

A 20: Poster – Atomic Clusters

Time: Wednesday 17:00–19:00

Location: Tent

A 20.1 Wed 17:00 Tent

Ab-initio study of the transition pathways for single and double interstitial solute (H, N, O, H-H, N-N and O-O) within bcc refractory metals (Mo and Nb) — ●HENRY ELORM QUARSHIE¹, HENRY MARTIN^{1,2}, ERIC KWABENA KYEH ABAVARE¹, and ALESSANDRA CONTINENZA³ — ¹Department of Physics, Kwame Nkrumah University of Science and Technology, Kumasi, Ghana — ²Center for Scientific and Technical Computing, National Institute for Mathematical Sciences, Kumasi, Ghana — ³Dipartimento di Scienze Fisiche e Chimiche, Università degli studi dell'Aquila, L'Aquila, Italy

This study investigates the diffusion pathways of single (H, N, O) and double (H-H, N-N, O-O) interstitial solutes in bcc molybdenum (Mo) and niobium (Nb). The aim is to understand how atmospheric gases rich in H, O, and N interact with metals. Ab-initio calculations were performed to determine equilibrium parameters, dissolution energetics, charge transfer, minimum energy paths, and diffusion coefficients. Single solutes exhibited site preferences, with H favouring tetrahedral sites (t-sites), N preferring octahedral sites (o-sites), and O showing material-dependent behaviour linked to the deformation behaviour of Mo and Nb. Diffusion energy barriers ranged from 0.10 eV to 1.34 eV, aligning with experimental results. The study also examined double interstitial solutes and found that a second solute significantly reduces activation energies, enhancing diffusion in most configurations, except for Mo-O. This effect is due to the second solute's influence on local lattice relaxations and interstitial interactions. The work further reveals that a second solute can alter the preferred diffusion pathways.

A 20.2 Wed 17:00 Tent

Design and Analysis of Metal-Organic Frameworks for Enhanced Water Purification — ●ABDUL RAHMAN JUNIOR MOHAMMED¹ and HENRY MARTIN^{1,2} — ¹Department of Physics, Kwame Nkrumah University of Science and Technology — ²Center of scientific and Technical Computing, National Institute for Mathematical Sciences Kumasi Ghana

This work is dedicated to the computational design and analysis of Metal-Organic Frameworks with the purpose of improving water purification processes. Increased concern about water quality, considering a wide range of contaminants, calls for urgent action toward efficient and sustainable methods of purification. Advanced computational capabilities involved in this study include molecular dynamics, density functional theory, and machine learning techniques employed to optimize structural properties and performance of selected MOFs. The synthesis and characterization of new MOFs, such as UiO-66-NH₂, possessing very good adsorption properties for pollutants of various origins, including heavy metals, dyes, and VOCs, are among the focuses of this work. We investigate how the variation of temperature, pressure, and interaction solvent through the simulation of different conditions of synthesis can impact stability and effectiveness. It follows that the tailored design of MOFs significantly improves their adsorptive efficiency and stability in an aqueous environment. Moreover, the embedding of ML techniques will allow the predictive modeling of MOF performances to enable them to identify crucial features of MOF structures responsible for enhancement in the purification capability.

A 20.3 Wed 17:00 Tent

Reconstructing the anisotropic expansion of a laser driven nanoplasma — ●PAUL TUEMMLER¹, FELIX GERKE², CHRISTIAN PELTZ¹, HENDRIK TACKENBERG¹, BJÖRN KRUSE¹, BERNHARD WASSERMANN², THOMAS FENNEL¹, and ECKART RÜHL² — ¹University of Rostock, D-18059 Rostock, Germany — ²Freie Universität Berlin, D-14195 Berlin, Germany

Coherent diffractive imaging (CDI) at X-ray free-electron lasers (FELs) has evolved into a well-established method for the structural investigation of unsupported nanoparticles. This inherently static method can be readily adopted to time-dependent studies by incorporating a

second pulse in a pump-probe scheme.

In a recent experiment at LCLS, we utilized this method to study the fundamental process of free plasma expansion into vacuum using the example of laser-pumped SiO₂ nanospheres. The resulting plasma expansion rapidly and isotropically softens the initial surface density step. This, in turn, increases the radial decay of the scattering signal eventually precluding meaningful measurements due to a diminishing signal-to-noise ratio within only a few hundred femtoseconds [1].

Here, we present the results of a follow-up experiment at the European XFEL where we revisited SiO₂ as a target, but operated in a weaker excitation regime. This approach allowed us to record images over far longer timescales and revealed a strong anisotropic expansion dynamic, as predicted by theory [2].

[1] C. Peltz *et al.*, New J. Phys. **24**, 043024 (2022).

[2] C. Peltz *et al.*, Phys. Rev. Lett. **113**, 133401 (2014).

A 20.4 Wed 17:00 Tent

Towards experimental studies of interatomic Coulombic electron capture (ICEC) — ●ANDRE MIRANDA ROCCO GIRALDI and ALEXANDER DORN — Max Planck Institut für Kernphysik, Saupfercheckweg 1, 69117 Heidelberg

This work targets the experimental detection of an environment assisted atomic decay mechanism [1], referred to in literature as excitation transfer ionization. The process constitutes the resonant excitation of a neon atom in a cluster by electron impact to a 2p5 3s or 2p5 3p state (excitation energy on the range of 16 to 19 eV), and subsequent deexcitation by ionizing a neighboring Ar atom (ionization potential of 15.8 eV). This reaction has been evidenced by laser-induced excitation of neon, but remains to be detected by means of an electron beam as the excitation mechanism. The confirmation of such process could provide insight into the role of the atomic environment on energy transfer and help gather information about ICD- and ICEC-like reactions. Presently we are adapting an electron and ion momentum spectrometer (reaction microscope) and are optimizing the formation of neon-argon dimers or bigger mixed clusters which requires the determination of the optimal conditions (nozzle temperature, gas pressure and mixing ratio). First results will be presented.

[1] Gokhberg, K. and Cederbaum, L.S. (2009). Environment assisted electron capture. Journal of Physics B: Atomic, Molecular and Optical Physics.

A 20.5 Wed 17:00 Tent

Disentangling hard x-ray induced relaxation mechanisms in atomic clusters using multiparticle coincidence spectroscopy — ●NIKLAS GOLCHERT¹, YUSAKU TERAOKA¹, EMILIA HEIKURA¹, MADHUSREE ROY-CHOWDHURY¹, MINNA PATANEN², OKSANA TRAVNIKOVA³, ARNO EHRESMANN¹, and ANDREAS HANS¹ — ¹Institut für Physik und CINsAT, Universität Kassel, Heinrich-Plett Str. 40, 34132 Kassel, Germany — ²Nano and Molecular Systems Research Unit, Faculty of Science, University of Oulu, PO Box 3000, Oulu 90014, Finland — ³Sorbonne Université, CNRS, UMR 7614, Laboratoire de Chimie Physique-Matière et Rayonnement, F-75005 Paris, France

Understanding the response of dense media to high-energetic photons, explicitly in the context of biological radiation damage, is essential for the targeted use of radiation therapy and the fundamental knowledge on electron correlations alike. Noble gas clusters often serve as prototype systems for fundamental research on dense media. For the analysis of the involved processes, electron spectroscopy is a sensitive tool, which is, however, challenged by the increasing number of possible mechanisms that accompany large amounts of stored energy. We employed multielectron-photon coincidence spectroscopy to investigate the behavior of prototypical argon clusters upon deep inner-shell ionization with hard x-rays to disentangle the consecutive relaxation mechanisms that may or may not involve neighboring constituents of a conglomerate of particles.