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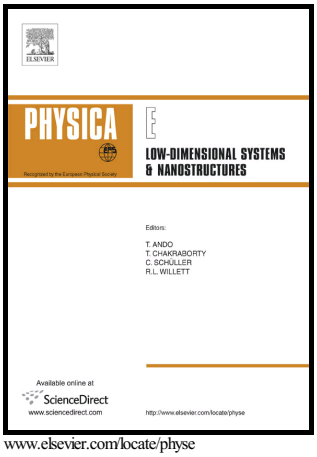

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PII: S1386-9477(16)31212-7
DOI: http://dx.doi.org/10.1016/j.physe.2016.12.014
Reference: PHYSE12688

To appear in: *Physica E: Low-dimensional Systems and Nanostructures*

Received date: 28 October 2016
Revised date: 21 December 2016
Accepted date: 30 December 2016

Cite this article as: Rui Li, Yaping Tao, Zhong-li Liu and Yonggang Tan, Edge-functionalization of blue phosphorene nanoribbons: Studied from first-principl methods, *Physica E: Low-dimensional Systems and Nanostructures* http://dx.doi.org/10.1016/j.physe.2016.12.014

Edge-functionalization of blue phosphorene nanoribbons: Studied from first-principle methods

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Abstract

Through density functional theory calculations, the impact of edge functionalization with O, OH, and alternate termination of them (OHO) on the structural stabilities, electronic and magnetic properties of blue phosphorene nanoribbons (BPNR) are mainly investigated. The formation energies demonstrate that the O-termination on the BPNRs is the most stable, and OHO-termination is more stable than OH-termination, besides the ab initio dynamic simulation show that they are all thermal dynamically stable at room temperature. Both the ground structures of O- and OH-BPNRs are spin-polarized semiconductors, while OH-functionalized BPNRs are nonmagnetic semiconductors. As the ribbon width increasing, the band gaps of O-aBPNRs tend to 1.04eV, but that of OH-aBPNRs tend to 1.97eV, comparable with the band gap of single-layer blue phosphorene, since it is dominated by pz electrons of the inner P atoms. In contrast, the influence of OHO-termination on GNRs, SiNRs, and black PNRs are also studied. Our results demonstrate that OHO-terminated GNRs and SiNRs are not a simple summation of O- and OH-terminated GNRs and SiNRs, and they are nonmagnetic stable both with zigzag and armchair edges, presenting metallic properties. While the OHO-terminated black PNRs present similar electronic and magnetic properties with OHO-terminated blue PNRs, and both the OHO-terminated zigzag and armchair edges are spin-polarized stable. These results provide potential help in the fields of band gap engineering and the designing of phosphorus-based spin devices with control over spin in spintronics.

Keywords: blue phosphorene; nanoribbons; chemical functionalization; energy dispersion; magnetic properties.

Ⅰ. Introduction

Two-dimensional (2D) materials (e.g. graphene, *h*-BN) have driven lots of interest from the past two decades due to their rich physics and potential for integration into next-generation electronic and energy conversion devices. Opposed to their bulk counterparts, the optical, electronic, mechanical and thermal properties of 2D materials can be easily tailored through numerical ways, such as the application of external strain, by cutting into narrow ribbons, or by stacking multiple layers of the same or different 2D materials [1-5].

Most recently, a 2D few-layer black phosphorus or phosphorene, has been fabricated by exfoliation [6]. The dubbed phosphorene, consisting of weakly stacked layers of a quasi-planar