

Accepted Manuscript

Full Length Article

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PII: S0169-4332(18)30383-0
DOI: <https://doi.org/10.1016/j.apsusc.2018.02.040>
Reference: APSUSC 38498

To appear in: *Applied Surface Science*

Received Date: 22 December 2017
Revised Date: 31 January 2018
Accepted Date: 4 February 2018

Please cite this article as: P. Panigrahi, S.R. Naqvi, M. Hankel, R. Ahuja, T. Hussain, Enriching the Hydrogen Storage Capacity of Carbon Nanotube Doped with Polyolithiated Molecules, *Applied Surface Science* (2018), doi: <https://doi.org/10.1016/j.apsusc.2018.02.040>

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Enriching the Hydrogen Storage Capacity of Carbon Nanotube Doped with Polyolithiated 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 polyolithiated molecules (PLMs). Van der Waals corrected calculations disclosed that various PLMs like CLi, CLi₂, CLi₃, OLi, OLi₂, OLi₃, 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 H₂ molecules adsorbed with each Li⁺ through the polarization of incident H₂ molecules via electrostatic and van der Waals type of interaction. With a maximum doping concentration, that is 3CLi₂/3CLi₃ and 3OLi₂/3OLi₃ a maximum of 36 H₂ molecules could be adsorbed that corresponds to a reasonably high H₂ storage capacity with the adsorption energies in the range of -0.33 to -0.15 eV/H₂. This suits the ambient condition applications.

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