MO 23: Resonant Energy Transfer and Interatomic Coulombic Decay II

Time: Friday 10:30–12:00 Location: PA 1.150

MO 23.1 Fri 10:30 PA 1.150

Intermolecular decay mechanisms in pure and doped helium nanodroplets — •Aaron LaForge[1], Rupert Michiels[1], Carlo Callegari[2], Michele Di Fraia[2], Marcel Drabbels[3], Bruno Langbehn[4], Marcel Mudrich[5], Veronica Oliver[3], Yevheniy Ovcharenko[4], Oksana Plekan[2], Kevin Prince[2], Thomas Möller[4], and Frank Stienkemeier[1] — [1]Universität Freiburg, GermanY — [2]Elettra-Sincrotrone Trieste, Italy — [3]EPFL Lausanne, Switzerland — [4]TU Berlin Germany — [5]Aarhus University, Denmark

As opposed to molecular systems where electron dynamics proceed only through intramolecular processes, weakly bound complexes create an environment in which locally excited electrons can additionally interact with neighboring molecules leading to new intermolecular decay mechanisms. Here, we present a systematic study of intermolecular decay mechanisms in pure and doped He nanodroplets using free electron laser radiation. When resonantly excited, the nanodroplets can either exchange energy with neighboring He atoms or through the acceptor dopants. By pump-probe techniques combined with photoelectron spectroscopy, we can fully characterize and energetically resolve the different decay paths.

MO 23.2 Fri 10:45 PA 1.150

Time-Resolved Interatomic Coulomb Electron-Capture by Ba^+ through Rb proximity — •Axel Molle[1], Oriol Vendrell[2], and Annika Bande[1] — [1]Institute for Methods for Material Development, Helmholtz-Zentrum Berlin f. Materialien & Energie, Berlin — [2]Department of Physics and Astronomy, Aarhus University, Aarhus, Denmark

In this work, we will present results of a time-resolved numerical investigation of the Ultrafast Interatomic Coulomb Electron Capture (ICEC) as a first attempt to predict experiments of the near future. A species A captures a free electron in the ICEC process by long-range energy transfer through Coulomb interaction to a bound electron in a neighbouring species B, which is then ionized.

From a theoretical perspective, even though first predicted for atoms and molecules through the asymptotic approximation of scattering theory [1], investigation of the time-resolved ICEC dynamics has been successful in lower-dimensional systems [2]. From the experimental side, on the other hand, techniques for trapping ultracold ions and atom clouds are advancing. This may enable investigating ICEC in an experiment in the near future.

We thus numerically study the dynamics of such an exemplary experiment at ultracold temperatures, with a barium cation trapped in a cloud of rubidium atoms, in order to predict and pave the way for time-resolved ICEC experiments.

[1] Gokhberg / Cederbaum, Phys. Rev. A **82** (2010).

[2] Pont *et al.*, J. Phys. Condens. Matter **28** (2016).

MO 23.3 Fri 11:00 PA 1.150

Evidence for direct detection of radiative charge transfer photons from Auger final states in neon clusters — •Andreas Hans[1], Vasili Stumpf[2], Xaver Holzapfel[1], Philipp Schmidt[1], Christian Ozga[1], Catmarna Küstner-Wetekam[1], Till Jahnke[3], Arno Ehresmann[1], Philipp V. Demekhin[1], Kirill Gokhberg[2], and André Knie[1] — [1]Institut für Physik und CINSaT, Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany — [2]Physikalisch-Chemisches Institut, Universität Heidelberg, Im Neuenheimer Feld 229, 69120 Heidelberg, Germany — [3]Institut für Kernphysik, Goethe-Universität, Max-von-Laue-Str. 1, 60438 Frankfurt, Germany

Non-local charge distribution processes in dense samples like clusters and liquids have recently attracted tremendous attention in atomic and molecular physics. As a result of progress in both theory and experiment a variety of mechanisms was predicted and observed. Among them is radiative charge transfer (RCT), in which the transfer of an electron from a neutral site of a cluster to a doubly charged site is accompanied by photon emission. The occurence of RCT has been experimentally deduced from energy conservation reasons by multi-particle coincidence detection after inner-shell ionization and subsequent Auger decay in noble gas clusters. However, direct observation of the emitted photons has not been reported so far, although this might be an advantageous method to track RCT in dense matter. Here, we report evidence for the first measurement of photons emitted in an RCT process in large neon clusters.

