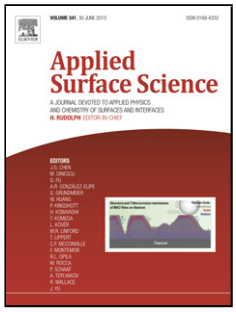

Title: DFT Study of Adsorption Behavior of NO, CO, NO_2, and NH_3 Molecules on Graphene-like BC_3: A Search for Highly Sensitive Molecular Sensor

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DFT Study of Adsorption Behavior of NO, CO, NO_2, and NH_3 Molecules on Graphene-like BC_3: A Search for Highly Sensitive Molecular Sensor

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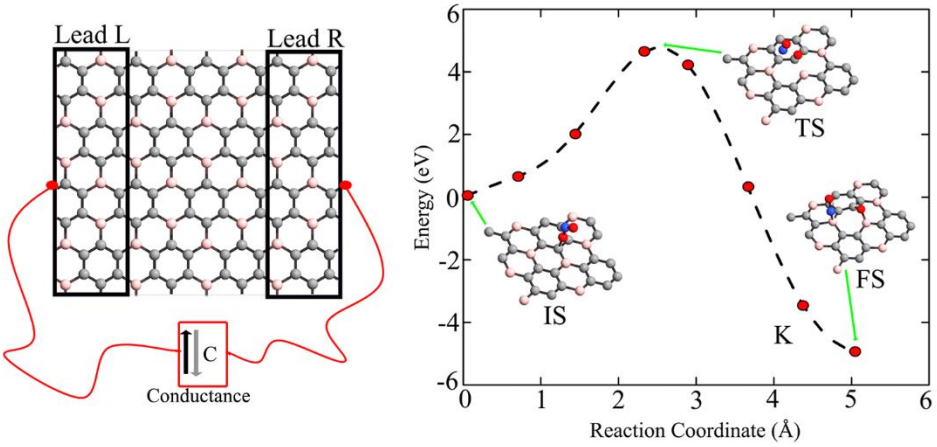
Graphical Abstract



Highlights:

- BC_3-based sensor has a low and moderate sensitivity to CO and NH_3, respectively.
- BC_3-based sensor has high potential for NO and NO_2 detection.
- NO_2 could be dissociated into NO and O species through the adsorption on the BC_3.
- BC_3 is a promising catalyst for dissociation of NO_2 gas molecule.

Abstract

The adsorption behaviors of toxic gas molecules (NO, CO, NO_2, and NH_3) on the graphene-like boron carbide (BC_3) are investigated using first-principle density functional theory. The graphene-like BC_3 monolayer is a semiconductor with a band gap of 0.733 eV. It is discovered that all the above gas molecules are chemisorbed on the BC_3 sheet while they retain their molecular forms. It is also revealed that the NO_2 gas molecule could be dissociated into NO and O species through the adsorption process. The amounts of charge transfer upon adsorption of CO and NH_3 gas molecules on the BC_3 are found to be small. The band gap changes in BC_3 as a result of interactions with CO and NH_3 are only 4.63% and 16.7%, indicating that the BC_3-based sensor has a low and moderate sensitivity to CO and NH_3, respectively. Contrariwise, upon adsorption of NO or NO_2 on the BC_3, significant charges are transferred from the molecules to the BC_3 sheet, causing a semiconductor-metal and semiconductor-p type semiconductor transition. Our study suggests that the BC_3-based sensor has a high potential for NO and NO_2 detection