Abstract Submitted
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First-Principles Study of Muon Trapping in Singlet and Triplet States of Oxyhemoglobin ROGER PINK, S.R. BADU, T.P. DAS, Department of Physics, University at Albany, SUNY, N. SAHOO, UTMD Anderson, LEE CHOW, Department of Physics, University of Central Florida, R.H. SCHEICHER, Uppsala University, K. NAGAMINE, Department of Physics, UCR — There is great current interest in the possibility of magnetic character in oxyhemoglobin (OxyHb) due to the detection [1] of muon spin-lattice relaxation in 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.

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