

A 12: Clusters I (with MO)

Time: Tuesday 11:00–13:00

Location: N 6

Invited Talk

A 12.1 Tue 11:00 N 6

Cryo Kinetics and Spectroscopy of 3d Metal Clusters and Alloys — JENNIFER MOHRBACH, SEBASTIAN DILLINGER, MATTHIAS KLEIN, AMELIE EHRRARD, and ●GEREON NIEDNER-SCHATTEBURG — Fachbereich Chemie, TU Kaiserslautern

The cluster surface analogy motivates us to utilize our hybrid tandem ion trap instrument (cryo-RF-hexapole and cryo-FT-ICR trap) for the study of adsorption and reaction kinetics of clusters under single collision conditions at 11–30 K, and for IR Photon Dissociation (IR-PD) spectroscopy initially focusing on the one and two colour investigations of metal organic complexes^[1] and lately extended towards their N₂ adsorption properties^[2].

We have started a systematic study of N₂ and H₂ cryo adsorption on size selected Fe, Co, and Ni clusters, and their alloys^[3]. Adsorption kinetics show mono layer like adsorbate shells. IR-PD spectra of cluster adsorbate complexes [M_n(N₂)_m]⁺ reveal complex patterns – DFT modelling providing some support. There are adsorbate coverage dependent spectral shifts and splittings that report on the cluster and adsorbate geometries. We compare to our synchrotron X-ray based studies of spin and orbital contributions to the total magnetic moments of the clusters^[4]. Supported by SFB 3MET.de.

[1] Y. Nosenko et al. PCCP **15**, 8171 (2013); J. Lang et al. PCCP **16**, 17417 (2014). [2] J. Lang et al., Chem.Comm 2016 (in print). [3] S. Dillinger et al. PCCP **17**, 10358 (2015); J. Mohrbach et al. JPC A 2016 (submitted). [4] S. Peredkov et al. PRL **107**, 233401 (2011); J. Meyer et al. JCP **143**, 104302 (2015)

A 12.2 Tue 11:30 N 6

Unusual magic numbers in Si_n⁺-Ar_m clusters — ●MARKO FÖRSTEL, BERTRAM JAEGER, PHILIPP SPORKHORST, and OTTO DOPFER — Institut für Optik und Atomare Physik, Technische Universität Berlin, Hardenbergstrasse 36, D-10623 Berlin

Silicon ions are found in the interstellar medium and in Earth's atmosphere. They are also involved in semiconductor manufacturing processes. The fundamental chemistry, behavior, and structure of Si_n⁺ ions are, however, still poorly understood. Here we probe the anisotropic electronic structure of the Si_n⁺ ion in form of the Si_n⁺-Ar_m potential energy surface by using argon ligands. Si_n⁺-Ar_m clusters are produced in a laser vaporization source and then analyzed in a mass spectrometer. Depending on the cluster source conditions we observe unusual magic numbers that cannot be explained satisfyingly by assuming an icosahedric argon shell. We interpret our observations as an effect of the strong anisotropy in the interaction potential of the Si⁺ ion caused by its unpaired electron. We present the observed magic numbers of Si_n⁺-Ar_m clusters and discuss the underlying structures with the help of quantum chemical calculations.

A 12.3 Tue 11:45 N 6

Absorption of diamondoid-noble metal cluster hybrids studied with ion yield spectroscopy — ●TOBIAS BISCHOFF¹, ANDRE KNECHT¹, ANDREA MERLI¹, VICENTE ZAMUDIO-BAYER², TOBIAS LAU³, BERND VON ISSENDORFF², MERLE RÖHR⁴, JENS PETERSEN⁴, ROLAND MITRIC⁴, THOMAS MÖLLER¹, and TORBJÖRN RANDER¹ — ¹TU Berlin, Germany — ²U Freiburg, Germany — ³Helmholtz-Zentrum Berlin, Germany — ⁴U Würzburg, Germany

The study of the radiative emission rate enhancement of molecules near metal surfaces has led to important applications such as single molecule spectroscopy. While interaction-induced amplification rates as high as 14 orders of magnitude have been already observed, there is still debate about the fundamental processes responsible for the enhancement. On the molecular size scale, small metal clusters may be used to systematically study the interaction between a metal subunit and a fluorophore. Diamondoids, perfectly shape and mass selected sp³ hybridized nanodiamonds, show intrinsic luminescence and can be selectively functionalized. We were able to synthesize hybrid systems of diamondoids and small metal cluster cations in the gas phase. This approach enables us to study the optical properties of tailored hybrid systems. Here, we present the UV/VIS absorption of adamantanethiol-Au₃/Ag₃ hybrid systems, measured through ion yield spectroscopy. An analysis of both the hybrid and single subunit absorptions shows significant differences in spectral composition depending on the type of metal cluster. We attribute these differences to charge transfer states

in the hybrid systems.

