Na atom and the excited He^* (short-range interatomic Coulombic decay). For Mg, we observe a pronounced enhancement of shake-up ionization where an excited Mg^+ ion is produced in the Penning process. Shake-up states are only weakly present in direct photoelectron spectra.

A 25.2 Wed 17:00 Philo 1. OG

Tracking Microhydration of Salt Molecules in Helium Nanodroplets and Commissioning a New Nanoparticle Injector System — •Mikkel Mortensen[1], Niklas Scheel[2], Marcel Mudrich[2], Henrik B. Pedersen[2], and Ltaief B. Ltaief[2] — [1]Institute of Physics, Kassel University — [2]Department of Physics and Astronomy, Aarhus University

The solvation of NaCl molecules in water, is an important process in chemistry. However, microscopic structures and energetics of the hydration complexes remain to be investigated. A recent study has quantified the number of water molecules needed, to form a complete hydration shell around NaCl in helium nanodroplets using Penning Ionization Electron Spectroscopy (PIES)[1]. Building upon this study, we investigate the microhydration dynamics of KBr, NaBr, and NaCl under comparable conditions at the XUV synchrotron light source, ASTRID 2. Our PIES measurements aim to investigate how different ionic constituents affect hydration structure and stability.

Furthermore, we are commissioning a new nanoparticle injector based on an aerodynamic lens system for producing aerosol beams of salt nanoparticles. This development will allow us to do experiments on salt hydration and electron spectroscopy in aerosols, including interactions with XUV radiation at ASTRID.

[1] L. B. Ltaief et al., submitted (2025), arXiv.2510.22000

A 25.3 Wed 17:00 Philo 1. OG

XUV photoionization of Microhydrated Biomolecules — •Niklas Scheel[1], Ltaief Ben Ltaief[1], Henrik B. Pedersen[1], and Marcel C. Mudrich[2] — [1]Department of Physics and Astronomy, Aarhus University, 8000 Aarhus C, Denmark — [2]Institute of Physics, University of Kassel, 34132 Kassel, Germany

Microhydrated biomolecules serve as valuable model systems for studying radiophysical processes in biologically relevant complexes, offering insights into the mechanisms of radiation damage in biological tissue. In this work, we present photoelectron-photoion coincidence (PEPICO) spectra of XUV-irradiated microhydrated thymine and uracil clusters, measured using the electron ion double-imaging endstation XENIA[1] at the ASTRID2 synchrotron.

We investigate outer-valence photoionization, confirming that attached water molecules stabilize the DNA bases against fragmentation[2] by acting as an efficient heat bath. At the same time, the data reveal a charge-transfer mechanism from the DNA base to the water: a charge hole initially created on a water moiety ultimately localizes on the DNA base.

Finally, we will present PEPICO spectra recorded at higher photon energies. These measurements probe inner-valence photoionization, where double ionization becomes accessible, leading to pronounced fragmentation and involving Intermolecular Coulombic Decay (ICD) as an efficient relaxation pathway.

[1] B. Bastian et al., Rev. Sci. Instrum., 2022, 93, 075110
[2] J. D. Asmussen et al., PCCP, 2023, 25, 24819-24828

A 25.4 Wed 17:00 Philo 1. OG

Novel Apparatus for Synchrotron X-ray Photoelectron Spectroscopy of Size-Selected Gas-Phase Clusters — Lotar Kurti, Phillip Stöcks, Fabian Bär, Lukas Weise, and •Bernd v. Issendorff — Physikalisches Institut, Universität Freiburg, Freiburg, Germany

A newly developed apparatus enables X-ray photoelectron spectroscopy on mass-selected cluster ions at synchrotrons. The heart of this system is a liquid nitrogen-cooled linear Paul trap, where stored cluster ions interact with synchrotron radiation. The emitted electrons are guided by a specially designed magnetic field into a Hemispherical Energy Analyzer, where the photoelectron spectra are recorded. Clusters are produced in a magnetron cluster source, mass-selected using a quadrupole mass spectrometer, and then introduced into the linear ion trap. This setup will allow for element-specific binding energy measurements of core levels and hence detailed insights into the chemical bonding of pure and mixed metal and semiconductor clusters. In this contribution, we present the current status of the new apparatus and some initial commissioning results.

A 25.5 Wed 17:00 Philo 1. OG

Single-shot imaging and modeling of individual water nanodroplets with an intense extreme ultraviolet laboratory source — •Lea Schüpke[1], José Gómez Torres[1], Linos Hecht[1], Frederic Ussling[1], Alessandro Colombo[1], Katharina Kolatzki[1], Indrani Dey[1], Changji Pan[1], Isabelle Bollier[1], Constantin Koch[1], Ehsan Hassanpour[1], Yves Acremann[1], Mario Sauppe[1], Björn Senfftleben[1], Hanchao Tang[2], Arnab Choudhury[2], Bruce Yoder[2], Ruth Signorell[2], and Daniela Rupp[1] — [1]ETH Zürich, DPHYS — [2]ETH Zürich, DCHAB

Our unique high-intensity extreme ultraviolet (XUV) beamline enables flash-imaging of individual free-flying nanoparticles in a lab environment, thus avoiding the severe access limitations of large-scale facilities. We have started to investigate the freezing dynamics of supercooled water droplets between few 100 nm and few μm in diameter. This size range is mostly unexplored due to the lack of suitable imaging methods. In this work, Mie-simulations are discussed that allow to understand subtle changes in the diffracted light distribution caused by aggregate state changes and droplet sizes.

