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Study of $B_{12}N_{12}$ and $AlB_{11}N_{12}$ fullerene as H_2S absorbent and sensor by computational method

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Abstract

The absorption of the H_2S on the small boron nitride fullerene ($B_{12}N_{12}$) 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 H_2S, using the monomer unit, were considered. Compared with the weak physisorption on the pristine $B_{12}N_{12}$, the H_2S 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 $B_{12}N_{12}$ presents high sensitivity to H_2S. Based on calculated results, the Al-inserted $B_{12}N_{12}$ is expected to be a potential novel sensor for detecting the presence of H_2S.

Keywords: Hydrogen Sulfide, Boron Nitride Fullerene, $B_{12}N_{12}$, Al-inserted, Density Functional Theory Calculations