عنوان مقاله:

Theoretical investigation into nano structures of Si substituted C20 fullerene and H2 Adsorption on them

محل انتشار:

اولین همایش نانومواد و نانوتکنولوژی (سال: 1390)

تعداد صفحات اصل مقاله: 5

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خلاصه مقاله:

The MPW1PW91/6-31++G** density functional calculations were used to obtain minimum geometries and interaction energies between the molecular hydrogen and nanostructures of fullerenes C20cage), C20(bowl), C20H10(bowl C19H10Si(bowl,penta) ,C19H10Si(bowl,hexa) ,by Gaussian 98 package. In each case, H2molecule is adsorbed above the pentagonal and hexagonal sites. Using NBO analysis, the net atomic charge electronic chemical potential (μ), hardness (η), and different of HOMO LUMO gaps (4 HLG) are obtained. All results shown that Si atom substitution in hexa site in C20 hydrogen molecule.

کلمات کلیدی:

DFT, H2 AdsorptionBowl Heterofullerene

لینک ثابت مقاله در پایگاه سیویلیکا: