

Abstract Submitted  
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**Study of Electronic Structures of Nucleobases and Associated Nuclear Quadrupole Interactions for  $^{14}\text{N}$ ,  $^{17}\text{O}$  and  $^2\text{H}$  in A-DNA and B-DNA** R.H. SCHEICHER, MTU Houghton, DIP N. MAHATO, R.H. PINK, M.B. HUANG, T.P. DAS<sup>1</sup>, SUNY Albany, ARCHANA DUBEY, H.P. SAHA, LEE CHOW, UCF Orlando — As part of a research program for first-principles investigation of electronic structures of A-DNA and B-DNA systems we have previously carried out studies of the magnetic hyperfine interactions for the spin-label[1] muonium attached to A-DNA and B-DNA. The present work involves the nuclear quadrupole interactions (NQI) of  $^{14}\text{N}$ ,  $^{17}\text{O}$  and  $^2\text{H}$  in these two systems. We will present the results of our investigations of the NQI properties using the Hartree-Fock-Roothaan procedure with many-electron correlations included using many-body perturbation theory. For the A-DNA and B-DNA systems we are using available structural data for the four nucleobases. For the free nucleobases, the geometry from the energy optimization procedure is being employed. Comparisons will be made with available experimental NQI data and planned future improvements will be discussed. [1] R.H. Scheicher, E. Torikai, F.L. Pratt, K Nagamine, and T.P. Das, *Hyperfine Interactions*, 158, 53 (2004); *Physica B, Physics of Condensed Matter*, 374, 448 (2006).

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