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Anisotropic electronic heat capacity and electrical conductivity of monolayer biased impurity-infected black phosphorus

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ABSTRACT

We theoretically investigate the electron-impurity interaction effects on the direction-dependent electronic heat capacity (EHC) and electrical conductivity (EC) of single-layer biased black phosphorus (BP) as a function of temperature. By means of the Born approximation besides the continuum approximation of the tight-binding Hamiltonian and the Green's function approach, we obtain a significant difference in the $x-$ and $y-$direction EHC and EC. Inherent higher value of the $y-$direction density of states around the Fermi energy in the valence band exhibits interesting anisotropic EHC and EC results. The Schottky anomaly in EHC quantity decreases slightly with impurity in $x-$direction of unbiased BP, whereas there is no change in $y-$direction. On the other hand, the probability of transition between energy levels provided by the decreased critical temperature decreases with impurity in $x-$direction EC and similarly there is no alteration in $y-$direction EC. We show that the Drude weight in EC appears with impurity in both directions. Furthermore, we study the influence of bias voltage on the EHC and EC of impurity-infected BP. Our findings showcase the increased (decreased) EHC (EC) of disordered BP and disappeared the Drude weight of EC in the presence of bias voltage.

1. Introduction

In the past decade, it has been seen the rapid development of two-dimensional (2D) materials such as graphene [1,2], hexagonal boron nitride [3], molybdenum disulfide (MoS_2) [4], silicene [5,6], germanane [7,8], and nanostructures based on phosphorous [9] in many fields owing to their remarkable mechanical, electrical, and thermal properties with potential applications in nanoelectronics, nanophotonics, and optoelectronics. Among these 2D materials, graphene attracted considerable attention because of its unique properties like high electronic and thermal mobility and high mechanical strength. However, the graphene electronic applications in high ON-OFF current ratio have been limited due to its zero band gap [1,10]. Also, device applications of MoS_2 with large band gap have been restricted because of its low mobility [11].

Most recently, researchers focused on new 2D-layered material BP named phosphorene. Some group fabricated monolayer BP using exfoliated BP [12,13]. The direct band gap [14], thermal conductivity, high carrier mobility [13,15], and a large ON-OFF current ratio [13], make BP a good candidate for nanoelectronics, thermoelectrics, and optoelectronics. The anisotropic structure is unique structural characteristic of BP which makes it distinguishable than other 2D materials and leads to the direction-dependent optical, thermal, mechanical, and electronic properties and thus, nanodevice can be designed utilizing this directional selectivity [16–22].

Electrical conductivity (EC) of BP 2D materials has been widely investigated [23] in recent years. The application of 2D materials in electronic and electrochromic devices increases by improving their EC via different methods, like strain [24,25], defect [27–29], and substitutional doping [30]. I. N. Kholmanov et al. [31] reported that the EC of graphene films improved by integration it with metal nanowires. Also, in Ref. [32], the EC of series of MoS_2 organic layer nanocomposites has been experimentally studied. Their results show that the EC of MoS_2-donor nanocomposites is more than the pristine MoS_2 at room temperature.

In Ref. [33], the authors theoretically studied the electronic and optical properties of a BP monolayer doped with tetracyanoquinodimethane (TCNQ), tetracyanoethylene (TCNE) and tetrathiafulvalene (TTF). They reported that the band gap of monolayer and bilayer BP reduce by TCNQ, TCNE and TTF doping due to charge transfer and strong interaction between BP and impurity molecules. E. Kutlu et al. [34] reported that the electronic and optical properties of BP have significantly changed by doping Au, Sn and I, also, the band structure of BP doped with Au and Sn show metallic behavior.

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Furthermore, BP is a promising candidate in battery electrode applications because of its high electrical conductivity [35,36], specific capacity, and significant high average voltage in comparison with TiO_2 and graphite [37].

Besides the electronic properties, yet, thermal properties of BP have not been investigated well. One of the thermal properties is heat capacity, which is a response function of the system as the ratio of the heat added to/removed from the matter to the resulting temperature change. Since charged impurity destroys the distribution of electronic density of states (DOS) of materials, one might study its effect on the EC and EHC quantities. In this work, using the tight-binding Hamiltonian, the Green's function approach, and the Born approximation, we study the effects of dilute charged impurities on the EC and EHC of monolayer biased BP. All calculations are carried out numerically.

Accordingly, the remainder of this paper is organized as follows: Secs. 2 and 3 introduce the required theoretical framework. In Sec. 4, we show the numerical results and finally, our main conclusions are concluded in Sec. 5.

2. Model and non-interacting Green's function

The top view of the real space of monolayer BP with an orthorhombic crystal structure and two different located phosphorus atoms in vertical heights have been illustrated in Fig. 1(a). The four phosphorus atoms at different sublayers of monolayer BP are represented by dark green and black symbols at the bottom and top sublayer, respectively. By taking into account the C_{2h} group invariance-included [38] tight-binding model proposed in Ref. [39] and using the expanded tight-binding model proposed by Rodin et al. [40] around the Γ point

