Ballistic electronic and thermal conductance of monolayer and bilayer black phosphorus

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ABSTRACT

We performed first principle calculations based on density functional theory and GW approximation with Landauer approach to study ballistic electronic conductance and ballistic thermal conductance of black phosphorus (BP) whose dimensions are smaller than the mean free path of carriers. Ballistic electronic conductance of monolayer BP and bilayer BP with four different stacking styles, and ballistic thermal conductance of monolayer BP were investigated. The electronic transmission value along armchair direction is found to be a little higher than that along zigzag direction near the band gap energy range. Our calculations showed that, the Γ point hole effective mass along zigzag direction is stacking-style sensitive, while other Γ point effective mass is independent of stacking style. We also reported the anisotropic ballistic thermal conductance of monolayer BP: the anisotropic ballistic thermal conductance ratio of zigzag-to-armchair approaches a constant (about 2.0) when the temperature is beyond 200 K. The reasons for these properties were discussed.

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1. Introduction

Since the fabrications of low dimensional materials became possible, low dimensional materials, especially two-dimensional (2D) materials have been expected to be bricks of next generation nanoelectronic, optoelectronic and thermoelectronic devices [1]. In the past few decades, many researchers focused on graphene and graphene-like materials, such as hexagonal boron nitride (*h*-BN) [2,3] and transition metal dichalcogenides (TMDCs) [4–8]. One of the characteristics these materials have in common is that they are rarely anisotropic. Very recently, some experimental research groups reported that BP has highly anisotropic properties both in electronic and thermal transportation [9–11]. It is believed that such unique anisotropic properties are desirable for the nano-electronic, optoelectronic, thermoelectronic and other novel devices.

The bulk structure of BP is a monolayer-stacking structure with van der Waals interactions between adjacent monolayer BP. Previous theoretical investigations show that the band gap of BP is

layer-number-dependent, varying from 0.15eV [12] for bulk BP to about 2.3 eV [13] for monolayer. It was reported that bulk BP has the band gap of range about 0.15−0.4eV both in experiments [14,15] and theoretical calculations [12,16,17]. Monolayer and few layers BP have much larger band gap. The band gap of monolayer BP had been predicted to be in the range 1.5−2.3 eV [13,18,19] with GW approximation while it was predicted to be about 1.0 eV [13,20,21] with the generalized gradient approximation (GGA) calculations. Recent theoretical calculations showed that the electronic structure and optical properties of the twisted bilayer BP largely depend on the twist angle [22]. The layer-number and stacking-style dependent electronic transport properties have been reported, but only the zigzag direction was investigated [23]. The wide layer-number-dependent band gap range makes monolayer and few layers BP more attractive and having great potential applications in electronic devices in the near future. Its high carrier mobility [24] and anisotropic in-plane properties [25] make it a potential ingredient for field-effect transistor(FET) [1] and thermoelectronic devices based on Seebeck effect [18]. However, there are contradictory experimental results about the anisotropic carrier mobility in literature [9,10]. There are also contradictory theoretical results about the anisotropy of thermal conductance in monolayer BP

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[18,26,27]. Furthermore, the role of stacking style of bilayer BP on its properties remains more open discussions.

Nowadays, it is possible to fabricate few layers BP structures whose dimensions are much smaller than the mean free path (MFP) of carriers. Therefore, it is essential to investigate the transport properties of BP in the ballistic regime. In this paper, using density functional theory (DFT) method and GW approximation plus Landauer approach [28,29], we have systematically investigated electronic transport properties of four different stacking style bilayer BP and thermal transport properties of monolayer BP in the ballistic regime. The A-C(I) and A-A stacking styles (Fig. 1(c)) of BP are most frequently investigated in literature. The former is the stacking style of bulk BP. In the Landauer formula, the key procedure is to evaluate the transmission function. In our work, both the electron transmission and the phonon transmission function were calculated using the band-counting method [30,31].

This paper is organized as follows: Section 2 gives a brief introduction of Landauer formula approach and the detailed calculation method. The electronic and thermal transport properties of monolayer and bilayer BP are shown in Sections 3 and 4, respectively, while the conclusions are given in Sec. 5.

2. Calculation method

The Landauer formula [28,29] for electron current (I_{el}) in the linear response regime is expressed as

$$I_{el} = \frac{e}{h} \int T_{el}(E)[f_L(E) - f_R(E)]dE \tag{1}$$

where $f(E)$ is the Fermi-Dirac distribution, the sub-indices L and R refer to the left and right hand side contacts, respectively. $T_{el}(E)$ is the transmission function at given energy E. In ref.30, the total transmission of electron $T_{el}(E)$ is described as $T_{el}(E) = \overline{T}_{el}(E)M_{el}(E)$. $\overline{T}_{el}(E)$ is the transmission per conduction channel at given energy E. $M_{el}(E)$ is the number of conduction channels at given energy E [29]. $\overline{T}_{el}(E)$ is given as $\overline{T}_{el}(E) = \lambda_{el}(E)/(L + \lambda_{el}(E))$ [28], where $\lambda_{el}(E)$ is the mean-free-path and L is the length of the conductor. In the ballistic limit ($L << \lambda_{el}(E)$), $\overline{T}_{el}(E)$ equals to 1, therefore the total transmission $T_{el}(E)$ depends on $M_{el}(E)$ only. $M_{el}(E)$ is expressed as [30,32].

