عنوان مقاله:

DFT Study of Phosgene Gas Adsorption on (Zn12S12)Fullerene like Nano cage

محل انتشار:

شانزدهمین کنگره ملی مهندسی شیمی ایران (سال: 1397)

تعداد صفحات اصل مقاله: 18

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خلاصه مقاله:

In this study, we used the theory of DFT and the function of B3LYP and ωb97xd to search for the properties of the adsorption of phosgene gas on the surface of Zn12S12 nano cage as a semiconductor. We found three stable structural arrangements of adsorbed phosgene gas on the surface of this semiconductor nanostructure. The energy levels of the adsorption of phosgene gas ranged from -86 ~ -148 kJ / mol based on B3LYP level and -137 ~ -208 kJ / mol based on ωb97xd level with the enthalpy of -130 ~ -186 kJ / mol, and the Gibbs free energy of -81 ~ -142 kJ / mol at a temperature of 298 K based on ωb97xd. The results indicated that this adsorption process is exothermic and spontaneous chemisorption. For all the structures, geometric parameters and some electrical properties were calculated by considering the boundary molecular orbital analysis and charge analyze study.

کلمات کلیدی:

Phosgene, Semiconductor, DFT, Nano cages, Spontaneous.

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