

QUANTUM MOLECULAR DYNAMICS FOR X-RAY INDUCED STRUCTURAL DAMAGE

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We will present a quantum dynamics theory for modelling the structural damage of molecules following the autoionization decay of molecular core-hole states generated by X-rays. Our theory will model the fundamental processes underlying the distortion of metalloprotein geometries characterized by X-ray crystallography, as well as the decay of radionucleotides used in highly targeted cancer-therapies. Both the absorption of X-rays and radionucleotide decay creates unstable core-hole states which can decay via autoionization involving the ejection of an electron and the collapse of another to the core-hole. The structural damage occurs via the Coulomb explosion of highly charged molecular cations created by the autoionization. Hence, simulations coupling the autoionization to structural dynamics will provide fundamental insight into this complex phenomenon. However, the required theoretical treatment is challenging, due to the complexity of autoionization and exponential scaling of possible decay channels with respect to the system size. Here we propose a quantum molecular dynamics method, which uses a time-dependent set of trajectory functions for modelling autoionization decay across multiple potential energy surfaces. The initial implementation of our method uses autoionization rates from atomic simulations, and our results are benchmarked against experimental x-ray/ion coincidence data of IBr molecule.

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