What happens to atoms and molecules during x-ray free-electron laser pulses?

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X-ray free-electron lasers (XFEL) open a new era in science and technology, offering many unique opportunities that have not been conceivable with conventional light sources. Because of their very high x-ray photon fluence within very short pulse duration, materials interacting with XFEL undergo significant radiation damage, i.e., they possibly become highly ionized and then explode. To comprehend underlying physics, it is crucial to understand detailed ionization and fragmentation dynamics of atoms and molecules during intense XFEL pulses. In this talk, I will present a theoretical framework to treat x-ray-induced processes and to simulate radiation damage dynamics, introducing two dedicated x-ray physics toolkits, XATOM and XMOLECULE. They can provide a fundamental insight to understand how matter interact with intense XFEL pulses. I will discuss how theory can explain recent experiments conducted at LCLS and SACLA, for instance, deep inner-shell multiphoton ionization and ultrafast x-ray-induced explosion of small polyatomic molecules, and how it can lead to new XFEL experiments.

References

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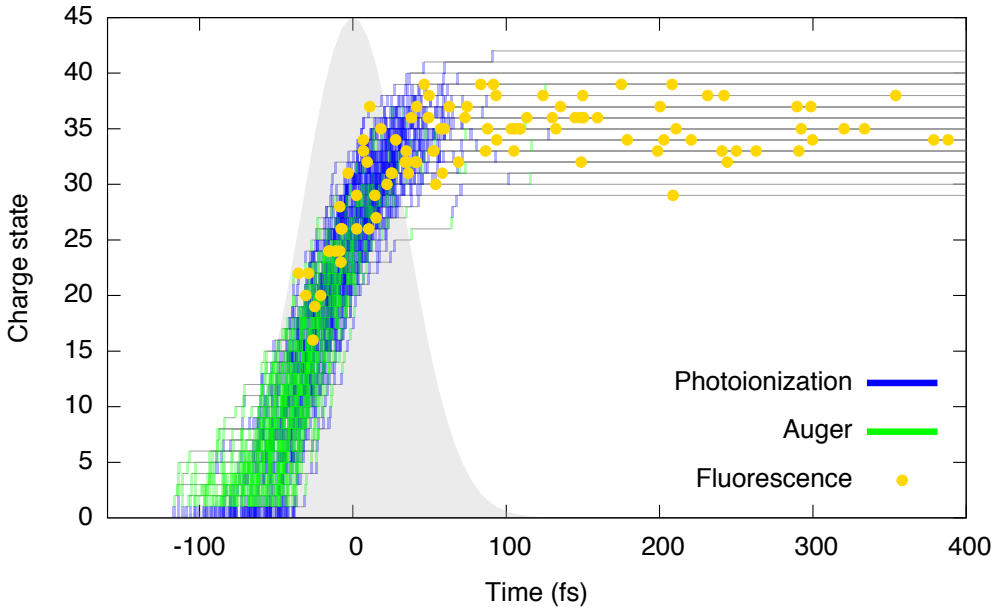

Figure: Exemplary pathways of multiphoton multiple ionization dynamics of Xe at 4.5 keV.