

## MULTIREFERENCE CALCULATIONS ON THE GROUND AND EXCITED STATES AND DISSOCIATION ENERGIES OF LANTHANIDE AND ACTINIDE OXIDES AND FLUORIDES

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High-level ab initio approaches are often necessary in detailing the many excited states and spin multiplicities of lanthanide and actinide species, while offering reliable routes towards calculating accurate spectroscopic properties. In this work, multi-reference methodologies including the complete active space self-consistent field (CASSCF) and multi-reference configuration interaction (MRCI) methods were utilized to calculate the ground and excited state properties of lanthanide and actinide oxides and fluorides. Potential energy curves for the ground state, several excited states, and different dissociation channels were determined. Spin-orbit corrections were performed by diagonalizing the MRCI wavefunction on the basis of the Breit-Pauli Hamiltonian. Bond dissociation energies (BDEs) of the lanthanide and actinide oxides and fluorides species were also determined, and the impact of core-valence, relativistic, and spin-orbit contributions to the ground state were considered. Density functional theory (DFT) and wavefunction method predictions were compared.