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Dynamical coupling of electrons and ions in Xray-induced dynamics

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Synopsis Photo-absorption from short and intense Xray pulses by a molecule or a cluster triggers a complicated electron and ion dynamics. Whereas the excitation process concerns largely core-shell electrons, there are various subsequent relaxation channels like electronic decays and ionic Coulomb explosion. We will discuss the interplay of those processes for molecular clusters and fullerenes.

Multiple ionization of a polyatomic system in an intense X-ray pulse lead — in contrast to narrow photo lines observed for atoms — to broad photo-electron spectra [1, 2], since the charge built-up modifies the overall potential, as shown in the figure below for a C_{60} molecule. Typically such spectra are difficult to interpret. Fullerenes offers a way to separate out the electron dynamics since the cage structure confines spatially the origin of photo and Auger electrons. Together with the sequential nature of the photo processes at intensities available at X-ray free electron lasers, this allows for a remarkably detailed interpretation of the photo-electron spectra [3]. The general features derived can serve as a paradigm for situations where an ion dynamics becomes relevant. For C_{60} this may occur already for pulses as short as 10 fs.

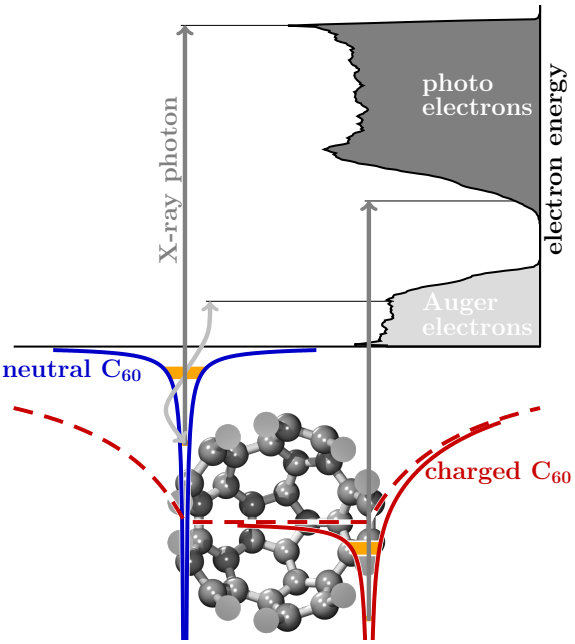

Figure: Sketch of the formation of broad electron spectra. The highest energy is observed for photo-ionization of core electrons from neutral C_{60} (blue solid line on the left). For a charged C_{60} (red solid line on the right) the energy is reduced due to the background potential (red dashed line).

The situation becomes more involved for clusters consisting of small molecules. We study systematically the electronic sequence of methane CH_4, ammonia NH_3, and water H_2O clusters, augmented by the "atomic limit" of neon clusters. Those containing hydrogen do eject fast protons when illuminated by short X-ray pulses. A suitable overall charging of the cluster controlled by the X-ray intensity induces electron migration from the surface to the bulk leading to efficient segregation of the protons. This "dynamical segregation" hinders globally the explosion of the heavy atoms even outside the screened volume. In contrast to core-shell systems where the outer shell is sacrificed to reduce radiation damage, the intricate proton dynamics of hydride clusters allows one to keep the entire backbone of heavy atoms intact [4]. Further studies on large molecules — being neither as homogeneous nor as spherical as the molecular cluster above — confirm this segregation effect [5].

References

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