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Coulomb explosion imaging of small organic molecules at LCLS

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Synopsis Fragmentation of small organic molecules by intense few-femtosecond X-ray free-electron laser pulses has been studied using Coulomb explosion imaging. By measuring kinetic energies and emission angles of the ionic fragments in coincidence, we disentangle different fragmentation pathways, for certain cases can reconstruct molecular geometry at the moment of explosion, and show how it depends on LCLS pulse duration.

The development of free-electron lasers (FEL) delivering intense ultrashort coherent X-ray pulses paves the way towards structural investigations of matter with atomic spatial and femtosecond time resolution. One of the basic underlying processes for all of these studies is an inner-shell (multi-) photon absorption followed by the Auger or radiative decay and structural rearrangement (atomic motion and charge redistribution), often proceeding on comparable femtosecond time scale.

Here we have studied multiple fragmentation of small organic molecules upon multiphoton inner-shell ionization by intense (> 10^{16} W/cm^2) short (3-200 fs) 2 keV pulses provided by the Linac Coherent Light Source (LCLS) at Stanford. In order to increase and localize X-ray absorption, we used methylselenol (CH_3SeH), ethylselenol (C_2H_5SeH) and phenylselenol (C_6H_5SeH) compounds containing high-Z selenium atom as a substitute for naturally occurring oxygen. The experiment was conducted in the CFEL-ASG Multi-Purpose (CAMP) end station [1] installed at the AMO beamline of LCLS. By measuring kinetic energies and emission angles of the ionic fragments in coincidence, we can separate different fragmentation pathways and, for certain cases, reconstruct molecular geometry (bond lengths and angles) at the moment of explosion. In particular, in case of methylselenol proton energies and emission angles in the molecular frame can be defined for each of the identified pairs of heavy ion fragments (shown in Fig. 1). Comparing these data for a given final state and different pulse durations, we observe lower proton energies for longer pulses. This indicates molecular deformation during the pulse, which has direct implications for the studies of radiation damage. Overall, the results yield unique information on the structural rearrangement the molecule undergoes upon few-photon absorption, in particular, pointing to the ultrafast charge redistribution within the molecule.

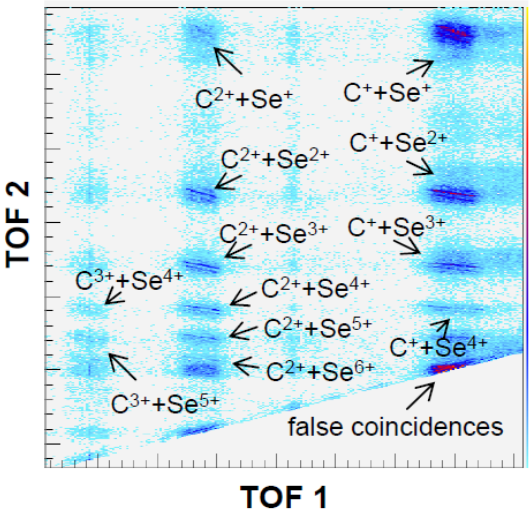

Figure 1. Photoion-photoion coincidence spectrum measured after Coulomb explosion of methylselenol by 3 fs LCLS pulses at 2 keV photon energy.

References

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