

MO 33: Cluster II

Time: Friday 14:00–15:30

Location: F 102

MO 33.1 Fr 14:00 F 102

The observation of electronic energy bands in argon clusters — ●MARKO FÖRSTEL^{1,2}, MELANIE MUCKE¹, TIBERIU ARION¹, TORALF LISCHKE¹, ALEX BRADSHAW^{1,3}, and UWE HERGENHAHN¹ — ¹Max-Planck-Institut für Plasmaphysik, 85748 Garching — ²Max-Planck-Institut für Kernphysik, 69117 Heidelberg — ³Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin

We have investigated the $3p$ valence band of argon clusters near the photoionization threshold. Detection of low kinetic energy electrons was achieved by using a newly constructed magnetic bottle type spectrometer. Ar clusters were produced in a supersonic expansion. In our experiments, we have varied the expectation value of the cluster size distribution, $\langle N \rangle$, from 50-1000 atoms by changing the expansion conditions. A strong feature at ca. 15 eV binding energy shows a photon energy dependence typical of electronic energy band dispersion. A feature with a similar dispersion occurs in the ordered solid at approximately the same photon energy. This first observation of band dispersion in a rare gas cluster indicates that bulk-like electronic properties are already present in clusters of a few hundred atoms. The cluster size dependence of the dispersion will be discussed in the presentation.

MO 33.2 Fr 14:15 F 102

IR spectroscopy on anionic cobalt(alcohol) clusters — ●PHILIP BIALACH¹, MARTIN WEILER¹, ANDREAS FUNK¹, ARNE LUECHOW², and MARKUS GERHARDS¹ — ¹TU Kaiserslautern, Physikalische und Theoretische Chemie, Erwin-Schrödingerstr. 52, 67663 Kaiserslautern — ²RWTH Aachen, Institut für Physikalische Chemie, Landoltweg 2, 52056 Aachen

Investigations on clusters containing transition metals and aliphatic ligands provide the opportunity to study the differences between small molecular systems and nanoscaled particles. The changes in physical and chemical properties by increasing the cluster size can be analyzed. The successive aggregation of ligands (e.g. alcohol molecules) on cobalt containing anionic metal clusters is investigated in a molecular beam experiment. Here the first IR spectroscopic analyses of anionic clusters containing cobalt atoms (1-4) and alcohol molecules (1-3 methanol, ethanol or n-propanol molecules) are presented. The anionic cobalt clusters are produced via a laser ablation source. To obtain structural information about the (cobalt) $n=1-4$ (alcohol) $m=1-3$ cluster anions the frequencies of the OH-stretching vibrations are probed by means of IR-photodetachment and IR-photofragmentation spectroscopy, respectively. The structural assignment is performed by comparing the experimental data with calculated frequencies obtained from ab initio and DFT calculations. It is shown that high spin complexes are preferred. In clusters containing at least two cobalt atoms the alcoholic OH groups are directed towards the Co-Co bonds.

MO 33.3 Fr 14:30 F 102

Elastic soft X-ray scattering from free nanoparticles — ●BURKHARD LANGER, EGILL ANTONSSON, RENÉ LEWINSKI, CHRISTINA GRAF, and ECKART RÜHL — Institut für Chemie und Biochemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin

For many years elastic light scattering from free micro particles has been successfully used to probe their properties such as size, shape, and index of refraction. Similar studies on nanoparticles require the wavelength of the incident light being shifted into the VUV or X-ray regime. Here, we report first experimental results on small angle X-ray scattering (SAXS) on free SiO₂ nanoparticles in the size regime between 100 and 250 nm. These particles are brought into the gas phase by using a continuous particle beam [1]. This beam is crossed by synchrotron radiation from an undulator beam line at BESSY II. The elastically scattered radiation intensity near forward direction is detected by an X-ray sensitive CCD-camera permitting the simultaneous measurement of photons in a range of $1.2^\circ - 9^\circ$ off the direct photon beam. Comparing the scattered intensities over a wide photon energy range (100-800 eV) to simple Mie calculations allows one to determine size distributions and optical properties of the nanoparticles. The results are in good agreement with transmission electron microscope (TEM) measurements, where these nanoparticles were deposited on a grid. In addition, we will discuss the resonant scattering in the Si $2p$ regime ($E \approx 100$ eV).

[1] H. Bresch *et al.* Faraday Discuss. **137**, 398-402 (2008).

