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A Quantum Mechanical Analysis of the Electronic Response of BN Nanocluster to Formaldehyde

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Abstract

It has been previously demonstrated that the electronic properties of pristine BN nanotubes and graphene-like sheets are not sensitive toward presence of H_2CO gas. Here, the adsorption of H_2CO on the external surface of $B_{12}N_{12}$ nano-cage is studied using X3LYP and Minnesota density functional calculations. Three different adsorption behaviors were found including physisorption, chemisorption, and chemical functionalization. Gibbs free energy changes at room temperature and 1 atm pressure is in the range of -0.07 to -2.00 eV (X3LYP). The HOMO-LUMO energy gap of the cluster dramatically decreases after the H_2CO chemisorption. Thus, $B_{12}N_{12}$ nanocluster may be used in gas sensor devices for H_2CO detection.

Key words: Nanostructures; Surfaces; Ab initio calculations; Electronic structure.