

Accepted Manuscript

Full Length Article

Modulating electronic and optical properties of black phosphorous carbide monolayers by molecular doping

Jing Zhang, Gui Yang, Junlong Tian, Yuanxu Wang, Dongwei Ma

PII: S0169-4332(18)31097-3
DOI: <https://doi.org/10.1016/j.apsusc.2018.04.137>
Reference: APSUSC 39136

To appear in: *Applied Surface Science*

Received Date: 3 February 2018
Revised Date: 26 March 2018
Accepted Date: 12 April 2018

Please cite this article as: J. Zhang, G. Yang, J. Tian, Y. Wang, D. Ma, Modulating electronic and optical properties of black phosphorous carbide monolayers by molecular doping, *Applied Surface Science* (2018), doi: <https://doi.org/10.1016/j.apsusc.2018.04.137>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.



**Modulating electronic and optical properties of black phosphorous carbide
monolayers by molecular doping**

Jing Zhang^a, Gui Yang^a, Junlong Tian^a, Yuanxu Wang^{a,b*}, and Dongwei Ma^{a*}

^a*School of Physics, Anyang Normal University, Anyang 455000, China*

^b*Institute for Computational Materials Science, School of Physics and Electronics,
Henan University, Kaifeng 475004, China*

Abstract

First-principles calculations have been performed to study the modulation of the electronic and optical properties of the black phosphorous carbide monolayer (b-PC) by the adsorption of O₂, H₂O, NO₂, and NH₃ molecules. All the molecules are weakly physisorbed on the surface of the b-PC, which act as electron acceptors except NH₃. Especially, O₂ and NO₂ molecules can introduce deep acceptor states in the bandgap of the b-PC. The effects of the external electric field and the in-plane strain were further studied. For the b-PC with the adsorbed O₂, the typical p-type doping can be achieved under an appropriate external electric field. However, the b-PC with the adsorbed NO₂ is the most susceptible to the in-plane strain, as evidenced by the significant changes in the adsorption energy and the charge transfer under the compressive strain. In addition, the optical absorption of the b-PC can be significantly enhanced upon the adsorption of O₂ and NO₂ molecules, which can be further modulated by the external electric field and the in-plane strain. Our calculations predict an effective method to modulate the electronic and optical properties of the b-PC, which may widen its applications in the future electronics and optoelectronics.

Keywords:

First-principle calculation; b-PC; molecular doping; electronic and optical properties

*Corresponding author. E-mail: wangyx@henu.edu.cn (Yuanxu Wang).

*Corresponding author. E-mail: dwmachina@126.com (Dongwei Ma).

Download English Version:

<https://daneshyari.com/en/article/7833786>

Download Persian Version:

<https://daneshyari.com/article/7833786>

[Daneshyari.com](https://daneshyari.com)