A 31: Interatomic and Intermolecular Coulombic Decay

Time: Thursday 11:00–13:00 Location: E 415

Invited Talk A 31.1 Thu 11:00 E 415

Ultralong range ICD in the He dimer, resonant Auger - ICD cascade processes — •Till Jahnke — IKF, Goethe Universität, Max-von-Laue-Str.1, 60438 Frankfurt

Interatomic (or intermolecular) Coulombic Decay (ICD) has become an extensively studied atomic decay process during the last 10 years. The talk will show examples of different systems in which ICD has been examined. In particular helium molecules (so called helium dimers) are presented in which ICD occurs over longest internuclear distances.

In ICD electrons of low energy are created as a typical decay product. Such electrons are known to effectively cause DNA double strand breakups suggesting ICD as a possible origin for radiation damage of living tissue. The group of L. Cederbaum recently suggested that ICD can be triggered efficiently and site-selectively by resonant excitation of molecules. They realized that this provides a unique tool to create low energy electrons at a specific site inside a biological system for example in order to damage malignant cells that are tagged using specific marker molecules.

Here we show experimentally that resonant Auger induced ICD can indeed be observed in model systems of small nitrogen and carbon monoxide clusters and - as expected - produces low energy electrons. Furthermore our simple model systems are able to prove the efficiency of ICD: it occurs before the individual molecule is able to undergo dissociation, i.e on a timescale <10 fs. Our findings therefore strongly support the idea of resonant Auger-ICD being a promising process to induce radiation damage at a specific site inside a high-Z-tagged cell.

Invited Talk A 31.2 Thu 11:30 E 415

Inter-atomic Coulombic decay in endohedral fullerenes — Narges Bahmanpour and •Vitali Averbukh — Department of Physics, Imperial College London, Prince Consort Rd, SW7 2AZ, London, UK

Interatomic Coulombic decay (ICD) in endohedral fullerene complexes presents a special interest due to its ultrafast and possibly non-destructive character [1]. Here we consider for the first time the variation of the decay width of the endohedral inner-valence vacancy with the displacement of the endohedral atom from the fullerene centre. Excitation of multipole fullerene plasmons by ICD in the off-centre geometry is predicted [2]. Distinction is made between averaging over classical ensemble of random displacements and over coherent vibrational state of the endohedral ion inside the cage. Finally, orbital overlap effect is considered within the lowest-order Wigner-Wesskopf theory.

[1] V. Averbukh and L. S. Cederbaum, Phys. Rev. Lett. 96, 053401 (2006).

[2] N. Bahmanpour and V. Averbukh, in preparation.

Invited Talk A 31.3 Thu 12:00 E 415

ICD-like decays in aqueous electrolytes — •Gunnar Öhrwall[1], Niklas Ottosson[2,3], and Olle Björneholm[2] — [1]MAX-lab, Univ. of Lund, Box 118, 22100 Lund, Sweden — [2]Dept. of Physics and Astronomy, Univ. of Uppsala, Box 516, 75120 Uppsala, Sweden — [3]FOM-institute AMOLF, Science Park 102, 1098 XG Amsterdam, The Netherlands

The first systems where it was predicted that inner valence-ionized states of condensed matter should relax efficiently to delocalized two-hole final states - Interatomic or Intermolecular Coulombic Decay (ICD), were hydrogen-bonded clusters, and recently the phenomenon has been observed following inner-valence ionization in hydrogen-bonded water clusters [1]. In 2005, Öhrwall et al. showed the existence of an ICD-like mechanism following O1s ionization of large water-clusters: In the de-excitation spectrum, features originating from final states delocalized over the ionized molecule and a neighboring molecule were observed, in addition to the normal Auger final states localized on the ionized species [2]. This has later also been observed in O1s ionization of liquid water.

Here, I will show examples of ICD-like decays in core-ionized aqueous ions, and in water molecules in aqueous electrolytes. I will also discuss how the efficiency for such decays depends on factors such as charge, polarizability, and solvated radius of the ionic solutes [3].

References [1] M. Mucke et al., Nat. Phys. 6 (2010) 143. [2] G. Öhrwall et al., J. Chem. Phys. 123 (2005) 054310. [3] N. Ottosson, G. Öhrwall, and O. Björneholm, Chem. Phys. Lett. 543 (2012) 1.

Invited Talk A 31.4 Thu 12:30 E 415

Intermolecular Coulomb decay at heterogeneous interfaces — •Thomas Orlando[1,2] and Gregory Grieves[1] — [1]School of Chemisty and Biochemistry, Georgia Institute of Technology, Atlanta, Georgia-USA — [2]School of Physics, Georgia Institute of Technology, Atlanta, Georgia-USA

We investigate low-energy (1-250 eV) electron interactions with complex targets with a particular emphasis on understanding correlated electron interactions and energy exchange in the deep valence and shallow core regions of the collision targets. Specifically, we demonstrate that ejection of $H^+(H_2O)_{n=1-8}$ from low energy electron irradiated water clusters adsorbed on graphite and graphite overlayers of Ar, Kr or Xe results from intermolecular Coulomb decay (ICD). Inner valence holes in water ($2a_1^{-1}$), Ar ($3s^{-1}$), Kr ($4s^{-1}$) and Xe ($5s^{-1}$) levels correlate with the cluster appearance thresholds and initiate ICD. Proton transfer occurs during or immediately after ICD and the resultant Coulomb explosion leads to $H^+(H_2O)_{n=1-8}$ desorption with kinetic energies that vary with initiating state, final state and inter-atomic/molecular distances. Since ICD can create reactive protons and low energy electrons locally, this process may contribute to radiation-induced damage of hydrated DNA.