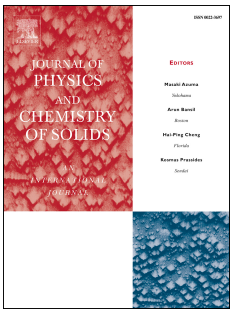
Accepted Manuscript



Structural, electronic, and magnetic properties of gas molecules on Mo-, Si-, and Pt-doped BC_3 sheets

Yanan Tang, Minghui Zhang, Weiguang Chen, Xiao Cui, Yi Li, Xianqi Dai

PII: S0022-3697(17)32263-1

DOI: 10.1016/j.jpcs.2018.05.037

Reference: PCS 8600

To appear in: *Journal of Physics and Chemistry of Solids*

Received Date: 23 November 2017

Revised Date: 24 May 2018

Accepted Date: 25 May 2018

Please cite this article as: Y. Tang, M. Zhang, W. Chen, X. Cui, Y. Li, X. Dai, Structural, electronic, and magnetic properties of gas molecules on Mo-, Si-, and Pt-doped BC_3 sheets, *Journal of Physics and Chemistry of Solids* (2018), doi: 10.1016/j.jpcs.2018.05.037.

Structural, electronic, and magnetic properties of gas molecules on Mo-, Si-, and Pt-doped BC_3 sheets

Yanan Tang [a,b,1*], Minghui Zhang [a], Weiguang Chen [a,1], Xiao Cui [a], Yi Li [b], and Xianqi Dai [a,b*]

[a] College of Physics and Electronic Engineering, Quantum Materials Research Center, Zhengzhou Normal University, Zhengzhou Henan, 450044, China

[b] College of Physics and Electronic Engineering, Henan Normal University, Xinxiang Henan, 453007, China

Abstract

In this study, based on first principles calculations, we compared the performance during the sensing of toxic gas molecules (NO, NO_2, HCN, and NH_3) by Mo, Si, and Pt dopants within BC_3 sheets (D-BC_3). Compared with the Pt-BC_3 sheet, the Si-BC_3 and Mo-BC_3 sheets exhibit a stronger affinity for the adsorption of gas molecules. The adsorbed NO and HCN had larger energy differences than those of the NO_2 and NH_3 molecules, thereby indicating that NO_2 and NH_3 could be detected readily as specific gas molecule on the D-BC_3 substrates. In addition, the adsorption of gas molecules induced great changes in the electronic structure and magnetic properties of the D-BC_3 systems. In particular, the adsorption of NO on the Pt-BC_3 and Si-BC_3 substrates yielded a larger magnetic moment (2.0 u_B) than those when the other gases were adsorbed on D-BC_3 sheets. These results may facilitate control over the adsorption properties of toxic gas molecules and the design of BC_3-based gas sensors or spintronic devices.

***Keywords*:** Adsorption stability; Electronic structure; First principles calculations; Graphene-like BC_3; Magnetic property;

*Corresponding author. Tel./Fax: +86 371 65502273. E-mail address: yntang2010@163.com (Y. Tang), xqdaizs@163.com (X. Dai)

[1]These authors contributed equally to this article and are considered co-first authors.