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First Principles Study of Muonium Trapping and Associated Magnetic Hyperfine Interactions in Nucleobases in Single and Double Chain DNA and Solid Nucleobases S.R. BADU, R.H. PINK, SUNY Albany, ARCHANA DUBEY, UCF Orlando, R.H. SCHEICHER, Uppsala University, Sweden, H.P. SAHA, UCF Orlando, K. NAGAMINE, UC Riverside, E. TORIKAI, Yamanashi University, LEE CHOW, UCF Orlando, M.B. HUANG, T.P. DAS, SUNY Albany — The trapping of muonium (Mu) and muon hyperfine interactions (HFI) are studied for free nucleobases and nucleobases in single and double strand DNA and in solid nucleobases. For our investigations we have utilized the Hartree-Fock procedure with many-body effects included using many-body perturbation theory. Results for the muon magnetic contact and dipolar HFI will be presented for the various environments. The trends among the different environments is rather different from those for the nuclear quadrupole interactions in the corresponding systems because of the differences in geometry of the Mu trapping sites in the various systems. Quantitative comparison will be made between our theoretical results and experimentally measured¹ muon HFI properties in the solid nucleobases.

¹Penny L Hubbard et al., J. Phys. Chem. A108, 9302 (2004).

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