عنوان مقاله:

DFT-D study of hydrogen storageonto Fe decorated monolayergraphenylene

محل انتشار:

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خلاصه مقاله:

Hydrogen has to be produced, since on the earth it only occurs in the form of water and hydrocarbons.For practical application of hydrogen as energy source, it must be stored, carried and released when it must be consumed. To date,there is no investigated material that exhibits all necessary properties. Moreover, for all methods of hydrogen storage by the structures, there are some key issues. In this work, porousgraphenylene (GPY) functionalized with Fe transition metal was considered for its potential as a high capacity hydrogen storage material.GPY or biphenylene carbon is a 2D sp2- carbon membrane contains three kinds of polygon [1]. GPY has a unique structure which is composed of dodecagonal, hexagonal and tetragonal rings that we nominated them as A, B and C, respectively.DFT calculations were done using DMol3package.We used generalized-gradient approximation (GGA) as well as the Perdew–Burke–Ernzerhof (PBE) exchange and correlation functionals with the double numerical polarized(DNP) basis set. A 6×6×1 Monkhorst–Pack k-point mesh with a 13.54 Å × 13.54 Å × 20.00 Å periodic boundary condition for the GPYsheet was applied. To accountVan der Waals forces and dispersion effects, the empirically-correcteddensity functional theory (DFT-D) method in Grimme scheme wasemployed in all computations [2].In this work, the first attempt was made to consider the best positions for iron atom and then the hydrogen molecule adsorption. Iron metal atomwas placed in five different positions with a different distance from the graphenylene plate, then,the bonding energy was calculated.It was seen that hexagonal ring is the best position with total adsorption energy of –2.66 eV in which distance of Fe from graphenylene sheet is about 1.5 Å.Also, the results show that band gap energy of GPYis 0.894 eV which does not significantly changeafter adsorption of the hydrogen molecule in the hexagonal ring. But, in the presence of Fe and H2, band gap decreases to 0.666 eV. The results confirm that Fe decoration can extremely improve hydrogenstorage capacity of the GPY and up to 16 H2 molecules could be adsorbed on Fe decorated GPY [3 .[that is very higher than that of alkali and alkaline earth metalsdecorated GPY

کلمات کلیدی:

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