THE ELECTRONIC STRUCTURE OF THE PLUTONYL ION

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Restricted Hartree-Fock (RHF) and spin-orbit configuration-interaction (SOCI) calculations were performed on the ground and low-lying excited states of the plutonyl ion, $PuO_2^{2+}$. These results are compared to density functional theory (DFT) results obtained using generalized gradient corrections. The low energy transitions are $f \rightarrow f$. Information on the vibrational modes will also be presented. For the ab initio work, the actinides are modeled with relativistic effective core potentials and Gaussian correlation consistent double-zeta plus polarization basis sets. The DFT work used Slater basis sets.