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Ab Initio Calculation of Zero Field Splitting Parameters of Iron Complexes and Molecular Magnets FREDY AQUINO, JORGE H. RODRIGUEZ, Department of Physics, Purdue University — Zero-Field Splittings (ZFS) in metal complexes arise from the combined action of crystalline fields acting on the metal valence shells and spin-orbit coupling, a relativistic effect. The Ab-Initio calculation of Zero-Field Splitting parameters, $H_{ZFS} = D[S_z^2 + \frac{1}{3}S(S+1)] + E(S_x^2 - S_y^2)$, of metal-containing molecules is a challenging computational problem of practical relevance to biology and molecular-based nanotechnology. Metal-containing molecular magnets, in particular, have been postulated as potentially useful highly dense memory storage devices depending on the magnitudes and signs of their ZFS parameters (i.e., magnetic anisotropies). We present results based on a computational methodology which treats the non-relativistic electronic structure of magnetic molecules within the framework of spin density functional theory (SDFT) and adds the relativistic effects of spin-orbit coupling via second order perturbation theory (PT). This combined SDFT-PT approach has allowed us to compute from first principles the ZFS parameters of iron-containing complexes with a fairly good degree of accuracy. We present results for some biologically relevant iron complexes which serve as models for metal centers in proteins and which display fairly large ZFS. The computed parameters depend strongly on the molecular geometries. Some functionals within the generalized gradient approximation of SDFT yield fairly satisfactory results. Supported by NSF.

Jorge Rodriguez
Department of Physics, Purdue University

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