Relativistic Multi-Reference *Ab Initio* Studies of Excited States of Heavy-Element Complexes

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Abstract

Electronic structures of heavy-element complexes are complicated due to significant relativistic effects and strong electron correlation. Theoretical investigations are required to provide a fundamental understanding of the ground-state and excited-state properties. While computational modeling of excited states of heavy-element complexes is challenging, progress has been made in the recent years in interpreting their electronic adsorption and emission spectra. In this talk we will present our computational investigation results on the structures, stabilities, excitation energies, and fluorescence spectroscopic properties of gold and actinide complexes using relativistic quantum chemistry methods. We have investigated the optimal structures and excitation energies of AuX_2^- (X = halogen, CN), UO_2^{2+}, NUO^+, UN_2, UF_6, $(Ar)_xUO_2Cl_2$, $NpO_2Cl_4^{2-}$ and hydrated uranyl-glycine-water complexes using relativistic wavefunction theory (WFT) and density functional theory (DFT).[1-5] The calculated excitation energies and simulated fluorescence spectra using a time-dependent theory of electronic spectroscopy and a spin-orbit state-interacting approach are in good agreement with experiments.

References:

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