Improving hydrogen physisorption energy using swcnts through structure optimization and metal doping substitution

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Abstrak

The effect of metal doping on the hydrogen physisorption energy of a single walled carbon nanotube (SWCNT) is investigated. Unlike many previous studies that treated metal doping as an ionic or charged element, in this study, lithium and magnesium are doped to an SWCNT as a neutral charged by substituting boron on the SWCNT (Boron substituted SWCNT). Using ab initio electronic structure calculations, the interaction potential energies between hydrogen molecules and adsorbent materials were obtained. The potential energies were then represented in an equation of potential parameters as a function of SWCNT diameters in order to obtain the most precise potential interaction model. Molecular dynamics simulations were performed on a canonical ensemble to analyze hydrogen gas adsorption on the inner and outer surfaces of the SWCNT. The isosteric heat of the physical hydrogen adsorption on the SWCNT was estimated to be 1.6 kcal/mole, decreasing to 0.2 kcal/mole in a saturated surface condition. The hydrogen physisorption energy on SWCNT can be improved by doping lithium and magnesium on Boron substituted SWCNT. Lithium-Boron substituted SWCNT system had a higher energy physisorption that was 3.576 kcal/mole compared with SWCNT 1.057–1.142 kcal/mole. Magnesium-Boron substituted SWCNT system had the highest physisorption energy that was 7.396 kcal/mole. However, since Magnesium-Boron substituted SWCNT system had a heavier adsorbent mass, its physisorption capacity at ambient temperature and a pressure of 120 atm only increased from 1.77 wt% for the undoped SWCNT to 2.812 wt%, while Lithium-Boron substituted SWCNT system reached 4.086 wt%.