A 25.6 Wed 17:00 Philo 1. OG

Detailed investigation of unexpected photoelectron spectra via angle-resolved spectroscopy of noble metal clusters — •Steve Takouan Tchounga, Lukas Weise, and Bernd von Issendorff — Physikalisches Institut, Albert-Ludwigs-Universität, Freiburg im Breisgau, Germany

Angle-resolved spectroscopy provides an important test of the theoretical description of clusters since these spectra carry more information than the bare electron binding energies. Specifically, the anisotropy of photoelectron spectra depends on the angular momentum state [1, 2].

The presented analysis utilizes the additional information from angle-resolved spectroscopy to gain a better understanding of the electronic structure of the cluster. For Au_{33}^- an electronic shell closing is expected, leading to the opening of a new shell for Au_{34}^-. The angular momentum character of this new shell is not in accordance with a simple shell model.

The Issendorff's model [2] was utilized to gain insight into the character of the orbital involved in the premature shell closing of Cu_{91}^-. The β parameter curve for this orbital exhibits a clear f-type character, indicating a premature filling of the next shell. The reason for this premature shell closing cannot be identified by this result, but the additional information on the character should help in finding the reason.

[1] Bartels et al., Science, 323, 5919 (2009). [2] Piechaczek et al., Phys. Rev. Lett. 126, 233201 (2021). [3] Bartels et al., Phys. Rev. A 88, 043202 (2013).

A 25.7 Wed 17:00 Philo 1. OG

HHG Coherent Diffraction Imaging of water nanodroplets — •José Gómez Torres[1], David Biner[1], Constantin Koch[1], Indrani Dey[1], Frederic Ussling[1], Linos Hecht[1], Yves Acremann[1], Isabelle Bollier[1], Alessandro Colombo[1], Ehsan Hassanpour[1], Katharina Kolatzki[1], Changji Pan[1], Mario Sauppe[1], Lea Schüpke[1], Björn Senfftleben[1], Hanchao Tang[2], Arnab Choudhury[2], Bruce Yoder[2], Ruth Signorell[2], and Daniela Rupp[1] — [1]D-PHYS, ETH Zürich — [2]D-CHAB, ETH Zürich

Homogeneous freezing of free-flying water droplets of 1μm radius and smaller remains largely not understood due to the resolution limit of optical imaging. A change in freezing dynamics is expected in respect to droplets over 10μm [1], but no experimental study has confirmed this. Ice nucleation rates are also uncertain, with previous studies not agreeing on a compatible value [2]. Using intense XUV pulses from our tabletop HHG source, we obtain single-shot diffraction patterns of individual nanodroplets injected using an aerodynamic lens, to investigate possible morphology changes related to freezing. Here, the first results from this measurement are shown.

[1] Buttersack, T et al., JPCB 120 (2016): 504
[2] Amaya, A. and Wyslouzil, B., J. Chem. Phys. 148.8 (2018)

A 25.8 Wed 17:00 Philo 1. OG

High-Resolution Electron Spectroscopy of Doped Helium Nanodroplets with a Hemispherical Electron Analyzer — •Narcis-Silviu Blaj[1], Niklas Scheel[2], Rajni Rajni[1], Asbjørn Laegdsmand[1], Aleksandar Milosavljevic[3], John Bozek[3], and Marcel Mudrich[1,2] — [1]Institute of Physics, University of Kassel, D-34132 Kassel, Germany — [2]Department of Physics and Astronomy, Aarhus University, 8000 Aarhus C, Denmark — [3]Soleil Synchrotron, 91190 Saint-Aubin, France

Helium nanodroplets (HNDs) have mostly been used as inert cryomatrices for spectroscopy of embedded molecules and clusters.

We performed the first high-resolution X-ray photoelectron spectroscopy (XPS) measurements of pure and doped helium nanodroplets at the PLEIADES beamline of SOLEIL Synchrotron using a hemispherical electron analyzer (HEA). In particular, we explored droplets doped with krypton and argon. The formation of Ar and Kr clusters was identified through the appearance of additional low-binding-energy features accompanying the spin-orbit doublets of the atomic photolines (Kr 3d and Ar 2p), in agreement with earlier observations of photoemission from pure small Kr and Ar clusters. We systematically recorded XPS spectra as a function of photon energy, droplet size, and doping level, allowing us to study the evolution of spectral line shifts and intensity ratios between atomic and cluster-specific components.

In addition, we plan further experiments at SOLEIL as well as at other synchrotron facilities to explore a wider range of photon energies, dopants, and cluster conditions.