عنوان مقاله:

Study of B12N12 and AlB11N12 fullerene as H2S absorbent and sensor by computational method

محل انتشار:

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خلاصه مقاله:

The absorption of the H2S on the small boron nitride fullerene (B12N12) and its Al-inserted analog was theoretically analyzed by density functional theory. The structural stability was based on the minimum energy and non-complex vibrational frequencies. Different sites and orientations of H2S, using the monomer unit, were considered. Compared with the weak physisorption on the pristine B12N12, the H2S molecule presents strong physisorption on both Al-inserted fullerene, as indicated by the calculated geometrical structures and electronic properties for these systems. It is suggested that the Al-inserted B12N12 presents high sensitivity to H2S. Based on calculated results, the Al-inserted B12N12 is expected to be a potential novel sensor for detecting the presence of H2S.

کلمات کلیدی:

Hydrogen Sulfide, Boron Nitride Fullerene, B12N12, Al-inserted, Density Functional Theory Calculations