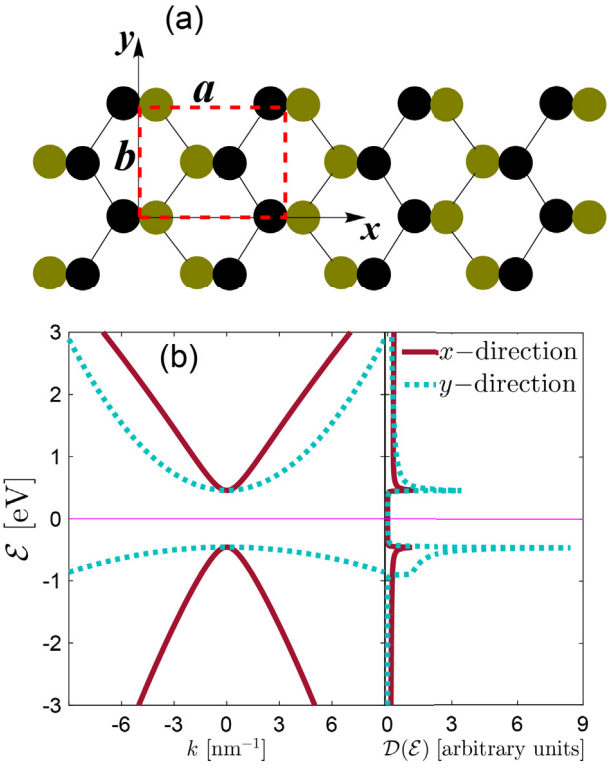

Fig. 1. (a) Top view geometry of single-layer BP. The red dashed lines illustrate the unit cell. Each cell includes four atoms shown by dark green and black circles. The lattice constants along the $x-$ and $y-$direction are labelled by $a = 4.63$ Å and $b = 3.3$ Å, respectively (taken from Ref. [40]). Panel (b) indicates the direction-dependent electronic band structure and density of states of monolayer BP. The Fermi level is set to zero (narrow solid magenta line). (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

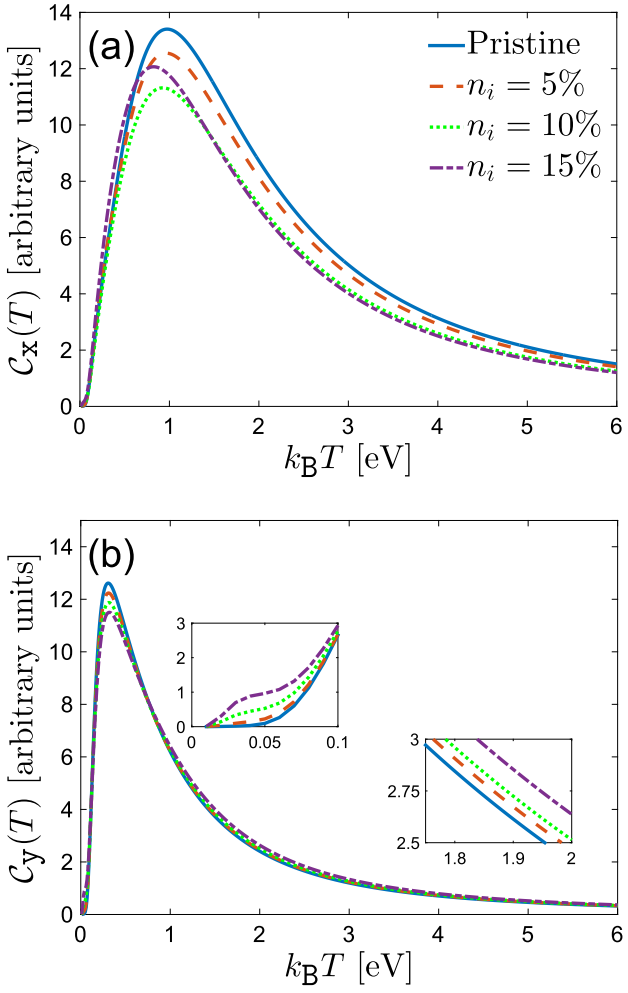

Fig. 2. (a) $\mathscr{C}_x(T)$ and (b) $\mathscr{C}_y(T)$ in monolayer unbiased BP for different impurity concentrations, namely $n_i = 0\%$, 5%, 10%, and 15%. The decreasing behavior of critical temperature with n_i is evident in $x-$direction.

(retaining the terms up to the second-order in momentum), the continuum approximation of phosphorene model Hamiltonian would be achieved as [40],

$$\mathscr{H}(\mathbf{k}) = \begin{pmatrix} \varepsilon_c + \eta_c k_x^2 + \nu_c k_y^2 & \gamma k_x + \alpha k_x^2 + \beta k_y^2 \\ \gamma k_x + \alpha k_x^2 + \beta k_y^2 & \varepsilon_v - \eta_v k_x^2 - \nu_v k_y^2 \end{pmatrix}. \tag{1}$$

which is in the basis of envelope functions ψ^c and ψ^v associated with the probability amplitude at the respective sublattice sites. In the equation above, $\varepsilon_c = -1.335$ eV and $\varepsilon_v = -0.423$ eV are the energies from the bottom of the conduction band and the top of the valence band at Γ point, respectively, with a direct energy gap $\mathscr{E}_g = |\varepsilon_c - \varepsilon_v| = 0.912$ eV and $\mathbf{k} = (k_x, k_y)$ is the momentum. Other coefficients can be extracted from the knowledge of density functional theory (DFT) results [41]: $\eta_c = 0.008187$, $\eta_v = 0.038068$, $\nu_c = 0.030726$, $\nu_v = 0.004849$ which are in units of eVnm^2, and $\gamma = 0.48$ eVnm. By considering $\alpha \ll \gamma$ and time-reversal invariant (TRI) in the system, one might delete terms including α and β. Thereby, the new Hamiltonian by considering V_{bias} as variable bias voltage can be rewritten as:

$$\mathscr{H}(\mathbf{k}) = \begin{pmatrix} \mathscr{H}_c & \mathscr{H}_{cv} \\ \mathscr{H}_{cv} & \mathscr{H}_v \end{pmatrix}, \tag{2}$$

where