Computing a Potential Bio-fuel Cell of BNNT- FAD Complex by Modeling Methods

F. Mollaamin[1]

Abstract: Due to this work, it has been investigated that single walled boron nanotube (SWBNNT) as an entrapped redox complex can be connected to flavin adenine dinucleotide (FAD) as a bio catalytic to be a promising material for the electronic industry according to their structure and physical properties.

In this study, the optimized geometry of BNNT- FAD complex was implemented at the framework of DFT using the three-parameter Beckes exchange and Lee-Yang-Parrs correlation non-local functional, usually known as BLYP and B3LYP methods by 6-31G* basis set dealing with description of electronic structure of BNNT-FAD complex. Eventually,NMR measurements on the basis of Gauge Including Atomic Orbital (GIAO) complemented the calculations on the mentioned model.

The data debated that the BNNT bio-fuel cell model can be applied for generating electric power in a lower resistance district with the best agreement based on the linear correlation of voltage-current directly from a sustainable fuel substrate such as FAD. These results depicted that the boron nitride nanotube is a progressing conductive compound for the direct electron transfer type bio-fuel cell. In fact, the potential efficiency, material flexibility and privileged stability of FAD and BNNT indicated the effective and practical electrochemical utilization of bio-fuel cell.Overall,through considering different situations of FAD atoms junction to BNNT and analysis of NMR parameters, it was evident that the electron transferring caused more structural stability to BNNT- FAD complex due to hydrogen bonding in solution.

[1] Department of Chemistry, Qom Branch, Islamic Izad University, Qom, Iran
smollaamin@gmail.com