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Auger spectrum of a water molecule after single and double core ionization LUDGER INHESTER, CARL F. BURMEISTER, GERRIT GROENHOF, HELMUT GRUBMUELLER, Max Planck Institut for Biophysical Chemistry — The high intensity of Free Electron Lasers (FEL) opens up the possibility to perform single-shot molecule scattering experiments. However, even for small molecules radiation damage induced by absorption of intense x-ray radiation is not yet fully understood. To provide insight into this process, we have studied the dynamics of water molecules in single and double core ionized states by means of electronic transition rate calculations and ab initio molecular dynamics (MD) simulations. From MD trajectories photoionization and Auger transition rates were computed based on electronic continuum wavefunctions obtained by explicit integration of the coupled radial Schrödinger equations. To account for the nuclear dynamics during the core hole lifetime, the calculated electron emission spectra for different molecular geometries were accumulated according to the obtained time-dependent populations. We find that, in contrast to the single core ionized water molecule, the nuclear dynamics for the double core ionized water molecule during the core hole lifetime leaves a clear fingerprint on the electron emission spectra. In addition, the lifetime of the double core ionized water was found to be significantly shorter than half of the single core hole lifetime.

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