

Abstract Submitted  
for the MAR11 Meeting of  
The American Physical Society

**First-Principles Study of Muon Trapping in Singlet and Triplet States of Oxyhemoglobin** S.R. BADU, Department of Physics and Astronomy, University of Utah, ACHANA DUBEY, Department of Physics, UCF, LEE CHOW, Physics Department, UCF, R.H. PINK, Physics Department, SUNY Albany, R.H. SCHEICHER, Department of Physics and Astronomy, Uppsala University, K. NAGAMINE, Physics Department, UCR, N. SAHOO, UTMD Anderson, T.P. DAS<sup>1</sup>, Department of Physics, SUNY Albany — Observation of muon spin-lattice relaxation effects in Oxyhemoglobin by the muon-spin rotation ( $\mu$ SR) technique [1] has sparked current interest in the possibility of magnetic character in Oxyhemoglobin (OxyHb). First-Principles variational Hartree-Fock Many Body Perturbation Theory (VHFMBPT) technique investigations on the singlet and triplet states of pure (OxyHb) have shown [2] that the triplet state is considerably higher than the singlet state ruling out magnetic character. However the charge distribution obtained by the VHFMBPT procedure in both states show a number of sites that have negative charges where the trapping of muon is being investigated to examine if the energy gap in the ordering of singlet and triplet states can be reduced or reversed leading to magnetic effects. Other possible sources of magnetism in Oxyhemoglobin will also be discussed. [1] K. Nagamine et al. Proc. Japan. Acad. B-Physics 83, 120 (2007); [2] S.R. Badu et al. Reported at Third Joint HFI-NQI International Conference, CERN, Geneva, September 2010.

<sup>1</sup>Also Department of Physics, University of Central Florida

T.P. Das  
Department of Physics, SUNY Albany

Date submitted: 22 Dec 2010

Electronic form version 1.4