Restricted Active Space (RAS) approach to uranium compounds: An effort towards multi-reference methods for more complex electronic structure or larger molecule

Fan Wei

Supercomputing Center, CNIC, CAS

E-mail: weifan@sccas.cn

Abstract

We have applied the restricted active space second-order perturbation theory (RASPT2) on a series uranium compounds, including uranium dinitride (UN_2), uranium hexafluoride (UF_6) and Uranium chloride anion, etc. We have evaluated some different construction of restricted active space, to make our method applicable for treating the electronic structure of central uranium and the ligands simultaneously under limited computational cost. The RASPT2 scheme has achieved comparable accuracy for complete active space (CASPT2) theory. We have modeled several electronic spectra of target compounds such as the absorption spectra, electron-impact spectra and photonelectron spectra (PES), which were consistent with experimental data.