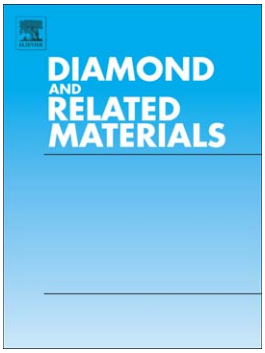

Structural, electronic and adsorptive characteristics of phosphorated holey graphene (PHG): First principles calculations

Li-Bin Shi, Yan-Yan Zhang, Xiao-Ming Xiu, Hai-Kuan Dong

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Structural, electronic and adsorptive characteristics of phosphorated holey graphene (PHG): First principles calculations

Li-Bin Shi [1*], Yan-Yan Zhang [2*], Xiao-Ming Xiu [1*], Hai-Kuan Dong [1]

[1] *School of Mathematics and Physics, Bohai University, Liaoning Jinzhou 121013, China*

[2] *School of New Energy, Bohai University, Liaoning Jinzhou 121013, China*

Abstract

Two-dimensional (2D) materials have attracted attention since the discovery of graphene in 2004. However, the zero band gap limits its application in the field of electronic devices. Opening graphene's band gap has become one of the most important subjects. Nitrogenated holey graphene (NHG) has been successfully synthesized in 2015. It has attracted much attention because of semiconducting properties. However, there is still a lack of detailed study on phosphorated holey graphene (PHG). In this paper, the structural, electronic and adsorptive characteristics of PHG are investigated by first principles calculations. First, we investigate the structural characteristics of PHG, and compare it with the previous discoveries of NHG and graphene. The stacking behavior of PHG is studied, and the most stable stacking order is obtained. Then, we study the band structure characteristics of PHG. Impact of the biaxial strain and vacancy defects on the band structure is discussed. Finally, we investigate atomic adsorption on PHG. Atomic adsorption energy, equilibrium distance, and charge transfer are analyzed. The effect of atomic adsorption on band structure is discussed. Our investigation can provide useful information for insight into the novel 2D materials of PHG.

Keywords: Phosphorated holey graphene, Structural characteristics, Electronic behavior, Atomic adsorption,

1. Introduction

With the development of society, the search for new materials has become a goal of scientific research [1, 2]. Two-dimensional (2D) materials have attracted intense attentions since graphene's discovery in 2004 [3–10]. However, the application of graphene in the field of electronic devices has been greatly limited due to its zero band gap properties [11]. 2D semiconductors, such as BN, AlN and MoS_2 have become the focus of research [12–14]. Very recently, phosphorene, a single layer of black phosphorus (BP), was successfully fabricated through exfoliation from the bulk black phosphorus and attracted much attention due to its direct band-gap semiconducting features [15–17].

At present, a series of covalent organic frame works have been designed to form two-dimensional structure similar to graphene [18, 19]. It is hoped that the band gap of graphene will be opened by changing its internal structure. Recently, a unique two-dimensional structure of nitrogenated holey graphene (NHG) with a stoichiometry of C_2N in the plane was synthesized by a simple wet-chemical reaction in 2015 [20]. The NHG is a direct band gap semiconductor with atomic structure of carbon atoms terminated by nitrogen atoms. Mortazavi et al. investigated thermal conductivity and mechanical properties in NHG [21]. They observed an overall decreasing trend in elastic modulus and tensile strength as temperature increased. The predicted thermal conductivity was about 64.8 W/m · K at 300 K. Tromer et al. discussed the atomic adsorption behavior on NHG [22]. It was found that H and B atoms prefered to adsorb on the top of N atom, while O atom prefered to adsorb on the top of C-C bond. Guan et al. investigated effects of strain on electronic and optic properties of NHG [23]. It was observed that the material was quite soft with a small stiffness constant, and it remained a direct gap semiconductor under strain. Li et al. had synthesized boron and nitrogen codoped holey graphene [24]. Omidvar et al. did a systematic study on the structure and stability of boronated holey graphene (BHG) [25].

Motivated by the recent synthesis of NHG, phosphorated holey graphene (PHG) with the stoichiometry of C_2P has also attracted much attention. Yagmurcukardes et al. investigated electronic, magnetic, and mechanical properties of NHG, PHG, and Arsenicated holey graphene (AsHG) [26]. However, they did not study the stacking orders and adsorptive behaviors of PHG. The electronic behavior for different layers of PHG is also lack of detailed research. In this study, we have made necessary supplements to previous investigation on PHG. First, the structural characteristics of PHG are analyzed. Stacking structures of PHG are studied, and the most stable stacking is obtained. Then, we investigate the band structures for different layers of PHG. Impact of the biaxial strain and defects on the band structures is investigated. Finally, we investigate the atomic adsorption characteristics on monolayer PHG. The effect of atomic adsorption on band structure is analyzed.

*Corresponding authors

Email addresses: slb0813@126.com (Li-Bin Shi [1]), dhk@bhu.edu.cn (Hai-Kuan Dong [1])