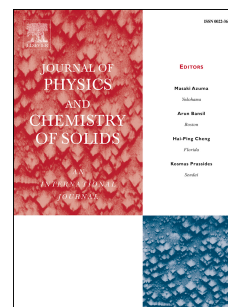


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Structural, electronic, and magnetic properties of gas molecules on Mo-, Si-, and Pt-doped BC₃ sheets

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, NO₂, HCN, and NH₃) by Mo, Si, and Pt dopants within BC₃ sheets (D-BC₃). Compared with the Pt-BC₃ sheet, the Si-BC₃ and Mo-BC₃ sheets exhibit a stronger affinity for the adsorption of gas molecules. The adsorbed NO and HCN had larger energy differences than those of the NO₂ and NH₃ molecules, thereby indicating that NO₂ and NH₃ could be detected readily as specific gas molecule on the D-BC₃ substrates. In addition, the adsorption of gas molecules induced great changes in the electronic structure and magnetic properties of the D-BC₃ systems. In particular, the adsorption of NO on the Pt-BC₃ and Si-BC₃ substrates yielded a larger magnetic moment (2.0 μ_B) than those when the other gases were adsorbed on D-BC₃ sheets. These results may facilitate control over the adsorption properties of toxic gas molecules and the design of BC₃-based gas sensors or spintronic devices.

Keywords: Adsorption stability; Electronic structure; First principles calculations; Graphene-like BC₃; Magnetic property;

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

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

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