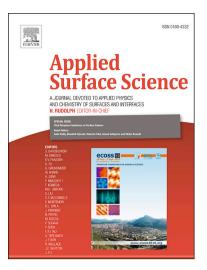
### Accepted Manuscript

#### Full Length Article

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

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## ACCEPTED MANUSCRIPT

## 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<sub>2</sub>, CLi<sub>3</sub>, OLi, OLi<sub>2</sub>, OLi<sub>3</sub>, 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<sup>+</sup> cations. This situation allows multiple H<sub>2</sub> molecules adsorbed with each Li<sup>+</sup> through the polarization of incident H<sub>2</sub> 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<sub>2</sub> molecules could be adsorbed that corresponds to a reasonably high H<sub>2</sub> storage capacity with the adsorption energies in the range of -0.33 to -0.15 eV/H<sub>2</sub>. This suits the ambient condition applications.

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