عنوان مقاله:

Can Nitride-boron Nanocage Sense or Capture Carbon Monoxide? A Density Functional Theory Study

محل انتشار:

چهارمین همایش پیل سوختی (سال: 1389)

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نویسندگان:

Fatemeh Cigarchi - *Master Student Molecular Simulation Research Laboratory, Department of Chemistry, Iran University of Science and Technology, Tehran, Iran*

S.Majid Hashemianzadeh - *Professor Seyed Majid Hashemianzadeh. Molecular Simulation Research Laboratory, Department of Chemistry, Iran University of Science and Technology, Tehran, Iran*

خلاصه مقاله:

Using first principles calculations, we have investigated the adsorption of CO molecule on boron-nitride nanocage (BN)36 as a adsorbent. Our calculations were performed at the B3LYP level of density functional Theory along with standard split valence basis set 6-31G*. By examining the molecular orbitals and binding energies our results indicate that B36N36 is not sensitive to carbon monoxide and just a physical adsorption occurs.

کلمات کلیدی:

greenhouse gas, (BN)n cluster, Inorganic fullerene, carbon monoxide,density functional theory

لینک ثابت مقاله در پایگاه سیویلیکا: