

عنوان مقاله:

Interacti on of CO with BN nanocluster surface

محل انتشار:

پانزدهمین سمینار شیمی فیزیک ایران (سال: 1391)

تعداد صفحات اصل مقاله: 3

نویسندگان:

Si ma Mehdi Shishvan - *Department of C hemistry, Shah idRajae Teacher Training U niversity, P.O . Box ۱۶۸۷۵-۱ ۶۳, Tehran, Iran*

Jav ad Beheshtian - *Department of C hemistry, Shah idRajae Teacher Training U niversity, P.O . Box ۱۶۸۷۵-۱ ۶۳, Tehran, Iran*

خلاصه مقاله:

Boron nitride (BN) nanomaterials are ex pected to have vast variety applications as electronic device s, high heat-resistance semiconductors, and i nsulator lub ricants because of prov iding convenient stability at high temperature s with hi gh electronic insulation in air and also hydrogen storage materials [۱]. Borone Nitride (BN) is a com pound of Bo rone and Nitride with a chemical f rmula BN. As a toxic gas, carbonm onoxide still remains as one of the major gaseo us pollutant s, When the concentration of CO increases, it is dangerous for human body. Sever al theoretic al researc hes for CO adsorption on various surfa ces have been reported[۲].We pe rformed DF T calculatio ns to study the adsorption of CO on the B_{۱۶}N_{۱۶} and B_{۲۴}N_{۲۴} fullerene-like nanocluster

کلمات کلیدی:

Boron e Nitride na nocluster, D ensity functional theor y, Adsorption, CO

لینک ثابت مقاله در پایگاه سیویلیکا:

<https://civilica.com/doc/1363790>

