

Nonlinear X-ray Spectroscopy of Molecules — Simulation Methods, Applications and Challenges

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The recently developed intense X-ray laser sources offer new opportunities to detect molecular structure and dynamics at an unprecedented level, thanks to the element selectivity and localized nature of core excitations generated by ultrashort X-ray pulses. Nonlinear infrared or optical spectroscopy techniques which have been proven successful are now extended to the X-ray regime. Here we briefly survey the quantum chemistry methods of nonlinear X-ray spectroscopy simulation of molecules, introduce the possible applications of nonlinear X-ray spectroscopy signals, and discuss the existing challenges in theoretical development.