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Si-decorated graphene: a promising media for molecular hydrogen storage

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Abstract

The adsorption of hydrogen molecules (H_2) on Si-decorated graphene was studied by using density functional theory calculations based on local density approximation (LDA). The accuracy of our method was validated by high level quantum chemical calculation result at MP2 level of theory for similar system. Our calculations show that Si-decorated graphene has high adsorption energy, high net charge transfer values and small connecting distances to graphene surface due to chemisorption. This makes adsorbed Si on the surface as a positive center which can adsorb considerably H_2 molecules. We find that up to 16 H_2 molecules can stably bind to two Si atoms on both side of the graphene sheet with slightly desirable adsorption energy which indicates that the resultant system facilitates the hydrogen desorption at near ambient conditions for practical applications. This newly developed Si decorated graphene with its hydrogen storage capacity of about 15 wt% would be an excellent candidate for hydrogen storage mediums.

Keywords: Hydrogen storage; Adsorption; DFT; Si-doped Graphene