

Abstract Submitted  
for the MAR12 Meeting of  
The American Physical Society

**Elucidating Structure and Catalytic Cycles of Anti- or Ferro-magnetic Iron Enzymes from Spin Density Functional Theory**<sup>1</sup> JORGE H. RODRIGUEZ, Department of Physics, Purdue University — Nature uses metal-containing enzymes to catalyze important biochemical reactions. Some enzymes, such as methane monooxygenase hydroxylase (MMOH), contain (anti)ferromagnetic binuclear iron centers that interact with dioxygen and/or other substrates to facilitate biochemical functions. We have studied the electronic and magnetic structures of several enzyme binuclear iron centers and predicted their spectroscopic properties. We have used spin density functional theory (SDFT) to predict <sup>57</sup>Fe Mössbauer and other spectral parameters of MMOH and structurally related iron-containing enzymes. Upon dioxygen binding, the diiron center of MMOH undergoes a ferromagnetic to antiferromagnetic transition which may play an important role in its catalytic activity. In addition, based on our ability to predict spectroscopic data, we have been able to predict the structure of a key reaction intermediate in the MMOH catalytic cycle for which there is no X-ray structure.

<sup>1</sup>Funded, in part, by NSF CAREER award CHE-0349189

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Date submitted: 11 Nov 2011

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