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Feasible of an ethanol perform on pristine and p-doped single walled carbon nanotubes

We study feasible of ethanol absorbed on pristine and impurity P-doped on armchair single walled carbon nanotubes(SWCNTs) by first principle based on DFT. Van der Waals corrected and spin polarized density functional theory calculations using plane wave approach with periodic boundary conditions were carried out to investigate the intermolecular interaction. The interaction between absorbate on the exterior surface and inner site of functionalized SWCNTs is revealed that it prefers to adsorb inner rather than outer of pristine and P-doped SWCNTs. Bader charge analysis and Noncovalent analysis (NCIplot) indicate that the binding energy of ethanol is significantly increased for adsorption on the sidewall of functionalized nanotubes. However, we observe that in inner case, the adsorbate rearranges structure on matching with vdW radius of SWCNTs in comparison to the exterior sidewall of the tubes that ethanol prefer to perform on low curvation. In conclusion, we state that the interaction between an ethanol and both functionalized and pristine SWCNTs is remarkable physisorption. Furthermore, the electronic structure of the considered complex system is not dramastically change in electronic properties.

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