

MO 7: Poster: Cluster

Time: Monday 16:00–18:00

Location: P1

MO 7.1 Mon 16:00 P1

Autoionization processes in homogeneous and heterogeneous clusters — ●TIBERIU ARION¹, MELANIE MUCKE¹, MARKO FÖRSTEL¹, HANS-PETER RUST¹, ALEXANDER M. BRADSHAW^{1,2}, and UWE HERGENHAHN¹ — ¹Max-Planck-Institut für Plasmaphysik, EURATOM Association, Garching, Germany — ²Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Experimental investigations of Interatomic/Intermolecular Coulombic Decay have gained considerable momentum in the last few years. We have investigated this novel autoionization process by electron and e^-, e^- coincidence spectroscopy, using a magnetic bottle spectrometer. We have revisited ICD in medium-sized homogeneous Ne clusters, and find a minimum kinetic energy of ICD of around 0.8 eV, different from earlier experiments on the Ne dimer. In heterogeneous clusters of Ne and Kr we have recorded an unusually high transition energy of about 10 eV. Here, the ICD process proceeds after Ne $2s$ photoionization, and leaves a final state with a Ne $2p^{-1}$ and a Kr $4p^{-1}$ vacancy. We have studied the dependence of the effect on photon energy, cluster composition and cluster size. Interestingly, the ICD electron energy increases slightly and grows a shoulder on going from 2% to 5% Kr in the co-expansion process, which we interpret in terms of surface vs. bulk effects. We have performed similar experiments on ArXe mixed clusters, where the ICD electron is expected to have a kinetic energy in the 0-2 eV range. Extending our earlier study on water clusters, we have also recently investigated ICD in water clusters as a function of the size of the cluster as well as of isotopic substitution.

MO 7.2 Mon 16:00 P1

Melting of size-selected, free water clusters — ●ADAM PIECHACZEK, CHRISTIAN HOCK, RAPHAEL KUHNEN, MARTIN SCHMIDT, and BERND V. ISSENDORFF — Fakultät für Mathematik und Physik, Universität Freiburg, Stefan-Meier Str.19, 79104 Freiburg

An experimental study on free, size-selected water clusters has been performed. Negatively charged water clusters are thermalized in a temperature controlled radio frequency multipole trap by collisions with helium buffer gas at a pressure of about 10^{-3} mbar, transferred into high vacuum, mass-selected, and photofragmented by a laser pulse (1064 nm). The recorded fragment mass spectra are sensitive to the inner energy of the thermalized clusters, which allows us to link temperature and energy and deduce caloric curves. The curves are bulk-like at low temperatures, demonstrating that the vibrational density of states of the clusters is similar to that of bulk ice. At particle-size specific temperatures, a sudden increase of the heat capacity occurs, which marks the onset of a gradual melting transition. Above the transition temperatures the caloric curves bend upwards and deviate significantly from that of the bulk. Recently the caloric curves have been measured for a wide range of cluster sizes. A strong size dependence of the melting temperature has been observed.

[1] C. Hock et al., Physical Review Letters **103**, 073401 (2009)

MO 7.3 Mon 16:00 P1

First evaluation of a new resolution enhancement method for the Magnetic Bottle Photoelectron Spectrometer (PES) — ●MORITZ WEIGT and BERND VON ISSENDORFF — Universität Freiburg, FMF, Stefan-Meier-Str. 21, 79106 Freiburg

We have developed a new method for improving the resolution of the magnetic bottle type photoelectron spectrometer. By applying a well defined time-variable voltage to a part of the flight tube, electrons of equal energy are time focused in the detector plane. This works for all energies in the relevant range (0 - 10 eV) without affecting linearity of the energy measurement. Simulations show that the new setup is theoretically capable of 1/1000 energy resolution. We will present first measurements evaluating the potential of the method under real conditions.

MO 7.4 Mon 16:00 P1

IR spectra of benzoic acid cation clusters with nonpolar ligands — ●MATTHIAS SCHMIES, ALEXANDER PATZER, and OTTO DOPFER — Optik und Atomare Physik, TU Berlin, Germany

IR spectra of clusters of the benzoic acid cation with Ar and molecular nitrogen are obtained by photodissociation of mass-selected complexes

in a tandem mass spectrometer. The IR spectra are analyzed by comparison with DFT calculations (M06-2X/aug-cc-pVTZ) and provide information about the interaction potential (ligand binding site and interaction energy) between this prototypical aromatic carbonic acid and a nonpolar environment. Interestingly, the ligands prefer binding to the aromatic ring rather than to the acidic functional group, demonstrating the importance of dispersion forces in this system. This is in contrast to complexes of other aromatic complexes with acidic OH groups, such as phenol, which show predominantly hydrogen bonding to Ar and molecular nitrogen.

