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First Principles Electronic Structure Investigation of Singlet and Triplet States of Oxyhemoglobin by Hartree-Fock Procedure Combined with Many-Body Perturbation Theory S.R. BADU, SUNY Albany, ARCHANA DUBEY, UCF Orlando, R.H. SCHEICHER, Uppsala University, Sweden, N. SAHOO, UTMD Anderson Cancer Center, Houston, R.H. PINK, SUNY Albany, A. SCHULTE, H.P. SAHA, LEE CHOW, UCF Orlando, K. NAGAMINE, UC Riverside, T.P. DAS, SUNY Albany — Interest in the possibility of magnetic character of oxyhemoglobin has been recently stimulated by spin-lattice relaxation effects studied [1] by the muon-spin rotation technique. In view of this, we have carried out first-principles electronic structure investigations involving Hartree-Fock theory combined with many body perturbation effects on the singlet and triplet states of oxyhemoglobin. Our results indicates using two recent x-ray structural data [2,3] for oxyhemoglobin that, using only Hartree-Fock theory without correlation effects included, the singlet state lies above the triplet state by about 0.08a.u.[2] and 0.13a.u.[3]. Incorporation of many body effects by perturbation methods reverses the order with the triplet state located 0.18a.u.[2] and 0.14a.u.[3] respectively above the singlet state. Physical reasons for these relative orderings of the singlet and triplet states will be discussed.

[1] K. Nagamine etal. Proc. Acad.Ser.B 83,120(2007).
[2] Massimo Paoli etal. J.Mol. Biol. 256,775(1996).
[3] Sam-Yong Park etal. J.Mol. Biol. 360,690(2006)

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