A 19: Atomic clusters I

Time: Thursday 10:30–13:00 Location: BAR 205

Invited Talk A 19.1 Thu 10:30 BAR 205

Cluster ionization in strong laser fields - NIR vs. XUV — •Thomas Fennel, Jörg Köhn, Christian Peltz, and Mathias Arbeiter — Universität Rostock, 18051 Rostock, Germany

Clusters in intense laser pulses are valuable model systems for exploring new frontiers of ultrafast strong-field many-particle physics [1]. The understanding of key processes like collective excitations, ultrafast plasma creation, field amplification, and electron rescattering in clusters may open up new routes for the analysis and control of nanosystems with light. The talk will focus on two aspects: (i) waveform control of resonance enhanced electron emission in near-infrared pulses (NIR); (ii) ionization and heating behavior at short wavelength (XUV).

The first part discusses a scheme for efficient electron acceleration via resonant plasmonic effects [2], i.e. due to high transient polarization fields from resonant interaction of the laser with free cluster electrons. Numerical results for the directional control of the electron emission from metal clusters by the carrier-envelope phase of few-cycle laser fields will be presented [3]. The second part focusses on the ionization and heating of rare-gas clusters at high photon energy [4], where plasma heating disappears and photoionization dominates the laser-matter coupling. A two-color pump-probe scheme for the time-resolved analysis of the cluster dynamics is proposed.

[1] Th. Fennel et al., Rev. Mod. Phys. 82:1793 (2010)
[2] Th. Fennel et al., Phys. Rev. Lett. 98:143401 (2007)
[3] J. Köhn et al., in preparation
[4] M. Arbeiter and Th. Fennel, Phys. Rev. A, 82:013201 (2010)

A 19.2 Thu 11:00 BAR 205

Imaginary time Gaussian dynamics of rare gas clusters — •Holger Cartarius and Eli Pollak — Chemical Physics Department, Weizmann Institute of Science, 76100 Rehovot, Israel

Semiclassical Gaussian approximations to the Boltzmann operator have become an important tool for the investigation of thermodynamic properties of clusters of atoms at low temperatures. Usually, numerically expensive thawed Gaussian variants are applied. We introduce a numerically much cheaper frozen Gaussian approximation to the imaginary time propagator with a width matrix especially suited for the dynamics of clusters. The quality of the results is comparable to that of thawed Gaussian methods based on the single-particle ansatz. We apply the method to small rare gas clusters and investigate their dissociation processes. We also discuss the influence of an artificial confinement of the atoms usually introduced to converge numerical computations. The results show that restrictive confinements often implemented in studies of clusters can influence the thermodynamic properties drastically. This finding may have implications on other studies of atomic clusters.

A 19.3 Thu 11:15 BAR 205

Dynamical structure factor of extended nano plasmas — •Thomas Raitza, Heidi Reinholz, and Gerd Röpke — Universität Rostock

The dynamical structure factor of bulk plasmas is related to correlation functions, see [1]. Clusters of solid state densities can form nano plasmas after laser irradiation with intensities of $10^{13}-10^{16}$ W·cm^{-2}, which were investigated via molecular dynamics (MD) simulations. Free cluster electrons relax within a few femto seconds into a local thermodynamic equilibrium (LTE) in [2]. A *restricted MD simulations* scheme for finite systems has been developed in [3]. The generalization of the dynamical structure factor via bi-local current-density correlation function is introduced. Investigations of dynamical correlations via *restricted MD simulations* are presented for 1D chains [4] and 3D clusters. Several excitation modes were found and characterized. Dispersion relations for resonance frequencies were investigated with focus on cluster size dependency. In particular, the role of collisions on resonance damping will be presented.

[1] H. Reinholz; *Ann. Phys. Fr.* **30**, N° 4 - 5 (2006).
[2] T. Raitza, H. Reinholz, G. Röpke, I. Morozov, and E. Suraud; *Contrib. Plasma Phys.* **49**, 498 (2009).
[3] T. Raitza, H. Reinholz, G. Röpke, and I. Morozov; *J. Phys. A* **42**, 214048 (2009).
[4] T. Raitza, H. Reinholz, and G. Röpke; *Int. J. Mod. Phys. B*, accepted (2010).

