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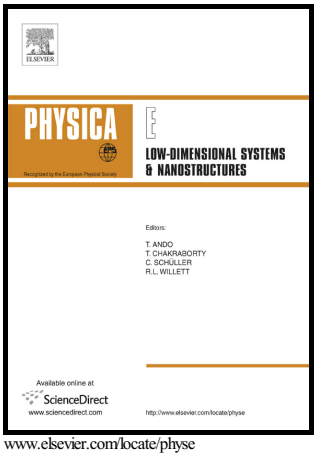

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Theoretical study on the phenylpropanolamine drug interaction with the pristine, Si and Al doped [60] fullerenes

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Abstract

Phenylpropanolamine (PPA) is a popular drug of abuse and its detection is of great importance for police and drug communities. Herein, we investigated the electronic sensitivity and reactivity of pristine, Al and Si doped C_{60} fullerenes to the PPA drug, using density functional theory calculations. Two adsorption mechanisms were predicted for PPA on the pristine C_{60} including cycloaddition and adsorption via $–NH_2$ group. It was found that the pristine C_{60} has a good sensitivity to this drug but suffers from a weak interaction (adsorption energy ~ -0.1 kcal/mol) because of structural deformation and aromaticity break. The PPA is adsorbed on the Al or Si doped C_{60} from its –OH or $–NH_2$ groups. The Al-doping significantly improves the reactivity of C_{60} but decreases its electronic sensitivity. Unlike the Al-doping, the Si-doping increases both the reactivity and electronic sensitivity to the PPA drug. At the presence of PPA drug, the conductivity of the Si-doped C_{60} considerably increases due to the HOMO-LUMO gap reduction by about 30.3%. Different analyses were used to obtain the results including nucleus independent chemical shift (NICS), density of states (DOS), molecular electrostatic potential (MEP), frontier molecular orbitals (FMO), etc.

Keywords

Sensor, Phenylpropanolamine, Abuse, Fullerene, DFT

1. Introduction