A GRAPHENE LAYER AND A CARBON NANOTUBE A NOVEL SYSTEM FOR HYDROGEN STORAGE

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ABSTRACT

It is shown that a periodic carbon atom system formed by a graphene layer and a carbon nanotube as the (6,6) or the (4,4) it is a feasible system for hydrogen storage purposes. This is an ab initio study using Density Functional Theory with local density approximation. The carbon system is inside a cubic cell of 25 or 30 a.u. sizes. Using the (4,4) nanotube the free interstitial space between the nanotube wall and the graphene plane is increased because the radii of the (4,4) nanotube is less than for the (6,6) nanotube. The total energy curves for the hydrogen molecule position with different axis orientations are presented for both carbon nanotubes. Comparison between the energy curves suggests that controlling the length of the interstitial space could be an efficient way to increase the hydrogen storage in this system. One principal result is the increase of the binding energy for the hydrogen molecule, respect to the binding energy of the hydrogen molecule above the graphene layer alone (70 to 85 mev)[1] or outside the (6,6) carbon nanotube alone (40 to 70 mev)[2]. For the computer simulations it has been used computer codes as fhi98md and quantum espresso.

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1. J. Chem. Phys., Vol. 112, No. 18, 8 May 2000
2. J. Chem. Phys., Vol. 117, No. 5, 1 August 2002

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