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Accurate computation and interpretation of spin-dependent properties in metalloproteins[1] JORGE RODRIGUEZ, Department of Physics, Purdue University — Nature uses the properties of open-shell transition metal ions to carry out a variety of functions associated with vital life processes. Mononuclear and binuclear iron centers, in particular, are intriguing structural motifs present in many heme and non-heme proteins. Hemerythrin and methane monooxigenase, for example, are members of the latter class whose diiron active sites display magnetic ordering. We have developed a computational protocol based on spin density functional theory (SDFT) to accurately predict physico-chemical parameters of metal sites in proteins and bioinorganic complexes which traditionally had only been determined from experiment. We have used this new methodology to perform a comprehensive study of the electronic structure and magnetic properties of heme and non-heme iron proteins and related model compounds. We have been able to predict with a high degree of accuracy spectroscopic (Mössbauer, EPR, UV-vis, Raman) and magnetization parameters of iron proteins and, at the same time, gained unprecedented microscopic understanding of their physico-chemical properties. Our results have allowed us to establish important correlations between the electronic structure, geometry, spectroscopic data, and biochemical function of heme and non-heme iron proteins.

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