

Accepted Manuscript

Title: DFT Study of Adsorption Behavior of NO, CO, NO₂, and NH₃ Molecules on Graphene-like BC₃: A Search for Highly Sensitive Molecular Sensor

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PII: S0169-4332(17)32371-1
DOI: <http://dx.doi.org/doi:10.1016/j.apsusc.2017.08.048>
Reference: APSUSC 36885

To appear in: *APSUSC*

Received date: 1-6-2017
Revised date: 3-8-2017
Accepted date: 7-8-2017

Please cite this article as: S.M.Aghaei, M.M.Monshi, I.Torres, S.M.J.Zeidi, I.Calizo, DFT Study of Adsorption Behavior of NO, CO, NO₂, and NH₃ Molecules on Graphene-like BC₃: A Search for Highly Sensitive Molecular Sensor, Applied Surface Science <http://dx.doi.org/10.1016/j.apsusc.2017.08.048>

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DFT Study of Adsorption Behavior of NO, CO, NO₂, and NH₃ Molecules on Graphene-like BC₃: A Search for Highly Sensitive Molecular Sensor

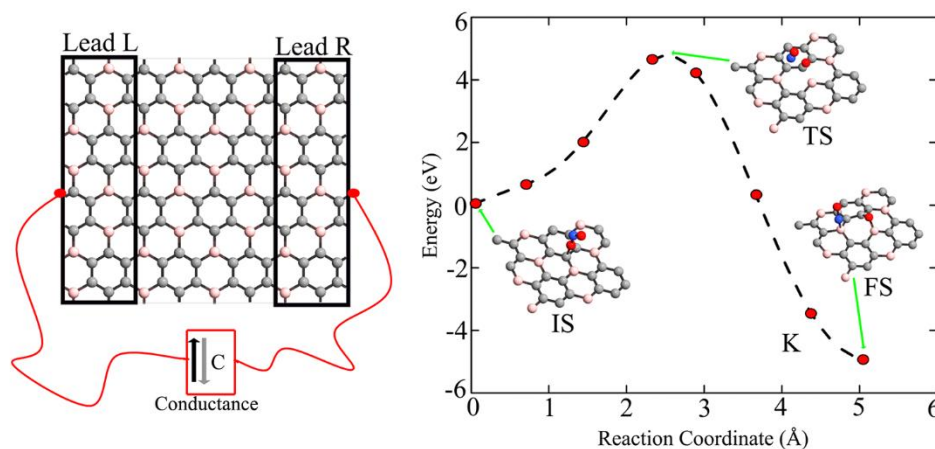
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Graphical Abstract



Highlights:

- BC₃-based sensor has a low and moderate sensitivity to CO and NH₃, respectively.
- BC₃-based sensor has high potential for NO and NO₂ detection.
- NO₂ could be dissociated into NO and O species through the adsorption on the BC₃.
- BC₃ is a promising catalyst for dissociation of NO₂ gas molecule.

Abstract

The adsorption behaviors of toxic gas molecules (NO, CO, NO₂, and NH₃) on the graphene-like boron carbide (BC₃) are investigated using first-principle density functional theory. The graphene-like BC₃ 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 BC₃ sheet while they retain their molecular forms. It is also revealed that the NO₂ gas molecule could be dissociated into NO and O species through the adsorption process. The amounts of charge transfer upon adsorption of CO and NH₃ gas molecules on the BC₃ are found to be small. The band gap changes in BC₃ as a result of interactions with CO and NH₃ are only 4.63% and 16.7%, indicating that the BC₃-based sensor has a low and moderate sensitivity to CO and NH₃, respectively. Contrariwise, upon adsorption of NO or NO₂ on the BC₃, significant charges are transferred from the molecules to the BC₃ sheet, causing a semiconductor-metal and semiconductor-p type semiconductor transition. Our study suggests that the BC₃-based sensor has a high potential for NO and NO₂ detection

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