$$M_{el}(E) = \sum_n \int \frac{L_\perp}{2\pi} dk_\perp \int \frac{L_{//}}{2\pi} dk_{//} \delta\left(E - \varepsilon_n\left(\vec{k}\right)\right) \frac{\pi\hbar|v_{//}|}{L_{//}}$$

$$= \sum_n \int \frac{L_\perp}{2\pi} dk_\perp \int_{\min \varepsilon_{n,k_\perp}}^{\max \varepsilon_{n,k_\perp}} \delta\left(E - \varepsilon_{n,k_\perp}\left(k_{//}\right)\right) d\varepsilon_{n,k_\perp}\left(k_{//}\right) \tag{2}$$

$$= \int \frac{L_\perp}{2\pi} dk_\perp N_{k_\perp}(E)$$

where $L_{\perp(//)}$ is the super cell size in the direction of perpendicular
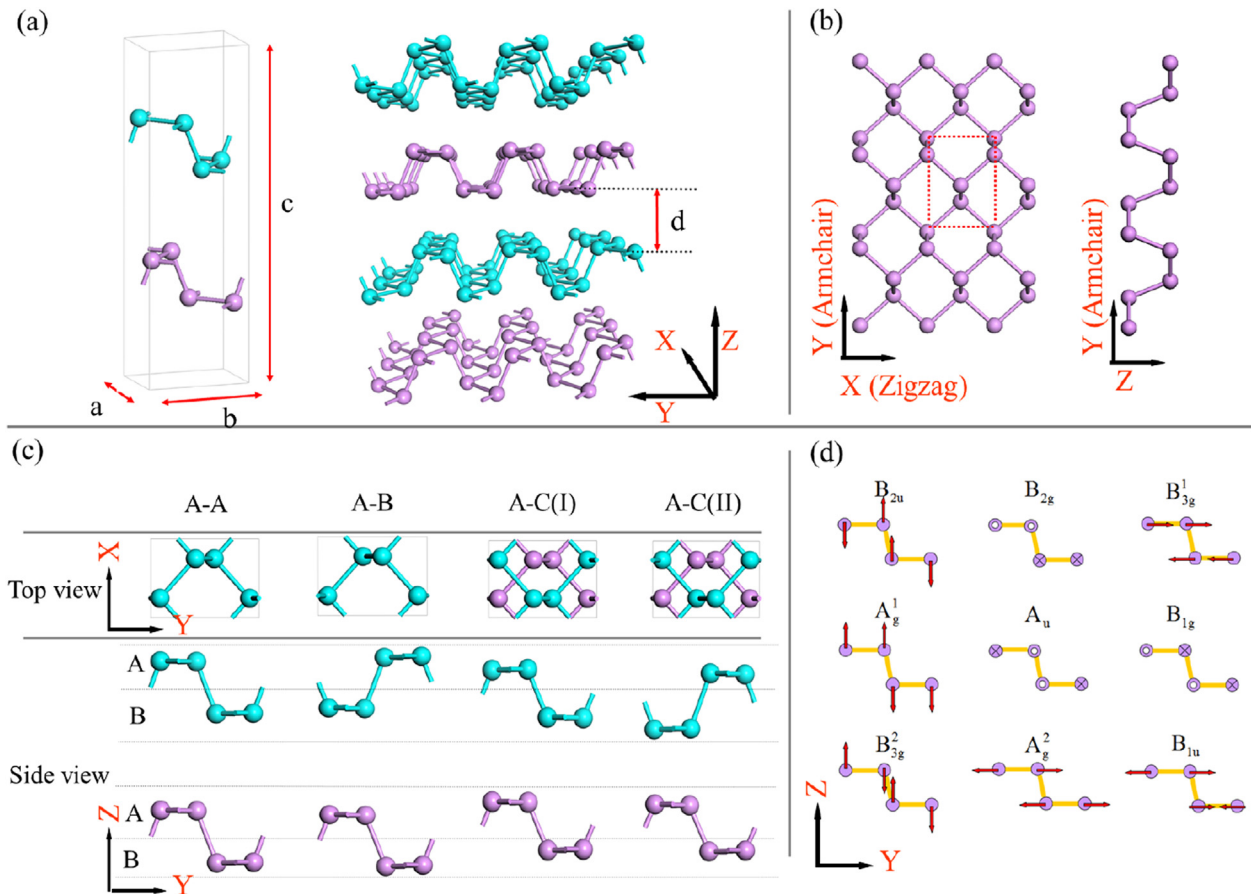
Fig. 1. (a) Crystal structure of bulk BP, *a*, *b* and *c* are the lattice constants along zigzag, armchair and z-direction respectively. *d* is the distance between the adjacent layers. (b) Top view and side view of the monolayer BP. The unit cell is indicated with a red rectangle. The X(zigzag), Y(armchair) and Z directions are indicated with black arrows. (c) Four different stacking styles of bilayer BP. Both the cyan and violet balls refer to phosphorus atoms. The cyan (violet) atoms belong to the top (bottom) layer. (d) Atomic displacements of the irreducible representations of 9 optical modes in monolayer BP. The dotted and crossed balls refer to vectors point in and out of the Y-Z plane respectively. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)