Electron impact ionization as a fundamental few-body reaction and a tool to study molecular dynamics

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Synopsis Progress in reaction microscope studies of atomic and molecular ionization by electron impact is discussed. Proceeding from simple atoms to small organic molecular clusters kinematically complete experiments allow to analyse few to many-body reactions which are relevant wherever ionizing radiation interacts with matter.

This talk discusses studies of electron impact ionization of atoms, molecules and clusters in which all momenta of the participating collision partners are specified. The early (e,2e) experiments using electrostatic electron spectrometers provided detailed insight in fundamental few-particle dynamics. Consequently theory advanced tremendously culminating, e.g., in exact solutions of the Coulombic three-body problem.

I will present investigations extending the limits of these conventional instruments by using multi-electron - ion imaging spectrometers (reaction microscopes). These allow accessing the full solid angle of particle emission, small cross sections down to 10^{-21} cm^2, coincident detection of up to five particles as well as usage of low-density targets like cluster beams and weak positron projectile beams.

Our earlier studies of few-body (e,ne) reactions confirmed that the most fundamental atomic systems are well understood in present days while there are open questions and challenges for larger atoms, for the four-body continuum (i.e. double ionization) and for reversing the projectile charge sign by studying positron impact. Proceeding to molecules with a number of more degrees of freedom it is intriguing to analyze the ionization dynamics as function of their spatial alignment. Likewise the binding energy of the ionized orbital determines the molecular fate concerning its dissociation and here molecular dynamics simulations can facilitate the interpretation.

We extended these investigations to molecules embedded in an environment like it is the case in weakly bound clusters where the ionization dynamics is modified and new reaction channels are emerging. On one hand we confirmed that molecular ions can stabilize by dissipating their internal energy to the environment. On the other hand we identified dimers where only the ionization-induced intermolecular vibrations initiate molecular fragmentation [1]. Other phenomena in ionized clusters are the suppression of molecular roaming [2] and the transfer of electronic energy to a neighbor ionizing it and initiating a Coulomb explosion. While this latter so-called inter-molecular Coulombic decay (ICD) process was mostly studied for photoionization, it is likewise important for electron impact. We have found ICD for a number of bio-relevant molecular dimers as hydrated pyridine, hydrated tetrahydrofuran and also for benzene dimers [3]. For these species the accessibility of the ICD channel delicately depends on the energy spectrum of the inner-valence vacancies and the lowest monomer and dimer double ionization energies [4].

From these observations it is expected that ICD is a widespread phenomenon in loosely bound matter and that ICD can initiate the direct damage of hydrated biomolecules such as DNA in the irradiation of biological tissue.

References

[1] Wang E *et al.* 2020 *Nat. Comm.* **11**:2194
[2] Wang E *et al.* 2021 *Phys. Rev. Lett.* **126** 103402
[3] Ren X *et al.* 2021 *Nat. Chem.* **14**, 232
[4] Skitnevskaya A D, *et al.* 2023 *J. Phys. Chem. Lett.* **14** 1418

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