Modeling of fundamental mechanisms initiated by x-ray irradiation: from atomic to nanometer scales

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Radiation-induced chemistry begins with electronic processes occurring on attosecond-to-femtosecond timescales [1-2] but evolves through molecular and chemical dynamics over picoseconds and beyond [3]. Establishing predictive connections across these disparate time and length scales remains a major challenge in modeling radiation–matter interactions. We are developing multiscale computational approaches [4-8] that connect the initial interaction of energetic photons with matter to electronic relaxation, secondary-electron production, and subsequent molecular dynamics. Electronic-structure calculations and Monte Carlo simulations yield evolving electronic configurations, charge states [4-7], and secondary-electron distributions that provide microscopic inputs for longer-timescale simulations [8].

Applications to x-ray-matter interactions will illustrate how local electronic processes couple to the surrounding environment [4-9]. X-ray spectroscopic observables provide sensitivity to electronic structure and local environments at atomic length scales [1-2], while x-ray scattering and reciprocal-space imaging provide complementary information on spatial correlations and structural dynamics at nanometer length scales [9]. Together, these complementary observables provide opportunities to test and constrain models across scales. Strategies for cross-scale modeling will be discussed, spanning electronic-structure and stochastic simulations, electron transport and energy deposition, molecular dynamics, and continuum descriptions. Such approaches could provide a microscopic foundation for understanding how radiation absorption ultimately leads to chemical and material transformations in complex environments.

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