CALCULATIONS OF ACTINIDE- AND LANTHANIDE-CONTAINING SMALL MOLECULES USING SPINOR-BASED RELATIVISTIC COUPLED-CLUSTER METHODS

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Neodymium and uranium mono-oxide (NdO and UO) and the corresponding anions and cations are of interest to both experimental and theoretical studies. These systems exhibit a high density of low-lying electronic states and strong correlation among valence f-type electrons. They thus emerge as challenging examples for electronic-structure calculations. In this presentation, we demonstrate the usefulness of coupled-cluster techniques in understanding many properties of low-lying electronic states including ionization energies, electron affinities, and geometrical constants. We show that the inclusion of spin-orbit coupling in orbitals plays an important role in the capability to treat dense electronic states using single reference methods. Possible extension to treat transuranium-containing small molecules is discussed.