Electronic structure at high x-ray intensity

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A unique opportunity offered by x-ray free-electron lasers is atomic-resolution imaging of individual macromolecular systems. It is well recognized that in such a single-shot single-molecule measurement, the x-ray pulse must be shorter than the time scale associated with the nuclear dynamics caused by the x-ray-driven electronic radiation damage. However, the x-ray-induced electronic damage itself, which directly affects the x-ray scattering pattern, is much more difficult to suppress. For this reason, a quantitative understanding of the electronic structure of polyatomic systems exposed to femtosecond x-ray pulses at intensities approaching (or exceeding) 10^20 W/cm^2 is crucial. To this end, we have been developing dedicated computational tools that allow us to predict the ultrafast molecular response at such unprecedentedly high x-ray intensities [1-4]. These tools, which represent the state of the art in modeling single-shot electronic damage in molecular matter, have been tested experimentally and have been instrumental in identifying new ionization enhancement mechanisms.

References:

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