MO 7.5 Mon 16:00 P1

Ultraviolet Photoluminescence of Ideal Nanodiamonds - Diamondoids — ●ROBERT RICHTER¹, DAVID WOLTER¹, LASSE LANDT¹, MATHIAS STAIGER¹, STEPHANIE WUTSCHIK¹, PETER R. SCHREINER², JEREMY E. DAHL³, ROBERT M. K. CARLSON³, CHRISTOPH BOSTEDT⁴, and THOMAS MÖLLER¹ — ¹Technische Universität, Berlin, Germany — ²Justus-Liebig-Universität, Gießen, Germany — ³Molecular Diamond Technologies, Richmond, USA — ⁴LCLS, Stanford, USA

Nanodiamonds, so called diamondoids are carbon clusters with perfect bulk diamond structure and complete hydrogen passivation. Diamondoids can be perfectly size-selected and isomer resolved even in their neutral state. This has made possible a variety of investigations on the size and shape dependence of their electronic structure and optical properties. We studied the photoluminescence of nanodiamonds and found intrinsic photoluminescence in the ultraviolet regime for various shapes and sizes of pristine hydrogen-passivated diamond clusters (diamondoids). The inclusion of high amounts of nitrogen into the nanodiamonds crystal lattice, using the example of urotropine (hexamethylenetetramine), is found to quench the luminescence. [1] L.Landt, D.Wolter et al. Phys. Rev. B **80**, 205323 (2009)

MO 7.6 Mon 16:00 P1

IR Spectroscopy of Microhydrated Nitrate Ions: Influence of Solvent and Temperature on Structure — ●NADJA HEINE¹, TORSTEN WENDE¹, LING JIANG¹, RISSHU BERGMANN¹, KENNETH D. JORDAN², GERARD MEIJER¹, and KNUT R. ASMIS¹ — ¹Fritz-Haber-Institut der MPG, Berlin — ²University of Pittsburgh, USA

Nitrate ions, NO_3^- , play an important role in atmospheric chemistry, nuclear waste treatment and biochemical processes. For instance, NO_3^- is one of the most abundant ions in the troposphere and can be formed by rapid acid dissolution of nitric acid in aerosol particles. For a molecular-level understanding of such processes the characterization of their hydration behavior is crucial. Here, we exploit infrared photodissociation (IRPD) spectroscopy for obtaining structural information on the nitrate-solvent complexes using a time-of-flight tandem mass spectrometer combined with an ion trap. We present IRPD spectra of $\text{NO}_3^-(\text{H}_2\text{O})_{1-4}$ as well as selected deuterated analogs, measured in the OH-/OD-stretching region (2400 - 3800 cm^{-1}) and at ion trap temperatures between 10 to 300 K. The present measurements complement our previous IRPD study of hydrated nitrate ions in the fingerprint region. The IRPD spectra of $\text{NO}_3^-(\text{H}_2\text{O})$ and $\text{NO}_3^-(\text{D}_2\text{O})$ in the OH-stretch region confirm a bidentate binding motif at low temperatures. At higher temperatures an additional isomer with just a single hydrogen bond is observed. The complex sequence in the OH-stretching region suggest a strong anharmonic coupling between the OH-stretch modes and low-frequency modes, which is modeled using vibrational CI calculations on a 15-dimensional potential energy surface.

MO 7.7 Mon 16:00 P1

Angular distribution of $(\text{CO}_2)_n$ scattered off a Si(111)/SiO₂ surface — WOLFGANG CHRISTEN, ●TIM KRAUSE, and KLAUS RADE-MANN — Humboldt-Universität zu Berlin, Institut für Chemie, Brook-Taylor-Str. 2, 12489 Berlin

Interest in cluster-surface collisions has mostly focused on rare gas and metal clusters, and precious little is known about the surface interaction of van der Waals bound molecular clusters at moderate energies.

Employing a specialized setup¹ for the experimental investigation of chemical processes occurring between neutral van der Waals bound clusters and a solid surface in the hyperthermal energy range we re-

port first results on the angular distribution of a pulsed supersonic beam of pure CO₂ scattered off a Si(111)/SiO₂ surface under ultrahigh vacuum conditions. Scattered particles are detected using time resolved mass spectrometry. A translator stage provides the possibility to sample either the incoming beam (target surface retracted) or to determine the angular and velocity distribution of scattered particles. Angular information is obtained by rotating the target surface, $\Theta_{\text{scatter}} = \Theta_{\text{in}} + \Theta_{\text{out}}$.

