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# Theoretical Study of Ethanol Interaction with Pristine and P-doped Single-Walled Carbon Nanotubes

Feasible interactions between metallic single-walled carbon nanotubes (SWCNTs) and ethanol gases were carried out via using theory of first principles based on DFT. Also, the vdW correction and spin polarized were included in this account. The equilibrium position, adsorption energy, charge transfer, density of states, and electronic band structure of ethanol rearranged inside and outside pristine also with P-doped nanotubes were calculated to estimate the responses of P-SWCNT. It was found that the ethanol preferred to absorb inside than outside the tube at diameter of 8.19 Å. Conversely, for nanotubes diameters with more 13.63 Å, the ethanol equivalently forms both inside and outside carbon nanotubes. The investigations on electronic properties have been shown that ethanol performed as electron-withdrawing group because of hydroxyl group attached with ethyl group. Then, the electron in SWCNTs moves toward the adsorbate thereby enhancing its conductivity. Furthermore, doping an impurity, Phosphorus, on the surface improved the absorption and the characteristic of all intermolecular interactions were types of physisorption.

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