MO 23.4 Fri 11:15 PA 1.150

Ultrafast intermolecular relaxation process in hydrated biomolecule cluster — •Xueguang Ren, Enliang Wang, Khokon Hossen, and Alexander Dorn — Max-Planck-Institut für Kernphysik, 69117 Heidelberg, Germany

It is accepted that DNA lesions are induced by secondary species like radicals and the abundant low-energy secondary electrons generated by the primary radiation. In the present work we report the observation of hitherto unrecognized damage mechanism in form of a non-local autoionizing process called intermolecular coulombic decay (ICD) which directly ionizes DNA constituents in an aqueous environment. As a model system hydrogen-bonded dimers are used which consist of one tetrahydrofuran (THF) molecule - a surrogate of deoxyribose in the DNA backbone - and one water molecule. After inner-valence ionization of water by electron impact the vacancy is filled by an electron from an outer-valence orbital and ultrafast energy transfer across the hydrogen bridge leads to ionization of the neighboring THF molecule and ejection of an electron. This energy transfer from water to THF is faster than the otherwise occurring intermolecular proton transfer. The signature of the ICD reaction is identified in triple coincidence measurements of both ions and one of the final state electrons.

MO 23.5 Fri 11:30 PA 1.150

Approaches to the Interatomic Coulombic Decay in neutral quantum dots — •Martin Lützner and Annika Bande — Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner Platz 1, 14109 Berlin, Germany

The interatomic Coulomb decay (ICD) is an ultrafast, radiationless energy transfer process between atoms and molecules. In ICD an electron in an innervalence state of an atom deexcites by transferring energy to an electron in another atom. This causes the second electron to leave the neighbouring atom if the excitation energy of the first atom lies above the ionization threshold of the second one. Recent theoretical investigations predicted ICD happening in a system of two neighbouring charged semiconductor Quantum Dots (QD).

In the current description of charged QDs electronically excited intraband states were considered. Since excitonic states are more long-lived and play a major role in the optical properties of semiconductors, it is desirable to describe neutral quantum dots. In this talk an approach on the description of ICD in neutral QDs will be given. The holes in this model are regarded as static pointlike particles. Furthermore the effects of Coulomb screening on the carrier dynamics is investigated.

MO 23.6 Fri 11:45 PA 1.150

Interatomic Coulombic Decay in Real-Life — •Robert Bennett[1], Joshua Leo Hemmerich[1], and Stefan Yoshi Buhmann[1,2] — [1]University of Freiburg, Germany — [2]Freiburg Institute for Advanced Studies (FRIAS), Freiburg, Germany

Interatomic Coulombic decay (ICD) is a mechanism by which energy can be very rapidly redistributed between molecular systems. The ICD process includes production of a free electron, which is normally of relatively low energy. These 'slow' electrons can cause damage to biological systems, in particular to DNA. Biological processes of course take place outside the idealised conditions studied so far in ICD, rather proceeding in non-trivial environments such as those found in solvent media, near a cell membrane or in a molecular chain.

In this talk I will present a newly-developed theory of ICD based on macroscopic quantum electrodynamics in media that naturally takes into account the effects of the environment, as well as those of relativistic retardation. It will be shown that orders-of-magnitude enhancement of the rate can be missed by ignoring retardation, and that the rate can be significantly enhanced or suppressed depending on the orientation of the decaying system relative to a nearby surface.