Radiation-induced collision cascades with ab initio informed two-temperature molecular dynamics

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The prediction of primary radiation damage formation is highly sensitive to how the incident projectile's kinetic energy is distributed between the atomic and electronic subsystems of the target material. However, accurately accounting for electronic effects in large-scale, multi-million atom simulations of radiation-induced collision cascades remains a persistent challenge in radiation damage modeling. Energetic projectiles lose kinetic energy quickly through electronic stopping as they move through a material, while in near-equilibrium conditions, electrons and ions interact via electron-phonon coupling, which has an effective strength much weaker than that of electronic stopping energy losses. Furthermore, neither electronic stopping nor electron-phonon coupling can adequately describe the energy losses for all atoms involved in the cascade process, where atoms transition continuously from a high-energy regime to equilibrium, while experiencing a highly disordered, under-dense state of the material during the heat spike phase.

Real-time time-dependent density functional theory (rt-TDDFT) has successfully calculated the electronic stopping power of ions along various trajectories and can also reveal how energy dissipation depends on the local atomic and electronic environment of the projectile. These rt-TDDFT results can be used to inform large-scale molecular dynamics simulations, applying a two-temperature model in which the coupling between the electronic and atomic subsystems varies with the local environment and is fitted to the *ab initio* data. In this talk, I will demonstrate that the essentially parameter-free model developed through this fitting process accurately captures the instantaneous energy losses of atoms throughout the highly non-equilibrium cascade process. The high-energy regime is validated through direct comparisons to ion range experiments, while the low-energy regime reflects the expected characteristics of electron-phonon coupling and phonon dispersion. Simulations of full collision cascades predict two distinct coupling regimes that operate on different time scales without requiring separate coupling terms. The model yields an effectively nonlinear velocity dependence of the dissipation for atoms in the heat spike phase of collision cascades.