A robust computational investigation on C_{60} fullerene nanostructure as a novel sensor to detect SCN^-

ABSTRACT

This study explored on the adsorption properties and electronic structure of SCN^- via density functional theory analysis on the exterior surfaces of C_{60} and CNTs using B3LYP functional and 6-31G** standard basis set. Then adsorption of SCN^- through nitrogen atom on the C60 fullerene is electrostatic (−48.02 kJ mol¯1) in comparison with the $C_{59}Al$ fullerene that shows covalently attached to fullerene surface (−389.10 kJ mol¯1). Our calculations demonstrate that the SCN^- adsorption on the pristine and Al-doped single-walled CNTs are −173.13 and −334.43 kJ mol¯1, indicating that the SCN^- can be chemically bonded on the surface of Al-doped CNTs. Moreover, the adsorption of SCN^- on the C_{60} surface is weaker in comparison with $C_{59}B$, $C_{59}Al$, and $C_{59}Ga$ systems but its electronic sensitivity improved in comparison with those of $C_{59}B$, $C_{59}Al$, and $C_{59}Ga$ fullerenes. The evaluation of adsorption energy, energy gap, and dipole moment demonstrates that the pure fullerene can be exploited in the design practice as an SCN^- sensor and $C_{59}Al$ can be used for SCN^- removal applications