A 19.4 Thu 11:30 BAR 205

Velocity-Map-Imaging Spectroscopy of Alkali Metals Embedded Inside Helium Nanodroplets — •Lutz Fechner, Marcel Mudrich, and Frank Stienkemeier — Physikalisches Institut, Universität Freiburg, 79104 Freiburg, Germany

Helium nanodroplets provide an 'ideal' matrix for spectroscopy of embedded molecules due to the low temperature conditions (400 mK) and extremely weak guest-host interactions. However, photoionization spectroscopy has mostly been hampered by the trapping of photoions in 'snowballs' that remain bound to the droplets which prevents efficient ion detection. Therefore, a new velocity-map-imaging spectrometer for photo-electrons has been built and characterized. In first experiments rubidium atoms are studied in a resonance-enhanced-multiphoton-ionization (REMPI) scheme by means of electron as well as ion imaging-spectroscopy. Gas-phase measurements are compared to spectra obtained with atoms attached to the surface of helium nanodroplets. These measurements pave the ground for future femtosecond photoionization studies of molecules embedded inside helium nanodroplets.

A 19.5 Thu 11:45 BAR 205

Ionization dynamics of doped helium nanodroplets in intense few-cycle IR laser fields — •Siva Rama Krishnan[1], Marcel Mudrich[2], Lutz Fechner[2], Vandana Sharma[1], Manuel Kremer[1], Bettina Fischer[1], Nicolas Camus[1], Jagannath Jha[3], Krishnamurthy Manchikanti[3], Robert Moshammer[1], Frank Stienkemeier[2], and Joachim Ullrich[1] — [1]Max Planck Institut für Kernphysik, Saupferchekweg 1, 69117 Heidelberg, Germany — [2]Physikalisches Institut, Universität Freiburg Hermann-Herder-Str. 3, 79104 Freiburg, Germany — [3]Tata Institute of Fundamental Research, 1 Homi Bhabha Road, Mumbai 400005, India

The ionization dynamics of two-component rare-gas clusters in intense laser fields has evoked recent interest due to the markedly different behaviour when compared to pristine clusters both in the intense IR [1,2] and intense VUV or soft X-ray domains [3,4]. We present studies on the ionization dynamics of helium nanodroplets (10^4 He atoms/droplet) doped with 1-100 atoms of other rare-gas dopants (Xe, Kr or Ar) which form embedded clusters at the center of the helium droplet. Intense few-cycle laser pulses (6 fs) with a central wavelength of 790nm and peak intensities in the range of 10^{14-15} W.cm^{-2} were used to ionize these droplets. Our studies reveal that the resulting ionization dynamics is very sensitive to the number of dopants in the droplets. [1]J. Jha and M. Krishnamurthy, J. Phys. B 41, 041002 (2008) [2]A. Mikaberidze et al., Phys. Rev. Lett. 102, 128102 (2009) [3]H. Thomas et al.,J. Phys. B. 42, 134018 (2009) [4]C. Gnodtke et al., Phys. Rev. A 79, 041201 (2009).

A 19.6 Thu 12:00 BAR 205

Rare-gas clusters in intense VUV, XUV and soft x-ray pulses: Signatures of the transition from nanoplasma-driven cluster expansion to Coulomb explosion in ion and electron spectra — •Mathias Arbeiter and Thomas Fennel — Institute of Physics, University of Rostock

We investigate the wavelength dependent ionization, heating, and expansion dynamics of medium-sized rare-gas clusters (Ar_N) under intense femtosecond short-wavelength free electron laser pulses by quasi-classical molecular dynamics simulations. A comparison of the interaction dynamics for pulses with $\hbar\omega$=20, 38, and 90 eV photon energy at fixed total excitation energy indicates a smooth transition from plasma-driven cluster expansion, where predominantly surface ions are expelled by hydrodynamic forces, to quasi-electrostatic behavior with almost pure Coulomb explosion[1]. Corresponding signatures in the time-dependent cluster dynamics as well as in the final ion and electron spectra support that this transition is linked to a crossover in the electron emission processes. This would be of interest for applications that are closely related to the correlation between ionization and expansion dynamics of many-particle systems in intense FEL pulses, such as single-shot diffractive imaging or time resolved x-ray holography.