MO 33.4 Fr 14:45 F 102

Inner-shell excitation of size-selected 10 nm silicon oxide nanoparticles in an aerodynamically focused particle beam — ●EGILL ANTONSSON¹, BURKHARD LANGER¹, JAN MEINER^{2,3}, SVETLANA KHASHINSKAYA³, MARKUS ERITT³, THOMAS LEISNER^{2,3} and ECKART RÜHL¹ — ¹Physical and Theoretical Chemistry, Institute for Chemie and Biochemistry, Freie Universität Berlin, Germany — ²Institute for Meteorology and Climate Research, Karlsruhe Institute of Technology (KIT), Germany — ³Institute for Environmental Physics, Prerecht-Karls-Universität Heidelberg, Germany

We present results from an experiment in which silicon oxide nanoparticles ($d: \approx 10$ nm) were studied in the gas phase in a particle beam by photoelectron spectroscopy. The particles were produced *in situ* in a plasma discharge reactor and aerodynamically focused. Pulsed injection into the interaction area allowed us to study nanoparticles with soft x-rays in a size regime in which it has proven notoriously difficult to attain sufficient target densities. The photo-emission of the nanoparticles was recorded after excitation near the Si $2p$ absorption edge using synchrotron radiation. Photon energies between 100 eV and 150 eV were used. The binding energy of Si $2p_{3/2}$ was determined to be 110.2 ± 0.2 eV relative to the vacuum level. The binding energy of Si $2p_{3/2}$ in bulk SiO₂ has been reported to be 103.8 eV relative to the Fermi level [1] which lies 5.1 eV below the vacuum level [2]. The higher binding energy in the nanoparticles will be discussed.

[1] D. G. J. Sutherland *et al.*, Phys. Rev. B, **48**, 14989-15001 (1993)

[2] F.J. Himpel *et al.*, Phys. Rev. B, **38**, 6084-6096 (1998)

MO 33.5 Fr 15:00 F 102

Optimierung der Translationskühlung von Überschallstrahlen durch reduzierte 'Skimmer'-Einflüsse — ●TIM KRAUSE, KLAUS RADEMANN und WOLFGANG CHRISTEN — Institut für Chemie, Humboldt-Universität zu Berlin, 12489 Berlin

Durch die adiabatische Kühlung einer Überschall-Expansion können sehr tiefe Translationstemperaturen erreicht werden^{1,2}. Um möglichst kalte Überschallstrahlen zu erzeugen, ist es notwendig, unerwünschte Wechselwirkungen zwischen Überschallstrahl und 'Skimmer' zu minimieren. Als ein Maß für niedrige Translationstemperaturen und die Strahlqualität kann das Geschwindigkeitsverhältnis $S = v/\Delta v$ dienen. Kommt es auf Grund von Streueffekten am 'Skimmer' zur Aufheizung des Strahls, vergrößert sich die Breite der Geschwindigkeitsverteilung, Δv . Bei konstanter Strömungsgeschwindigkeit, v , sinkt als Folge das Geschwindigkeitsverhältnis, S . Wir stellen Flugzeitspektren metastabiler Heliumatome zur Untersuchung der Wechselwirkung gepulster Überschallstrahlen mit einem 'Skimmer' als Funktion des Düsen-'Skimmer'-Abstands für Stagnationsdrücke im Bereich von 0,6 – 9,6 MPa vor. Durch die experimentelle Möglichkeit, bei veränderlicher Düsen-'Skimmer'-Distanz die gesamte Flugstrecke konstant zu halten, können Auswirkungen der Wechselwirkung des Überschallstrahls mit dem Skimmer quantitativ bestimmt werden.

¹J. Wang *et al.* Phys. Rev. Lett. **60**, 696 (1988)

²W. Christen, K. Rademann *J. Chem. Phys.* **125**, 174307 (2006)

MO 33.6 Fr 15:15 F 102

Protonated Water Clusters – a XAS Study — ●J. WITTICH², J. RITTMANN¹, F. AMESSEDER², K. HIRSCH², CH. KASIGKEIT², A. LANGENBERG¹, M. LEETMAA⁴, H. ÖBERG⁴, L.G.M. PETTERSSON⁴, J. PROBST², M. VOGEL², PH. WERNET¹, V. ZAMUDIO-BAYER², TH. MÖLLER², B. VON ISSENDORFF³, and J.T. LAU¹ — ¹Helmholtz-Zentrum Berlin für Materialien und Energie, Albert-Einstein-Str. 15, 12489 Berlin, Germany — ²Technische Universität Berlin, Institut für Optik und Atomare Physik, Hardenbergstr. 36, 10623 Berlin, Germany — ³Universität Freiburg, Fakultät für Physik, Stefan-Meier-Str. 21, 79104 Freiburg, Germany — ⁴Stockholm University, Fysikum, AlbaNova, Stockholm, Sweden

The electronic and geometric structures of size selected protonated water clusters are studied with X-ray absorption spectroscopy at the oxygen K-edge. Transitions from oxygen 1s electrons into unoccupied molecular orbitals are particularly sensitive to hydrogen bonding of water molecules and give information on the local electronic structure of protonated water clusters. Results on size selected H⁺(H₂O)_n ($n = 4 - 14$) clusters indicate size dependent shifts of the resonant X-ray absorption lines. Spectral signatures in this size range are rather

similar to gas-phase water molecules or the ice Ih surface than to liquid water. We will discuss our results in comparison to theory and experiments on gas phase water, liquid water, and ice. Additionally,

an insight into our XAS studies on the coordination of solvated ions in water clusters will be given.