

MO 7: Clusters II (joint session MO/A)

Time: Tuesday 14:00–15:45

Location: f142

MO 7.1 Tue 14:00 f142

Molecular Rotation in floppy Molecules: He-H₃⁺ — THOMAS SALOMON¹, IGOR SAVIC², OSKAR ASVANY¹, DIETER GERLICH³, AD VAN DER AVOIRD⁴, MICHAEL E. HARDING⁵, JÜRGEN GAUSS⁶, FILIPPO LIPPARINI⁷, and ●STEPHAN SCHLEMMER¹ — ¹I. Physikalisches Institut, Universität zu Köln — ²Department of Physics, University of Novi Sad, Serbia — ³Institut für Physik, Technische Universität Chemnitz — ⁴Theoretical Chemistry, Radboud University Nijmegen, The Netherlands — ⁵Fakultät für Chemie und Biowissenschaften Karlsruhe Institut für Technologie (KIT) — ⁶Department Chemie, Johannes Gutenberg-Universität Mainz — ⁷Dipartimento di Chimica e Chimica Industriale, Università di Pisa, Italy

The ro-vibrational predissociation spectrum of He-H₃⁺ has been recorded via the ν_2 vibrational mode in a cold 22-pole ion trap. The spectrum for the bare H₃⁺ consists of only a few ro-vibrational lines. Instead, the spectrum of the complex is very rich (~ 465 lines) even at the low temperature (4 K) of the experiment. Part of this complexity is associated with the (almost) free internal rotation of H₃⁺. The experimental results are compared to theoretical predictions of ro-vibrational spectra on the basis of ab initio calculations of the He-H₃⁺ potential energy surface. The energy levels result in transitions which agree in many cases with experimental results within a few wavenumbers. In addition, an experimental energy term diagram is reconstructed from the observed transitions. The influence of the Coriolis interaction resulting from the H₃⁺ internal rotation in a rotating He-H₃⁺ frame will be discussed.

MO 7.2 Tue 14:15 f142

Competition between inter- and intra-atomic ionization phenomena: Observation of Electron-Transfer-Mediated decay and Auger decay in Xenon-doped water clusters — ●AARON NGAI¹, RUPERT MICHIELS¹, NORA BERRAH², CARLO CALLEGARI³, EDWIN CHAPMAN¹, RAIMUND FEIFEL⁴, MICHELE DI FRAIA³, JAKOB KRULL¹, AARON C. LAForge², PAOLO PISERI⁵, OKSANA PLEKAN³, KEVIN PRINCE³, RICHARD J. SQUIBB⁴, VIT SVOBODA⁶, DANIEL UHL¹, HANS-JAKOB WÖRNER⁶, ANDREAS WITUSCHEK¹, and FRANK STIENKEMEIER¹ — ¹Institute of Physics, University of Freiburg — ²Department of Physics, University of Connecticut — ³Electro-Sincrotrone Trieste — ⁴Department of Physics, University of Gothenburg — ⁵Dipartimento di Fisica and CIMaINa — ⁶Laboratorium für Physikalische Chemie, ETH Zürich

Electron-transfer-mediated decay (ETMD) is a subset of the more general inter-coulombic decay (ICD). In condensed-matter or cluster systems, ETMD competes with other ionization processes such as autoionization (e.g. Auger decay). Using XUV-XUV pump-probe spectroscopy, we observe the competition between ETMD and Auger decay of Xe⁺ (4d_{3/2} and 4d_{5/2}) embedded in water clusters. In particular, we can distinguish between these two similar processes by observing the resulting Xe^{N+} ions in addition to time-resolving their femtosecond dynamics. In our experiment using the FERMI FEL at Elettra, two main features differentiating these decays are expected: the charges of the final Xe^{N+} ions, and kinetic energy broadening of Auger electrons through post-collision interactions (PCI).

MO 7.3 Tue 14:30 f142

Cryogenically Cooled Beams of Bio-Nanoparticles — ●LENA WORBS^{1,2}, JANNIK LÜBKE^{1,2,3}, ARMANDO ESTILLORE¹, AMIT K. SAMANTA¹, and JOCHEN KÜPPER^{1,2,3} — ¹Center for Free-Electron Laser Science, Deutsches-Elektronen-Synchrotron DESY, Hamburg — ²Fachbereich Physik, Universität Hamburg — ³Center for Ultrafast Imaging, Hamburg

Coherent diffractive imaging at free-electron lasers promises to allow the reconstruction of the three-dimensional molecular structures of isolated particles at atomic resolution [1]. However, because of the typically low signal to noise ratio, this requires the collection of a large amount of diffraction patterns. Since every intercepted particle is destroyed by the intense x-ray pulse, a new and preferably identical sample particle has to be delivered into every pulse.

We present novel approaches for the production of high density particle beams of shock-frozen bio-nanoparticles using a cryogenic buffer-gas cooling technique [2]. We have also developed a numerical simulation infrastructure that allows quantitative simulation of isolated par-

ticle trajectories inside the buffer-gas cell. The cryogenically-cooled nanoparticle beams are characterized using laboratory-based light-scattering [3]. To further improve the resulting particle beam, an aerodynamic lens is implemented to increase its density.

[1] M. M. Seibert, et al., *Nature* **470**, 78 (2011).

