A 11: Atomic clusters I (with MO)

Time: Monday 16:30–18:30 Location: B 302

Invited Talk A 11.1 Mon 16:30 B 302

Spectra of cold molecular ions from hot helium nanodroplets — •Marcel Drabbels — EPFL, Lausanne, Switzerland

The function of a molecule is intimately related to its structure. Accordingly, in the quest for a better understanding of molecular function, the development of spectroscopic methods to elucidate molecular structures increasingly takes central stage. The amount of detail that can be derived from spectra depends on the experimental conditions, most notably on the temperature of the sample and the intermolecular interactions a molecule experiences. Helium nanodroplets provide in this respect an almost ideal matrix. For neutral molecules, helium nanodroplet spectroscopy thus has led to important discoveries related to the structure of key molecular systems and has provided insight into the mechanisms underlying chemical reactions.

Compared to the level of sophistication that has been reached for neutrals, the spectroscopic exploration of ions is still in its infancy. The use of helium droplets as a cryogenic matrix could potentially solve many of the technical challenges associated with recording high-resolution spectra of cold molecular ions. Here, we will present a method to record spectra of ion containing helium nanodroplets that finds its roots in the nonthermal cooling dynamics of excited molecular ions. In addition, spectra of several molecular ions will be present and the influence of the helium environment on these spectra will be discussed.

A 11.2 Mon 17:00 B 302

Angular resolved photoionization study of C60 in ultrashort (4 fs) and short (40 fs) laser pulses — •S. Skruszewicz[1], H. Li[2], S. Zherebtsov[3], R. Irsig[1], F. Süssmann[3], Th. Fennel[1], J. Tiggesbäumker[1], M. F. Kling[2,3], and K.-H. Meiwes-Broer[1] — [1]Institut für Physik, Universitätsplatz 3, 18051 Rostock, Germany — [2]J.R. Macdonald Laboratory, Department of Physics, Kansas State University, Manhattan, KS 66506, USA — [3]Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Str. 1, 85748 Garching, Germany

Recently, the existence of Superatom Molecular Orbitals (SAMO) bound to the core of the hollow C_{60} cage has been reported [1,2]. Few-cycle as well as two-color pulses (w/2w) [3] are applied to study angule-resolved photoelectron emission from C_{60} in order to characterize SAMO in more details. As tool we utilize Velocity Map Imaging spectrometer to map angular dependence in the photoelectron emission. Multiple nodal structures appear in the angular signal distribution as we excite C_{60} with few-cycle laser pulses. At pulse durations of 40 fs, one observes distinct changes in the photoelectron angular distribution. We also made attempt to compare the CEP dependence on the electron emission to the result obtained with w/2w pulses of 40 fs.

[1] M. Feng et.al., Science **320**, 359 (2008)
[2] O. Johansson et.al., Phys. Rev. Lett. **108** 173401 (2012)
[3] N. Dudovich et. al., Nature **2**, 781 (2006)

A 11.3 Mon 17:15 B 302

Magnetic Moments of Chromium-Doped Gold Clusters: Anderson Impurity Model in Finite Systems — Konstantin Hirsch[1,2], Vicente Zamudio-Bayer[1,2], Andreas Langenberg[1,2], Markus Niemeyer[1,2], Bruno Langbehn[1,2], Thomas Möller[1], Akira Terasaki[3,4], Bernd von Issendorff[5], and •Tobias Lau[2] — [1]Institut für Optik und Atomare Physik, Technische Universität Berlin, 10623 Berlin — [2]Institut für Methoden und Instrumentierung der Forschung mit Synchrotronstrahlung, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, 12489 Berlin — [3]Cluster Research Laboratory, Toyota Technological Institute, 717-86 Futamata, Ichikawa, Chiba 272- 0001, Japan — [4]Department of Chemistry, Kyushu University, 6-10- 1 Hakozaki, Higashi-ku, Fukuoka 812-8581, Japan — [5]Fakultät für Physik, Universität Freiburg, 79104 Freiburg

The interaction of a single magnetic impurity with a free electron gas is a long standing problem in condensed matter physics. It results in interesting phenomena like the Kondo effect or Friedel oscillations. In recent years substantial progress was made by studying these phenomena in atomic scale systems. Here we follow this approach and investigate the interaction of a single magnetic impurity with a finite free electron gas. $CrAu_n^+$ clusters serve as a model system. We show that the size dependence of the local spin magnetic moment of $CrAu_n^+$ can well be described within in the Anderson impurity model, where the interaction of the localized impurity states with the electron bath of the gold matrix is governed by quantum confinement in the host, which is abscent in the corresponding bulk material.

