Contribution ID: **10** Type: **not specified**

DNA through the Eyes of Computational Chemistry and Muon Science

Friday, 6 September 2024 10:45 (25 minutes)

Deoxyribonucleic acid (DNA) is a complex molecule composed of nucleotides that store genetic information used in the development of all living things. Nitrogenous bases can be either guanine (G), adenine (A), cytosine (C), or thymine (T). The properties of DNA have attracted considerable interest from physicists, chemists, and material scientists due to its capability to act as a medium for electron transport and its potential in industrial applications as microdevices. Muon Spin Resonance (μSR) experimental technique has been successfully applied to study the microscopic properties and processes of different materials including molecules of biological importance. The hyperfine interaction between the muon's dipole moment and the surrounding unpaired electron can be measured using ALC-μSR spectroscopic technique and can be calculated using DFT quantum mechanical procedure. In DFT calculation, a basis set is an important factor in determining the quality of results, especially for hyperfine interaction where changes in the local geometry and electronic structure can have a big impact. The use of extensive basis sets is always desirable and is expected to produce better results. However, for DNA molecules of more than 10 base-pairs, all-electron geometry optimization calculation using large basis sets such is prohibitively difficult even on a supercomputer. An alternative is to use smaller basis sets. Combination of various basis set and functional were used to determine several properties of short DNA molecules. Some of the studied properties are optimized geometry, HOMO-LUMO gap, atomic charge, and muon trapping sites. The effect of different basis set and functional on the associated muon hyperfine interactions was also investigated. The ranking of muon stable sites is not affected by the different choice of basis set or functional. Other properties are affected at varying degrees.

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Session Classification: Science Session

Track Classification: Computational