¹W. Christen, K. Rademann, *Rev. Sci. Instrum.* **77**, 015109, 2006.

MO 7.8 Mon 16:00 P1

Gas Phase Vibrational Spectroscopy of Cerium Oxide Cluster Cations — •TORSTEN WENDE¹, ASBJÖRN BUROW², PIETERJAN CLAES³, MAREK SIERKA², GERARD MEIJER¹, PETER LIEVENS³, JOACHIM SAUER², and KNUT R. ASMIS¹ — ¹Fritz-Haber-Institut d. MPG, Berlin — ²Humboldt Universität Berlin — ³K.U. Leuven, Belgium

Cerium oxide is one of the most reactive rare earth metal oxides and play an important role in many catalytic applications. A key property of ceria (CeO₂) is the ability to release, store and transport oxygen ions which relies on the accommodation of electrons in localized f-orbitals. The theoretical description of localized Ce-4f states is a demanding task. Infrared photodissociation spectroscopy (IRPDS) of gas phase clusters can provide reliable data to test different DFT approaches.

Ce-containing clusters have not been spectroscopically studied in the gas phase yet. Here, we employ IRPDS combined with DFT calculations to characterize the structure of cationic cerium oxide clusters. Vibrational predissociation spectra of rare-gas tagged (CeO₂)_mCeO⁺ ($m=0,1,\dots,4$) and Ce_nO_{2n-2}⁺ ($n=2,3$) clusters are measured in the 400-1000 cm⁻¹ region. Structures containing a terminal Ce=O bond show a characteristic absorption band between 800-900 cm⁻¹. Larger clusters have common geometrical building units similar to bulk ceria leading to intense signals around 500 and 650 cm⁻¹. The results emphasize the importance of global optimization schemes and show that B3LYP does not always predict the correct global minimum structure.

MO 7.9 Mon 16:00 P1

Field enhancement around gold nanoparticles — •MADJET MO-

HAMED EL-AMINE — Free University Berlin, Institute of Chemistry and Biochemistry, Fabbeckstr. 36a, D-14195 Berlin

Using Time-dependent local density approximation, we investigated the optical properties of small gold nanoparticles. The dynamical response of the valence electrons responsible for the collective excitations is strongly influenced by the polarization of the core electrons [1] through screening effects [2]. This screening results in a shift of the surface plasmon to lower energy. The field enhancement factors were calculated for different nanoparticle sizes. We investigated also the dependence of the field enhancement factor on the distance from the surface of the nanoparticle and on the surrounding medium.

[1] L. Serra and A. Rubio, *Phys. Rev. Lett.* **78**, 1428 (1997)

[2] Lerne et al, *Eur. Phys. J. D* **4**, 95 (1998)

MO 7.10 Mon 16:00 P1

Size dependent luminescence of silicon clusters in neon matrices — •VICENTE ZAMUDIO-BAYER^{1,3}, STEFAN MINNIBERGER², ALEXANDRE RYDLO², KONSTANTIN HIRSCH^{1,3}, THOMAS MÖLLER³, BERND VON ISSENDORFF⁴, WOLFGANG HARBICH², and TOBIAS LAU¹ — ¹Helmholtz-Zentrum Berlin für Materialien und Energie, Wilhelm-Conrad-Röntgen Campus / BESSY II, Institut für Methoden und Instrumentierung der Synchrotronstrahlung (G-I2), Albert-Einstein-Str. 15, D-12489 Berlin — ²Institut de Physique des Nanostructures, EPFL, CH-1015 Lausanne — ³Technische Universität Berlin, Institut für Optik und Atomare Physik, EW 3-1, Hardenbergstraße 36, D-10623 Berlin — ⁴Albert-Ludwigs-Universität Freiburg, Fakultät für Physik/FMF, Stefan-Meier-Straße 21, D-79104 Freiburg

The optical properties of silicon are of great interest because of future possible applications compatible with existing silicon based electronics technology. Especially its light emitting characteristics have been studied to great extent. A large portion of these studies deal with the luminescence in the visible range of small ($d \geq 1$ nm) silicon structures, which has been linked to quantum confinement and/or the presence of defects. In order to better understand the underlying effects, it would be interesting to investigate smaller structures down to the molecular limit. Therefore we have measured the luminescence of very small ($n \leq 18$) size selected, pristine silicon clusters embedded in a neon matrix. Experimental details and some first results are presented.