

Abstract Submitted
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Radiation damage dynamics of light and heavy atoms of biological significance in Hartree-Fock and Kohn-Sham models¹ ALEXANDER KOZLOV, HARRY M. QUINEY, Univ of Melbourne — Simulations of radiation damage in single molecule imaging using X-ray free electron laser use atomic rates calculated in the lowest order [?, ?]. We investigate the difference in ionization dynamics predicted by Hartree-Fock and Kohn-Sham methods for light and heavy elements of biological significance. These methods produce very similar results for light atoms in short and bright pulses. For heavy atoms and light atoms in pulses with smaller peak intensity the predictions of the models may differ considerably. The presented analysis allows us to predict if two approaches will produce similar results for a given atom and a pulse with specified parameters. We demonstrate the sensitivity of the charge state dynamics to Auger rates and discuss the choice of effective potential and gauge for fluorescence and photoionization processes.

K. Moribayashi, X-Ray Spectroscopy (2012).

P. J. Ho and C. Knight, J. Phys. B. **50**, 104003 (2017).

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