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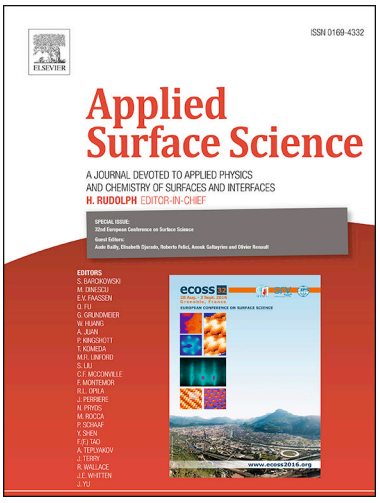

Full Length Article

Enriching the Hydrogen Storage Capacity of Carbon Nanotube Doped with Polylithiated Molecules

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Enriching the Hydrogen Storage Capacity of Carbon Nanotube Doped with Polylithiated Molecules

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ABSTRACT

In a quest to find optimum materials for efficient storage of clean energy, we have performed first principles calculations to study the structural and energy storage properties of one-dimensional carbon nanotubes (CNTs) functionalized with polylithiated molecules (PLMs). Van der Waals corrected calculations disclosed that various PLMs like CLi, CLi_2, CLi_3, OLi, OLi_2, OLi_3, bind strongly to CNTs even at high doping concentrations ensuring a uniform distribution of dopants without forming clusters. Bader charge analysis reveals that each Li in all the PLMs attains a partial positive charge and transform into Li^+ cations. This situation allows multiple H_2 molecules adsorbed with each Li^+ through the polarization of incident H_2 molecules via electrostatic and van der Waals type of interaction. With a maximum doping concentration, that is $3CLi_2/3CLi_3$ and $3OLi_2/3OLi_3$ a maximum of 36 H_2 molecules could be adsorbed that corresponds to a reasonably high H_2 storage capacity with the adsorption energies in the range of -0.33 to -0.15 eV/H_2. This suits the ambient condition applications.