XATOM: AN INTEGRATED TOOLKIT FOR X-RAY AND ATOMIC PHYSICS

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X-ray free-electron lasers (XFEL) open a new era in science and technology, offering many possibilities that have not been conceivable with conventional light sources. Because of their very high fluence within very short pulse duration, materials interacting with XFEL undergo significant radiation damage with ejection of electrons, leading to the creation of warm dense matter or plasma. To comprehend the underlying physics, it is crucial to understand detailed ionization and relaxation dynamics in individual atoms during XFEL pulses.

Here we present an integrated toolkit to investigate x-ray–induced atomic processes and to simulate electronic damage dynamics. This toolkit can easily handle all possible electronic configurations of all atom/ion species, and calculate physical observables during/after intense x-ray pulses. Based on nonrelativistic quantum electrodynamics and perturbation theory within the Hartree–Fock–Slater model, the toolkit can compute the photoionization cross sections, Auger and Coster–Kronig decay rates, fluorescence rates, shake-off branching ratios, and elastic x-ray scattering form factors and their dispersive correction. For electronic dynamics during intense x-ray pulses, it employs the rate equation approach with all computed cross sections and rates for all possible configurations, and then produces charge state distribution, electron and fluorescence spectra, scattering signals, and so on.

This XATOM toolkit has been successfully applied to study many XFEL-related phenomena: for instances, scattering dynamics in relation to hollow-atom formation [1], nonlinear x-ray absorption processes [2], multiphoton ionization of heavy noble gases [3], and molecular imaging with multi-wavelength anomalous diffraction at high x-ray intensity [4]. The toolkit enables us to connect details of electronic dynamics in atoms and the evolution of atomic processes in plasmas generated by XFEL.

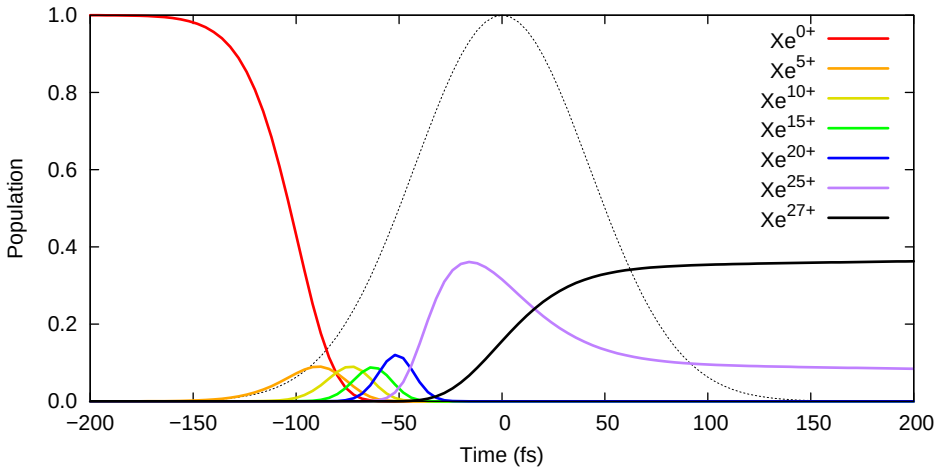

Figure 1. Time evolution of populations of several selected charge states of Xe in an XFEL pulse.

References

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