A DFT study on Water adsorption on Boron doped Carbon nanotubes

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Carbon nanotubes have been demonstrated as a promising nanoscale molecular sensors for detecting gas molecules becaouse of its high surface area, strength and outstanding physical properties. [1] However, pristine carbon nanotubes show little or no response to many pollutant gases. In earlier, different strategies have adopted to enhance the sensitivity of the CNTs. Among them, doping of Boron or Nitrogen is more popular in increasing the gas sensitivity of CNTs. Recent studies showed that boron-doped carbon nanotubes have significantly modified physical and chemical properties, and notably it increased surface reactivity. Futhermore, the electronic properties of B-CNT and N-CNT are sensitive to the presence of H_2O.[2] Thus, in study, we investigated the interactions between B-CNT and water molecules using periodic density functional theory calculations. For this, we considered metalic type (5,5) SWNTs, which is hydrophobic and revealed the interaction of water/water dimers with boron doped SWNT. We also calcualted the adsorption energy of water/water dimers with different boron concentration on CNT to know the dopant effect. Our results indicate that the water dimers are having larger adosprtion energy on B-CNT than the water monomer and also we found that Boron doping concentration of 4% has higher affinity towards water dimers molecules.

References

[1] Peng S, Cho K. Ab Initio Study of Doped Carbon Nanotube Sensors. Nano Lett., 2003; 3, 513.

[2] Adjizian JJ, Leghrib R, et al.Boron- and nitrogen-doped multi-wall carbon nanotubes for gas detection. CARBON 2014; 66,662.

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