عنوان مقاله:
Quantum chemical study hydrogen storage on the C3N nanotube

محل انتشار:
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خلاصه مقاله:
We performed a density functional theory study to investigate the storage of hydrogen molecule on the interiorand exterior of C3N nanotubes (C3NNTs). Adsorption energy values corresponding to the adsorption of H2 onthe pristine C3NNT were calculated to be in the range of +3.21 to -5.27 kcal/mol for the interior and -1.22 to -2.13 kcal/mol for the exterior of the nanotube. The second adsorption of H2 is site-selective so that the H2prefers to be adsorbed on two N atoms as far as possible from the first adsorbed-molecule with the adsorptionenergy of -1.61 kcal/mol. By increasing the coverage of adsorbed H2 molecules, the adsorption energy permolecule is less exothermic. The electrical conductivity of the C3NNT is not sensitive to the presence of H2molecules and its value slightly changed after the .hydrogen adsorption

کلمات کلیدی:
hydrogen, C3N nanotubes, sensitive