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Ab Initio Computation of Spin Orbit Coupling Effects on Magnetic Properties of Iron-Containing Complexes and Proteins FREDY AQUINO, JORGE H. RODRIGUEZ, Department of Physics, Purdue University, West Lafayette, IN 47907-2036 — Zero-Field Splittings (ZFS) in metalloproteins and other metal complexes arise from the combined action of crystalline fields acting on the metal valence electrons and spin-orbit coupling (SOC), a relativistic effect. The ab-initio calculation of ZFS parameters of metal-containing (bio)molecules is a challenging computational problem of practical relevance to metalloenzyme biochemistry, inorganic chemistry, and molecular-based bio- nanotechnology. We have implemented a methodology which treats the nonrelativistic electronic structure of magnetic (bio) molecules within the framework of spin density functional theory (SDFT) and adds the relativistic effects of SOC via perturbation theory (PT). This combined SDFT-PT approach allowed us to compute the ZFS parameters of iron-containing complexes and non-heme iron proteins with a good degree of accuracy. We also developed a semiquantitative approach to elucidate the physico-chemical origin of the magnitudes of ZFS parameters. We present results for biochemically relevant iron complexes and for nitric oxide-containing non-heme iron proteins, such as isopenicillin N synthase, which have unusually large ZFS. The computed ZFS parameters are in good agreement with experiment. Supported by NSF CAREER Award CHE- 0349189 (JHR).

Jorge H. Rodriguez
Purdue University

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