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First principles study of Interaction of H2 with doped Carbon Nanotube and Graphite Surfaces LI CHEN, YIMING ZHANG, NIKIHIL KORATKAR, PURU JENA, SAROJ NAYAK, RENSSELAER POLYTECHNIC INSTITUTE TEAM, VIRGINIA COMMONWEALTH UNIVERSITY COLLABORATION — Using first principles density functional theory based on gradient corrected approach we have studied interaction of H2 molecule with doped carbon nanotube and graphite surfaces. In agreement with earlier study we find that H2 physorbs on carbon nanotube and graphite surfaces while the binding increases dramatically when H2 binds to Li atoms decorated on carbon nanotube surfaces: the binding further enhances with Li atoms on fullerene doped nanotube pea-pod structures. The increase in binding in the latter structures arises due to charge transfer between the nanotube and dopants and the bonding is primarily in electrostatic in nature. The binding is further improved with decrease in diameter of nanotube suggesting a combination of various effects could be exploited for engineering suitable graphitic surfaces for molecular hydrogen storage.

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