[1] M. Arbeiter, Th. Fennel, submitted 2010

A 19.7 Thu 12:15 BAR 205

Resonant charging of Xe clusters in Helium nanodroplets under intense laser fields — •Christian Peltz and Thomas Fennel — Institute of Physics, University of Rostock, Germany

When exposed to intense laser fields, mixed clusters in core-shell configuration are expected to show multiple plasmon resonances[1]. There is an ongoing debate on the resulting signatures in the final emission spectra of ions and electrons. To study the microscopic interaction dynamics, we theoretically investigate Xe clusters embedded in He nanodroplets under pump-probe laser excitation ($\tau = 25\,\mathrm{fs}$, $I_0 = 2.5 \times 10^{14}\mathrm{W/cm}^2$, $\lambda = 800\,\mathrm{nm}$). Our molecular dynamics simulations on $Xe_{309}He_{10000}$ and comparison to simulation results for free Xe_{309} give evidence for the presence of selective resonance heating in the He shell and the Xe cluster, while a corresponding double hump feature in the final Xe charge spectra is absent. The pump-probe dynamics of the Xe spectra from the embedded system is qualitatively similar to that of the free species. In strong contrast to that, the predicted electron spectra do show well-separated and pronounced features from highly efficient plasmon assisted electron acceleration for both resonances in the embedded clusters. A detailed analysis of the ionization and recombination dynamics explains the apparent discaccord between the resonance features in ion and electron spectra[2].

[1] A. Mikaberidze et al. , Phys. Rev. A **77**, 041201 (2008)
[2] Ch. Peltz and Th. Fennel, arXiv:1009.4546v1

A 19.8 Thu 12:30 BAR 205

Condensation properties of single clusters under extreme conditions — •Marcus Adolph[1], Daniela Rupp[1], Tais Gorkhover[1], Sebastian Schorb[1], Heiko Thomas[1], David Wolter[1], Robert Hartmann[2], Nils Kimmel[2], Christian Reich[2], Rolf Treusch[3], Thomas Möller[1], and Christoph Bostedt[4] — [1]IOAP/TU-Berlin, Berlin, Germany — [2]MPG-HLL, München, Germany — [3]DESY, Hamburg, Germany — [4]SLAC, Palo Alto, USA

Free Electron Lasers (FEL) produce high energy XUV pulses and offer a new tool for exploring ultrafast motions in molecular systems and condensed matter. Currently a fast development of FELs towards shorter wavelength and higher pulse energies is taking place. The Free Electron Laser in Hamburg (FLASH) has been extended to seeded lasing and facilities in USA (LCLS) and Japan (Spring8) came into operation.

Using the short wavelength and high power densities of the FEL, we performed the first imaging experiments on single nanometer size rare gas clusters. This technique helps to gain insight into the basic interaction between FEL XUV radiation and matter which is especially important with regard to the imaging of bio molecules. The scattering images also allows us to reconstruct the size of free single clusters in the gas phase. This was used to study the process of clustering of single particles on a single shot basis. We observed the condensation characteristics of Xenon gas and growing processes of Xenon clusters under extreme pressure conditions, close to the vapor pressure curve.

A 19.9 Thu 12:45 BAR 205

X-ray and VUV Absorption Spectroscopy on Size Selected Chromium and Copper Clusters — •Felix Ameseder[2], Christof Ebrecht[2], Konstantin Hirsch[2], Christian Kasigkeit[2], Andreas Langenberg[1], Markus Niemeyer[2], Jochen Rittmann[1], Vicente Zamudio-Bayer[1], Marlene Vogel[1], Bernd von Issendorff[3], Thomas Möller[2], and Tobias Lau[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Institut für Methoden und Instrumentierung der Synchrotronstrahlung, Albert-Einstein-Straße, D-12489 Berlin — [2]Technische Universität Berlin, Institut für Optik und Atomare Physik, EW 3-1, Hardenbergstraße 36, D-10623 Berlin — [3]Albert-Ludwigs-Universität Freiburg, Fakultät für Physik/FMF, Stefan-Meier-Straße 21, D-79104 Freiburg

Studies on clusters reveal important information, including changes of the electronic structure from atomic to bulk like properties with increasing cluster size. Here we present the first X-ray and VUV absorption spectra on free size selected chromium and copper clusters. The clusters 2nd ionization potentials were determined from photoionization efficiciency curves. According to the Liquid Drop Model (LDM) a metal cluster can be described as a metallic sphere and thus its ionization potential scales linearly with cluster size over the inverse cluster radius. The results of 3d/4s valence and 2p core level photoionization will be discussed. By comparing the size dependence of the ionization potential derived from valence and core level photoionization insight into the effects of charging energy according to the LDM as well as shifts of electronic level of transition metal clusters can be obtained.