

عنوان مقاله:

(A DFT study on nitric oxide (NO) monitoring via borospherene (B40

محل انتشار:

هجدهمین همایش شیمی فیزیک ایران (سال: 1394)

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خلاصه مقاله:

In this work the adsorption of NO molecule on the surface of borospherene is investigated using DFT calculation for testing its potential capability as nanosensors. It is found that the NO is favorably chemisorbed on the borospherene, with adsorption energy -0.85 eV at M06-2X/6-31+G(d) level together with significant electronic response

کلمات کلیدی:

لینک ثابت مقاله در پایگاه سیویلیکا:

<https://civilica.com/doc/552591>

