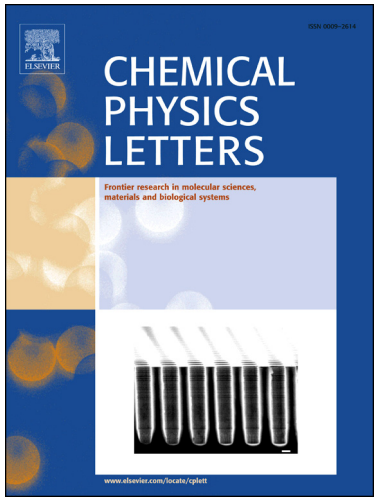

Research paper

Enhanced hydrophilic and conductive properties of blue phosphorene doped with Si atom

W.X. Zhang, J.W. Zhao, W.H. He, L.J. Luan, C. He

PII: S0009-2614(17)30203-8
DOI: http://dx.doi.org/10.1016/j.cplett.2017.02.078
Reference: CPLETT 34591

To appear in: *Chemical Physics Letters*

Received Date: 21 December 2016
Revised Date: 24 February 2017
Accepted Date: 26 February 2017

Please cite this article as: W.X. Zhang, J.W. Zhao, W.H. He, L.J. Luan, C. He, Enhanced hydrophilic and conductive properties of blue phosphorene doped with Si atom, *Chemical Physics Letters* (2017), doi: http://dx.doi.org/10.1016/j.cplett.2017.02.078

Enhanced hydrophilic and conductive properties of blue phosphorene doped with Si atom

W.X. Zhang [1*], J.W. Zhao [1], W.H. He [1], L.J. Luan [1], C. He[2*]

[1] School of Materials Science and Engineering, Chang'an University, Xi'an 710064, China;

[2] State Key Laboratory for Mechanical Behavior of Materials, School of Materials Science and Engineering, Xi'an Jiaotong University, Xi'an 710049, China;

Abstract

In this paper, the electronic, magnetic properties and the effect of Si-doped blue phosphorene on the adsorption of a H_2O molecule have been investigated using density functional theory with van der Waals corrections. The results indicate that doping Si into blue phosphorene can facilitate the dissociative adsorption of H_2O molecules. The dissociative energy barrier is reduced from 2.45 eV on pristine blue phosphorene to 0.19 eV on Si-doped blue phosphorene, which indicates a smooth dissociative adsorption. In addition, the dissociative adsorption of H_2O molecules can convert the Si-doped blue phosphorene from hydrophobic to hydrophilic with a semiconductor-to-metal transition.

Keywords: Blue phosphorene; Electronic properties; First principles calculations; Adsorption

[*] Corresponding Authors: W. X. Zhang (wxzhang@chd.edu.cn) or C. He (hecheng@mail.xjtu.edu.cn)