ACTINIDE M-EDGE X-RAY SPECTROSCOPY USING SPINOR-BASED COUPLED-CLUSTER TECHNIQUES

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We present spinor-based relativistic equation-of-motion coupled-cluster (EOM-CC) calculations for the actinide M-edge x-ray absorption spectra for uranyl, neptunyl, and plutonyl-containing molecules. An efficient implementation of core-valence separation for the spinor-based EOM-CC methods have enabled the calculations of the x-ray absorption spectra with rigorous treatments of relativistic and correlation effects. The benchmark calculations demonstrate the importance of the spin-orbit coupling and solvation effects on the computed spectra. The computed spectra are then compared with high-resolution x-ray absorption spectra extracted from the resonant inelastic x-ray spectroscopy (RIXS) map. The covalency of actinide 5f electrons is discussed.