[2] A. K. Samanta, et al., arXiv:1910.12606 [physics.bio-ph]

[3] L. Worbs, et al., *Opt. Expr.*, arXiv:1909.08922 [physics.optics]

MO 7.4 Tue 14:45 f142

Ultrafast Spectroscopy of Perylene Derivative Nanoparticles — ●CHRIS REHHAGEN^{1,2}, SHAHNAWAZ RAFIQ², STEFAN LOCHBRUNNER¹, and GREGORY SCHOLLES² — ¹Institute for Physics and Department of Life, Light and Matter, University of Rostock, 18051 Rostock, Germany — ²Frick Laboratory, Princeton University, 08540 Princeton, USA

Organic dye nanoparticles and nanostructures are of increasing interest in opto-electronic applications due to their potentially large exciton mobilities. While as inorganic nanoparticles are already applied in many scenarios, the properties of organic nanostructures are yet to be explored. Among a breadth of organic systems available, Perylene derivatives especially attract much interest as they provide a high oscillator strength, photostability, and a tuneability of the transition energy and supramolecular structure by changing the bay-substitutes.

We use flash precipitation to prepare nanoparticles of the Perylene Red (PR) and Perylene Orange (PO) dyes and correlate their optical spectra, quantum yields, emission lifetimes and their size. Ultrafast pump-probe spectroscopy is then performed on samples of different size classes to characterize their excited state dynamics. In PR nanoparticles, a new electronic state, formed after photoexcitation, was observed. Remarkably, no such intermediate state was observed in the PR monomer. In PO nanoparticles, we observe an ultrafast excimer formation. In both systems and for different size classes, we characterize the exciton diffusion in the nanoparticles by analyzing signatures in the transient dynamics resulting from exciton-exciton annihilation.

MO 7.5 Tue 15:00 f142

Spectroscopic investigation of gas-phase silvercluster-porphyrin hybrids — ●CARL FREDERIC USSLING¹, TOBIAS BISCHOFF¹, ANDRE KNECHT¹, ANDREA MERLI¹, MERLE I. S. RÖHR², POLINA G. LISINETSKAYA², ROLAND MITRIĆ², and THOMAS MÖLLER¹ — ¹Institut für Optik und Atomare Physik, Technische Universität Berlin — ²Institut für Physikalische und Theoretische Chemie, Universität Würzburg

In the last decades the size and structure-dependent optical properties of noble metal clusters have been widely investigated [1][2].

In the smallest size regime, both the cluster geometry and optical properties turned out to be particularly effected by the number of constituents [3]. Due to their strong UV and Vis absorption it has been predicted, that small silver clusters could be useful to develop new biomolecular sensors [4]. Hybrid systems consisting of small metal clusters and small molecular units have been developed and their optical behavior experimentally explored [5]. We investigated the possibility to combine small cationic silver clusters with single porphyrins in a collision cell and studied first the optical properties of Ag₃[Ag(OEP)]⁺ in the UV range.

[1] E. M. Fernández et al., *Phys. Rev. B* **70**, 165403 (2004)[2] C. Sönnichsen et al., *New J. Phys.* **4**, 93 (2002)[3] K. L. Kelly et al., *J. Phys. Chem. B* **107**, 668 (2003)[4] T. Tabarin et al., *J. Chem. Phys.* **127**, 134301 (2007)[5] V. Bonačić-Koutecký et al., *Phys. Chem. Chem.* **14**, 9282 (2012)

MO 7.6 Tue 15:15 f142

Investigation of isolated aggregates of coumarin derivatives in the gas phase by applying combined IR/UV spectroscopy — ●POL BODEN, ANKE STAMM, MICHAEL BORCHERS, DOMINIC BERNHARD, DOMINIQUE MAUÉ, and MARKUS GERHARDS — TU Kaiserslautern and State Research Center OPTIMAS, Germany

Coumarin and its derivatives are well known for their photo-induced reactivity leading to their importance as photobiological and photochemical substances. Here we report on 7-Hydroxy-4-methylcoumarin (7-H4MC) and its amino analogue 7-amino-4-methylcoumarin (7-

A4MC). The examination of 7-A4MC is of great interest because aminocoumarins show an intramolecular charge-transfer (ICT) between the amino group and the benzopyrone unit in solvents of moderate to high polarity. In order to investigate intrinsic effects with respect to ICT and structure of the 7-A4MC dimer in the neutral and cationic ground states as well as in the S_1 state, combined IR/UV spectroscopy is applied in molecular beam experiments. A comparison of the measured IR transitions with calculated frequencies and optimized structures allows clear structural assignments. Furthermore the 7H4MC dimer and its mono- and dihydrate are investigated both in their neutral and cationic ground state with regard to structural changes occurring upon UV photoionization. The tendencies of coumarins for self-aggregation observed in aqueous solution are investigated in detail on isolated species giving (in combination with hydration) a closer look on structure and function of coumarins.

MO 7.7 Tue 15:30 f142

Rayleigh scattering of a pulsed supersonic jet of Ar and CO₂ at high particle densities — ●SARA FAZLI and WOLFGANG CHRISTEN — Humboldt-Universität zu Berlin, Institut für Chemie, Brook-Taylor-Straße 2, 12489 Berlin

We present an experimental setup for the investigation of Rayleigh scattering of a pulsed supersonic jet and present first results for the scattered light intensity as a function of cluster source conditions. A jet of pure Ar or CO₂, respectively, is expanded through a parabolic nozzle at source temperatures between 230 K and 410 K and source pressures between 2 MPa and 10 MPa. The change of the Rayleigh scattering signal with source pressure and temperature is compared with the prediction of Hagena's scaling law (J. Chem. Phys. 56, 1793, 1972). Results show a pronounced dependence of the scaling parameters on the aggregation state (gas versus liquid) of the expanding fluid.