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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

Summary

DNA is the most important molecule for biology in particular and for life in general. Owing to its great importance for life processes, any unchecked damage in DNA molecules can have dramatic consequences for the affected organism. For understanding the origin of the damage at an electronic level, it is important to have a detailed knowledge of the electronic structure of DNA and related systems
We have presented our systematic study of the Nuclear Quadrupole Interaction (NQI) in another Abstract at this conference. Here we present the results of our investigations on the trapping of muonium (Mu) in the free nucleobases, nucleobases in single and double chain DNA and in solid nucleobases. The study of Mu trapping and the associated muon hyperfine interaction complements the (NQI) study in the diamagnetic DNA systems by providing magnetic information dependent on the electronic structure of the systems associated with the unpaired spin electron provided by the trapped Mu. It also provides insights into the nature of the trapping process and associated hyperfine properties for impurities in general and the procedure for studying them.
For our investigation, we have used the first-principles procedure of Hartree-Fock theory combined with many-body perturbation theory (MBPT) to include many-body electron correlation effects. These latter effects are very important because they influence both the stabilities of the Mu trapping sites and the associated hyperfine interaction properties. It was also important to introduce relaxation effects in the positions of the nearest neighbors of the trapped Mu impurity. These effects were found to be sizable and influenced the strengths of the trapping of Mu at the sites found, however they are not sensitive to manybody correlation effects, an important result for the future in making careful trapping studies more practicable.
Results obtained for muonium hyperfine interaction at the trapped muonium sites will be presented. The main contributor to the hyperfine interaction properties is found to be the Fermi Contact isotropic term. However electron-nuclear dipole-dipole hyperfine interaction also makes significant contributions. The predicted hyperfine constants for the Muonium and the nearest neighbor nuclei are utilized to obtain theoretical values of the level crossing frequencies in the presence of applied magnetic fields and compared with available experimental data [2].

References

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[2] Penny L Hubbard et al., J. Phys. Chem. A108, 9302 (2004).

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