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**Evaluation of density functionals using valence and core excited spectra of Ni(II) tetrahlides** MATT QUEEN, Montana State University, Bozeman, MT, HARLAN BYKER, Pleotint, LLC, ROBERT SZILAGYI, Montana State University, Bozeman, MT — We present a systematic evaluation of the performance of various density functional theories using the series of tetrahalide complexes of nickel(II). We report the accuracy of the ground state electronic structure from calculations employing gradient corrected (GGA), hybrid GGA, and meta-GGA functionals with systematic variation of exchange and correlation functions. Reference data for these calculations included valence and core excitation spectroscopic results and molecular geometry data. The core excitation spectra at the Ni L-edges and Cl K-edges were analyzed for extracting experimental orbital coefficient information of the lowest lying unoccupied frontier orbitals. Both the core and valence excitation spectra were simulated using time dependent density functional theory. In order to probe the basis set saturation effect *ab initio* calculations were also performed. The theoretically converging series of post-SCF methods allowed us for the evaluation of basis set saturation. The calculated atomic spin densities, orbital energies, and excitation data are compared to those from density functional calculations. A new hybrid functional is presented for the most reasonable description of the ground state of nickel(II) complexes.

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