عنوان مقاله:

A computational study of aniline adsorption on pure and doped surfaces of B40 borospherene

محل انتشار:

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نویسندگان:

Davood Farmanzadeh - *Department of Physical Chemistry, Faculty of Chemistry, University of Mazandaran, Babolsar*

Masoomeh Keyhanian - *Department of Physical Chemistry, Faculty of Chemistry, University of Mazandaran, Babolsa*

خلاصه مقاله:

B40 borospherene is the first all-boron fullerene which has been received considerableattention in boron chemistry [1] and experimentally observed using laser vaporization in 2014 [2].This box-like fullerene with D2d symmetry is composed of four hollow heptagons and twohollow hexagons. In present work, a theoretical study has been performed using Dmol3 programpackage for investigation of the adsorption of aniline on the surface of pristine and dopedborospherene with Fe and Co transition metals based on density functional theory (DFT). Forthis purpose, different possible orientations of aniline were considered in various situations offullerenes for investigation of the most stable configuration which is related to above of center ofhexagon or heptagon rings, above of six types of nonequivalent boron atoms, the bridges ofbonds and above of dopant atoms. The results reveal that aniline have been chemisorbed on thepristine B40 with significant adsorption energy. On the other hand, doping B40 with Fe and Cotransition metals leads to dramatically improvement in aniline adsorption and sensitivity. Theseobservations propose that depended to kind of dopant atoms, doped borospherene can showbetter adsorption or sensor applications than pristine B40 for adsorption and detection of aniline.

کلمات کلیدی:

Borospherene, Fullerene, Density Functional Theory, Dmol3 Program

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