Muon and Muonium in Nucleic Acid Bases studied from First Principles

S. R. Badu[1], R. H. Pink[1], Archana Dubey[2], Lee Chow[2], K. Nagamine[3,4,5], E. Torikai[6], R. H. Scheicher[7], and T. P. Das[1,2]

[1]*State University of New York at Albany, USA*
[2]*University of Central Florida, Orlando, USA*
[3]*Atomic Physics Laboratory, RIKEN, Saitama, Japan*
[4]*KEK-MSL, Tsukuba, Ibaraki, Japan*
[5]*University of California, Riverside, USA*
[6]*Yamanashi University, Kofu, Japan*
[7]*Uppsala University, Sweden*

DNA and RNA can certainly be seen as two of the most relevant molecules for biology in particular and for life in general. Owing to their huge importance for life processes, any unchecked damage in these molecules can have dramatic consequences for the affected organism, with cancer being the most commonly associated outcome. For an effective treatment and possible prevention of such diseases, it is essential to have a detailed understanding of the electronic structure of DNA and RNA and their encoding units, the base molecules, both in the state of damage as well as in their natural configuration.

Here, we present results from our systematic first-principles study of muon (μ^+) and muonium (μ^+e^-) adducts in the nucleobases of DNA and RNA. For our electronic structure investigations, we have employed the Hartree-Fock-Roothaan procedure supplemented with many-body perturbation theory as implemented in the well-known GAUSSIAN set of programs. The major aim of our study is to assess the influence of the interaction between the nucleobases and sugar rings and phosphate groups in DNA and RNA on the electronic structure using muon spin relaxation (μSR). To this end, we are considering the influence of the interaction between a nucleobase and a sugar ring by attaching a CH_3 group to the base, thus simulating the effect of the sugar ring presence without actually including all atoms in the calculation.

In our study, we distinguish between *indirect* and *direct* effects on the hyperfine interaction at the μ^+ site, with the former referring to the influence of changes in molecular geometries produced by the CH_3 group while the direct effect is considered to be due to the electronic interaction between the CH_3 group and the nucleobase. Furthermore, we have also investigated the solid-state structure of nucleobases using the first-principles Hartree-Fock cluster procedure and will compare the results with those obtained for individual bases and with those for the nucleobases attached to the DNA and RNA backbone as simulated by the CH_3 group.