A 35: Cluster and Nanoparticles (joint session MO/A)

Time: Thursday 15:15–16:45 Location: P 105

Invited Talk A 35.1 Thu 15:15 P 105

Charge and electronics in molecule activation by transition metal clusters — •Gereon Niedner-Schatteburg, Nils Wolfgramm, and Christoph van Wüllen — Fachbereich Chemie, RPTU Kaiserslautern-Landau, 67663 Kaiserslautern

Isolated transition metal clusters (TMCs) serve as well established proxys for the characterization of elementary reaction steps and intermediates. The charge states of such clusters are subject of debate ever since. We have developed and applied a cryo trapping technique [1] that allowed us to characterize size selected TMCs and their adsorbates for their kinetic and spectroscopic properties [2-8]. Electronic characterization arose through novel X-ray techniques which we have brought to gas TMCs [9]. We have recently started a systematic quantum chemical survey of electronic effects along the N_2 activating reaction pathways of some selected clusters [10], and the conceptual findings of this survey shall be presented and discussed. [1] 10.1016/B978-0-12-814013-0.00019-3; [3] 10.1039/c5cp00047e; [2] 10.1021/acs.jpcc.6b12167; 10.1063/1.4997403 ; 10.1063/1.4997407; [5] 10.1007/s11244-017-0865-2 ; 10.1080/00268976.2021.1953172; [4] 10.1063/5.0064965 ; 10.1063/5.0064966; [5] 10.1063/5.0075289 ; 10.1063/5.0075286; [7] 10.1039/D0CP06208A ; 10.1063/5.0157218 ; 10.1063/5.0157217; [8] 10.1021/acs.jpclett.8b00093 ; submitted to Helv. Chim. Act. (2025); [9] 10.1103/PhysRevLett.107.233401 ; 10.1039/C5CP01923K ; 10.1063/1.4929482; [10] to be published

A 35.2 Thu 15:45 P 105

Size characterization of doped rare-gas clusters utilizing rotational coherence spectroscopy — •Arne Morlok[1], Grzegorz Kowzan[2], Ulrich Bangert[1], Yilin Li[1], Frank Stienkemeier[1], and Lukas Bruder[1] — [1]University of Freiburg, Institute of Physics, Hermann-Herder-Straße 3, 79104 Freiburg, Germany — [2]Nicolaus Copernicus University in Torun, Institute of Physics, Grudziadzka 5, 87-100 Torun, Poland

A prominent challenge in spectroscopy is to investigate individual molecules or their aggregates in a well-defined and controlled environment. This goal can be accomplished with cluster-isolation spectroscopy, a technique in which molecules are isolated in or on the surface of rare-gas clusters. A complication of this technique is that the clusters, which are produced in a supersonic expansion, do not have a uniform size but follow a broad size distribution dependent on the expansion conditions. Although semi-empirical scaling laws based on the expansion parameters have been derived in order to predict the mean cluster size, results seem to underestimate the actual cluster size in comparison with experimentally determined size distributions. In this contribution, a novel spectroscopic approach is discussed to determine the mean cluster size of neutral rare-gas clusters. The technique is based on already known methods from rotational coherence spectroscopy. Results suggest a new scaling regime for the mean cluster size in the already established model in a certain parameter range.

A 35.3 Thu 16:00 P 105

Measuring the speed of interatomic Coulombic decay in helium nanodroplets — •Asbjørn Ørnemark Laegdsmand[1], Ltaief Ben Ltaief[2], Eva Klimesova[3], Keshav Sishodia[3], Martin Albrecht[3], and Marcel Mudrich[1] — [1]Institute of Physics, University of Kassel, 34132 Kassel, Germany — [2]Department of Physics and Astronomy, Aarhus University, 8000 Aarhus C, Denmark — [3]ELI Beamlines, The Extreme Light Infrastructure ERIC, Za Radnicí 835, 252 41 Dolní Břežany, Czech Republic

Helium nanodroplets are an interesting *test tube* for many types of interatomic reactions. In this work we have looked at both interatomic Coulombic decay (ICD) and laser-assisted electron scattering (LAES). We have measured the rate of ICD in lithium-doped helium nanodroplets by an EUV-pump NIR-probe scheme.

The nanodroplets are resonantly excited into the 1s 2p ^{1}P state with a 21.6 eV pump pulse and multi-photon ionized with an 1.56 eV probe pulse. ICD and LAES electrons are detected with in a magnetic bottle electron spectrometer. Arrival of the probe pulse ionizes most of the 1s 2p ^{1}P He, quenching the ICD process. Thus by varying the time delay between pump and probe we measure the speed of the ICD for different droplet sizes.

From the resulting electron spectra we distinguish several ionization pathways, such as ICD, LAES and above threshold ionization. We model the dynamics of the different pathways by rate equations and estimate their contribution to the total electron yield as a function of pump-probe delay time.

A 35.4 Thu 16:15 P 105

An optical laser blade setup for the detection of isolated nanoparticles — •Constantin Koch[1], José Gómez Torres[1], David Biner[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 Zurich — [2]D-CHAB, ETH Zurich

Coherent diffraction imaging (CDI) of free-flying water nanodroplets with our high-intensity extreme ultraviolet (XUV) beamline requires optimal overlap of droplet beam and micrometer-sized XUV focus. So far, this was difficult to achieve because of the small hitrates and large variability of the single-shot signals from XUV diffraction. We present the design, setup and comissioning of an optical laser blade, that makes nanoparticles in the interaction region directly visible and enables a quantitative characterization of the water source. A continuous-wave 450 nm laser is shaped into a thin horizontal laser sheet crossing the droplet beam. The scattered light is recorded with a CMOS camera adapted for vacuum compatibility. We observe clear signal from single droplets in the few hundred nm range and achieved a fast and reliable alignment procedure. The consistent signal also allowed us identify previously overlooked problems in the injector system and to obtain a three-dimensional density distribution of the droplet beam in our vacuum chamber.

A 35.5 Thu 16:30 P 105

Uptake of Ammonia onto Mixed Sodium Sulfate/Bisulfate Cluster Ions Studied in a Cryogenic Ion Trap — •Kevin Li, Yihui Yan, and Jozef Lengyel — School of Natural Sciences, Technical University of Munich, Garching, Germany

Understanding the earliest stages of atmospheric new particle formation (NPF) requires direct measurements on sub-nanometer molecular clusters, yet such studies remain experimentally challenging. To investigate this size range, we have developed a cryogenic ion trap mass spectrometer for kinetic studies with mass-selected cluster ions under multicollisional conditions. The instrument utilizes a ring-electrode ion trap, which enables stable confinement and allows for long reaction times of up to seconds. Therefore, the trap provides a powerful platform for investigating reaction pathways relevant to atmospheric aerosol formation.

In this study, we characterize the performance of the cryogenic ion trap and show its capabilities in a model study measuring uptake of gaseous ammonia onto mixed sodium sulfate and bisulfate ions. We further highlight that investigating mixed multicomponent clusters can reveal synergistic effects in NPF, where different components jointly enhance the uptake efficiency. In mixed sodium sulfate-bisulfate clusters, bisulfate units govern the number of uptaken ammonia molecules, whereas sulfate units control the reaction rate. With these experiments, we demonstrate the instrument's ability to investigate reaction pathways relevant to NPF.