

Abstract Submitted
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First-principles Study of Muon and Muonium in A- and B-form DNA E. TORIKAI, Yamanashi University, Kofu, Japan; RIKEN, Wako-shi, Japan, R.H. SCHEICHER, Uppsala University, Uppsala, Sweden, T.P. DAS, State University of New York at Albany, Albany NY; University of Central Florida, Orlando FL, F.L. PRATT, ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, UK, K. NAGAMINE, KEK-MSL, Tsukuba, Japan — We have carried out a systematic first-principles study of muon (μ^+) and muonium (μ^+e^-) adducts in A-form and B-form DNA. All potential trapping sites in the four bases ADE, CYT, GUA, and THY were considered. Our results indicate that the difference in structural geometry between A- and B-form DNA can lead to substantial deviations in the hyperfine fields at the μ^+ sites. This could have important implications for the interpretation of Muon Spin Relaxation measurements that have shown evidence for an enhanced electron mobility in A-form DNA, but implicitly assume a negligible difference in the magnitude of the hyperfine fields at the trapped μ^+ site between A- and B-form DNA.

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