

MS 4: Clusters and Molecules

Time: Tuesday 14:00–15:15

Location: f128

Invited Talk

MS 4.1 Tue 14:00 f128

Multi-reflection time-of-flight mass spectrometry for cluster research — ●PAUL FISCHER, GERRIT MARX, and LUTZ SCHWEIKHARD — Institut für Physik, Universität Greifswald, 17487 Greifswald, Germany

Multi-reflection time-of-flight mass spectrometry (MR-ToF MS) is known as a powerful tool for precision mass measurements [1] and high-resolution isobar separation [2] in nuclear physics. In atomic and molecular physics, MR-ToF devices are appreciated for their characteristics as electrostatic ion traps [3], however, they are often operated in non-bunching mode, abandoning high resolving powers in favor of easier interaction prerequisites.

At the University of Greifswald, MR-ToF MS is applied for high-resolution investigations of atomic clusters. To this end, a series of techniques for the work with ion bunches exhibiting large mass differences is developed. This includes in-trap photodissociation [4] and the introduction of a novel tandem MR-ToF MS scheme [5]. As a first case of interest, the dissociation behavior of bismuth clusters and the change thereof resulting from doping with a single lead atom is investigated.

[1] F. Wienholtz et al., *Nature* 498:346 (2013)

[2] R.N. Wolf et al., *Phys. Rev. Lett.* 110:041101 (2013)

[3] D. Zajfman et al., *Phys. Rev. A* 55:R1577 (1997)

[4] P. Fischer et al., *Eur. Phys. J. D* 73:105 (2019)

[5] P. Fischer et al., *Phys. Rev. Research* 1:033050 (2019)

MS 4.2 Tue 14:30 f128

Nitrophobia of size selected iron clusters under cryo conditions — ●ANNIKA STEINER¹, CHRISTOPHER WIEHN¹, MATTHIAS P. KLEIN¹, DANIELA V. FRIES¹, PETER B. ARMENTROUT², and GEREON NIEDNER-SCHATTEBURG¹ — ¹Fachbereich Chemie und Forschungszentrum OPTIMAS, Technische Universität Kaiserslautern, 67663 Kaiserslautern, Germany — ²Department of Chemistry, University of Utah, Salt Lake City, Utah 84112, USA

We utilize a modified FT-ICR MS to characterize the interaction of N₂ with transition metal surfaces and clusters in detail. With this tandem cryo trap (T < 11 K) instrument we have investigated the N₂ adsorption on Co, Ni, Rh and N₂ and H₂ co-adsorption on Ru₈⁺.

In continuation of these studies, we conduct investigations of N₂ adsorption on Fe_n⁺ clusters. We investigate kinetic studies of N₂ adsorption and found size and pressure dependent effects. Thereby, we unravel otherwise unpredictable cluster size effects as e.g. very slow N₂ adsorption on Fe₁₇⁺, and an isomerism of the Fe₁₈⁺ cluster.

Furthermore, we present gas phase IR spectra of N₂ adsorption on isolated Fe_n⁺ clusters at cryo temperatures. The complex variations in terms of single or multiple IR active N₂ stretching bands are significantly red shifted with respect to the IR inactive stretching mode of free N₂ (2330 cm⁻¹). Based on this we compare the IR spectra of the “normal” Fe₁₃⁺ cluster with those of the nitrophobic Fe₁₇⁺ cluster. In combination with DFT studies, we try to interpret these size effects in terms of size dependent spin repulsion and to unravel cluster

morphologies in more detail.

MS 4.3 Tue 14:45 f128

A gas-phase soft X-ray study on the metal active site of metalloporphyrins and metalloproteins — ●KAJA SCHUBERT¹, KAAAN ATAK¹, LUCAS SCHWOB¹, SIMON DÖRNER¹, MARTIN TIMM², CHRISTINE BÜLOW², VICENTE ZAMUDIO-BAYER², XIN WANG³, TOBIAS LAU², THOMAS SCHLATHÖLTER³, and SADIA BARI¹ — ¹Deutsches Elektronen-Synchrotron, Hamburg — ²Institut für Methoden und Instrumentierung der Forschung mit Synchrotronstrahlung, Helmholtz Zentrum Berlin für Materialien und Energie, Berlin — ³Zernike Institute for Advanced Materials, University of Groningen, Groningen

Metalloporphyrins (MPs) are organometallic molecules widely found in nature and composed of a porphyrin ring coordinating a metal ion in the ring's cavity center. Their particular electronic structure makes MPs ideally suited for a number of applications, from biological functions to the usage in electronic devices. Electronic structure and functional activity of MPs are determined by the type of the metal, its oxidation and spin state as well as axial ligands around the metal center. For understanding the properties of MPs, it is hence of great importance to probe the local electronic structure of the metal ion. In this study electrospray ionization (ESI) tandem mass-spectrometry and synchrotron-based light were combined and site-selective excitation at the metal L-absorption edges was used for probing the metal site of several MPs. Similar measurements were performed for the MP-containing protein cytochrome c (12.4 kDa).

MS 4.4 Tue 15:00 f128

Dissociative Electron Attachment Studies with 2-Nitrofurane — ●MUHAMMAD SAQIB, EUGENE ARTHUR-BAIDOO, MILAN ONCAK, and STEPHAN DENIFL — University of Innsbruck, 6020 Innsbruck, Austria

Nitrofurans belong to the class of drugs typically used as antibiotics or antimicrobials. The defining structural component is a furan ring with a nitro group attached. In the present investigation, dissociative electron attachment (DEA) to 2-Nitrofurane (C₄H₃NO₃), which is considered as a potential radiosensitizer candidate for application in radiotherapy, has been studied in a crossed electron* molecular beams experiment. The present results indicate that low-energy electrons with kinetic energies from about 0 - 14 eV effectively decompose the molecule by DEA. In total, fifteen fragment anions were detected within the detection limit of the apparatus, as well as the parent anion of 2-Nitrofurane. Two major resonance regions, at which the anions are formed, are observed, one between ~0 eV and 5 eV and a second one in the range from 7 eV to 10 eV. (NO₂)⁻, (C₄H₃O)⁻, and (C₄H₃NO₃)⁻ is the most abundant fragment anion observed. The experimental results are compared with calculations of the thermochemical thresholds of the anions observed. The current study shows that low-energy electrons very effectively decompose the 2-Nitrofurane molecule upon attachment of low energy electrons, producing a large variety of charged fragments and radicals. This work was supported by the FWF, Vienna (P30332).