A 11.4 Mon 17:30 B 302

Clusters in intense femtosecond XUV pulses: Direct simulation of light scattering — •Christian Peltz[1], Charles Varin[2], Thomas Brabec[2], and Thomas Fennel[1] — [1]Institute of Physics, University of Rostock, Germany — [2]Department of Physics and Centre for Photonics Research,University of Ottawa, Canada

Recent XUV experiments on rare gas clusters at FLASH have proven that single-shot imaging of clusters contains valuable information on transient matter properties under intense XUV excitation [1]. These advances show that IR-XUV pump-probe experiments are in reach to illuminate the ultrafast dynamical evolution of highly excited nanosystems via the XUV scattering. However, so far no well established theory exists to fully describe the light scattering of strongly dynamical systems including nonlinear and transient effects. We propose a route to such theoretical analysis based on the recently introduced microscopic particle-in-cell (MicPIC) approach [2]. MicPIC enables us to simultaneously account for the nonlinear laser-cluster interaction dynamics including ionization, heating, and expansion along with light propagation on the fully microscopic level and without any restrictions on particle geometry. We report first theory results on XUV only and IR-XUV pump probe scenarios for large rare gas clusters up to (D∼80nm), which show the typical geometry-induced Mie scattering as well as elastic and inelastic XUV light scattering signals stemming from nonlinear effects and plasmonic excitations of the nanoplasma.

[1] C. Bostedt et al., Phys. Rev. Lett. **108**, 093401 (2012)
[2] C. Varin et al., Phys. Rev. Lett. **108**, 175007 (2012)

A 11.5 Mon 17:45 B 302

Time resolved electron spectra from clusters in the light of FLASH — •M. Müller[1], D. Rupp[1], T. Oelze[1], M. Sauppe[1], L. Flückiger[1], T. Gorkhover[1], A. Przystawik[2], M. Adolph[1], U. Frühling[2], M. Wieland[2], B. Schütte[3], A. Al-Shemmary[2], N. Stojanovic[2], S. Toleikis[2], J.-P. Müller[1], M. Krikunova[1], T. Laarmann[2], and T. Möller[1] — [1]TU Berlin, Hardenbergstr. 36, 10623 Berlin — [2]HASYLAB (DESY), Notkestr. 85, 22607 Hamburg — [3]Max-Born-Institut, Rudower Chaussee 17, 12489 Berlin

During the last ten years free-electron lasers (FEL) made highly intense and short pulses from the soft to the hard X-ray regime for the first time accessible. Facilities like FLASH opened a wide range of new research fields concerning the interaction of light with matter for example in physics, chemistry and biology.

We use rare gas clusters as a model system to study the complex interaction, which proceeds on different time scales. At first the cluster is ionized. Due to the loss of electrons and further ionization the Coulomb potential of the cluster gets deeper and the electrons are trapped in the cluster - a nanoplasma is built up. Finally the cluster is destroyed either by coulomb explosion or hydrodynamic expansion of the nanoplasma. By measuring electron and ion spectra, further insight into the ionization and recombination processes can be gained. The temporal evolution of the FEL induced plasma dynamics in clusters was further investigated by means of streaking the photoelectrons with a THz pulse, a very promising new tool at FLASH. We will give an overview of our setup and discuss first results.

A 11.6 Mon 18:00 B 302

Non-adiabatic quantum molecular dynamics with trajectory surface hopping — •Michael Fischer[1,2], Jan Handt[2], and Rüdiger Schmidt[2] — [1]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, D-01187 Dresden, Germany — [2]Institut für Theoretische Physik, Technische Universität Dresden, D-01062 Dresden, Germany

We present a simple and straightforward extension of non-adiabatic quantum molecular dynamics to approximately include electron-nuclear correlations by combining electron dynamics within time-dependent density functional theory with trajectory surface hopping dynamics for the nuclei. This approach allows for the qualitative understanding of experimentally measured collision spectra as well as

photoinduced processes as radiationless electron-nuclear relaxation. Benchmark examples from collision physics and photochemistry illustrate the improvements gained over ordinary non-adiabatic quantum molecular dynamics.

A 11.7 Mon 18:15 B 302

Die Greifswald EBIT — •Stephan Gierke[1], Christoph Biedermann[2], Gerrit Marx[1], Birgit Schabinger[1] und Lutz Schweikhard[1] — [1]Institut für Physik, Universität Greifswald, Felix-Hausdorff-Str. 6, 17489 Greifswald — [2]Max-Planck-Institut für Plasmaphysik, Wendelsteinstr. 1, 17491 Greifswald

In einer Elektronenstrahl-Ionenfalle (EBIT) werden Ionen mittels eines hoch- und monoenergetischen Elektronenstrahls erzeugt und gespeichert. Mit einem starken magnetischen Feld von 3 Tesla wird der Elektronenstrahl komprimiert, wodurch Stromdichten von 4000 A/cm^2 erreicht werden. In radialer Richtung erfolgt der Einschluss der Ionen durch die Raumladung des Elektronenstrahls und eines elektrostatischen Speicherpotentials an drei Driftröhren. Neutrale Atome werden durch Elektronenstoßionisation in der Falle schrittweise ionisiert. Der maximale Ladungszustand der erzeugten Ionen lässt sich über die Energie des Elektronenstrahls kontrollieren.
Die erzeugten hochgeladenen Ionen sollen in einem ersten Schritt in Wechselwirkung mit Fullerenen gebracht und deren Reaktionsprodukte mit einem Flugzeit-Massenspektrometer gemessen werden. Erste Voruntersuchungen mit der in Greifswald wieder in Betrieb genommenen ehemaligen Berlin EBIT [1] werden vorgestellt.
[1] C. Biedermann *et.* al, Phys. Scr. T. 73 (1997) 360