A 12.4 Tue 12:00 N 6

Disentangling water cluster beams — ●HELEN BIEKER^{1,2}, DANIEL HORKE^{1,2}, DANIEL GUSA¹, BORIS SARTAKOV³, ANDREY YACHMENEV¹, and JOCHEN KÜPPER^{1,2,4} — ¹Center for Free-Electron Laser Science, DESY — ²The Hamburg Center for Ultrafast Imaging, University of Hamburg — ³General Physics Institute, Russian Academy of Sciences — ⁴Department of Physics, University of Hamburg

To unravel the microscopic details of intermolecular interactions in water, we prepare controlled samples of size- and isomer-selected water clusters. Inhomogeneous electric fields allow us to create pure samples of individual structural isomers or of size-selected molecular clusters and to disperse molecules in a beam according to their quantum states [1].

Here, we aim to develop an understanding of the structures of water clusters containing a few monomer units. We present our first results on the production of size-selected samples using supersonic expansions, subsequent dispersion of the various clusters in strong electric fields, extending previous studies [2]. We introduce a simple theoretical description of water dimer in an electric field. Future experiments aim at utilizing x-ray and electron diffractive imaging to study the structures and ultrafast dissociation dynamics of these polymolecular systems.

[1] Y.P. Chang, D. A. Horke, S. Trippel and J. Küpper, *Int. Rev. Phys. Chem.* **34**, 557-590 (2015)

[2] R. Moro, R. Rabinovitch, C. Xia, and V.V. Kresin, *Phys. Rev. Lett.* **97**, 123401 (2006)

A 12.5 Tue 12:15 N 6

D-Dimensional Fourier Grid Hamiltonian Method with Potential-Adapted Grid for Hydrogen Isotopologue Cluster Computations — ●ALEXANDER KRAUS, ROBIN GRÖSSLE, and SEBASTIAN MIRZ — Karlsruhe Institute of Technology, Institute for Technical Physics, Tritium Laboratory Karlsruhe

In order to determine the systematic effect of molecular hydrogen clusters on the neutrino mass measurement with KATRIN, a computational method is needed that can be used for a calculation of initial and final beta decay states.

For this purpose, the Fourier Grid Hamiltonian Method has been generalized to *d* dimensions. A grid generation algorithm has been introduced that chooses sparse sampling points which represent the potential sufficiently to save computation time. The *d*-dimensional inverse FFT is used for fast computation of matrix elements. Eigenvalues and Eigenstates are approximated by parallel Lanczos diagonalization.

An overview of the constructed algorithm is given and first results and benchmarks are shown in this talk.

This method could also be useful to infrared spectroscopy of liquid hydrogen isotopologues for a better quantitative understanding of cluster excitations.

A 12.6 Tue 12:30 N 6

Highly nonlinear optical response of organotin cluster molecules — ●NILS W. ROSEMAN^{1,3}, JENS P. EUSSNER², ANDREAS BEYER³, STEPHAN W. KOCH³, KERSTIN VOLZ³, STEFANIE DEHNEN², and SANGAM CHATTERJEE¹ — ¹Institute of Experimental Physics I, Justus-Liebig-Universität Giessen, Heinrich-Buff Ring 16, D-35392 Giessen, Germany — ²Faculty of Chemistry and Materials Sciences Center, Philipps-Universität Marburg, Hans-Meerwein-Straße, D-35043 Marburg, Germany — ³Faculty of Physics and Materials Science Center, Philipps-Universität Marburg, Renthof 5, D-35032 Marburg, Germany

Organotin-based cluster molecules exhibit a large variety of physical properties. These depend on the clusters chemical composition as well as the spatial arrangement of the constituents. Variation of these two parameters usually results in highly complex electronic landscapes. Consequently, such cluster molecules exhibit a very specific linear response and ultimately nonlinear optical properties.

Here, we present the extreme nonlinear optical response of a cluster molecule composed of a SnS cluster-core decorated with styryl-ligands. The ligands, on the one hand, prevent crystallization and provide delocalized electrons that are responsible for the nonlinear response on

the other hand. These peculiarities result in low-threshold white-light generation. The latter is simulated numerically using an anharmonic oscillator model and experimental parameters only.

A 12.7 Tue 12:45 N 6

Infrared spectra and structures of boron-doped silicon clusters — •BERTRAM KLAUS AUGUST JAEGER¹, NGUYEN XUAN TRUONG¹, SANDY GEWINNER², WIELAND SCHÖLLKOPF², ANDRE FIELICKE¹, and OTTO DOPFER¹ — ¹IOAP, TU Berlin, Germany — ²FHI, Berlin, Germany

Silicon-based nanostructures have gained interest for nanoelectronics and nanophotonics. Therefore, the investigation of controlled change

of physical and chemical properties of silicon clusters by doping will aid in developing novel cluster-containing nanostructures. Here we study neutral silicon-rich silicon-boron clusters (Si_nB_m , $n=3-8$, $m=1-2$) via mass spectrometry, resonant infrared-ultraviolet two-color ionization (IR-UV2CI) spectroscopy and quantum chemical calculations [1]. The most stable isomers are found utilizing global energy optimization. Their linear IR absorption spectra are compared to the IR-UV2CI spectra, thus determining the geometries of the observed Si_nB_m clusters. Different physical properties such as charge distributions, ionization energies and bond energies will be discussed. As the B-B bond is stronger than the B-Si and Si-Si bonds, boron segregation is observed for Si_nB_m clusters with $m=2$.

[1] N.X. Truong et al., Int. J. Mass Spectrom., 2016, 395, 1-6