



Tuning carrier mobility of phosphorene nanoribbons by edge passivation and strain



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ABSTRACT

Using first-principles calculations, we have studied the effects of different edge passivation groups on the carrier mobility of the phosphorene nanoribbons (PNRs) and strain effect on the transport property in passivated PNRs. The numerical results show that the size-dependent carrier mobility of passivated PNRs is not very sensitive to the different passivation groups, such as hydrogen (H), fluorine (F) and chlorine (Cl), but strongly associated with the orientation of nanoribbons. Passivated armchair-PNR has much larger carrier mobility than passivated zigzag-PNR at the similar ribbon width. With increasing ribbon width, the electron mobility of passivated PNRs can be further enhanced. We also find that the anisotropy of carrier mobility in passivated PNRs can be reversed by applying tensile strain resulting from order switching of the conduction bands around Fermi level.

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Two-dimensional (2D) materials such as graphene [1–3] and transition metal dichalcogenides (TMDs) [4–6] have attracted intensive research interest due to their high surface-volume ratio and unique electronic properties distinguished from their bulk counterparts. It is well-known that a high-performance device such as a field-effect transistor (FET) requires a moderate electron band gap and reasonably high carrier mobility of the channel material [7–13]. Pristine graphene offers extremely high carrier mobility, however, its performance in nanotransistors is limited due to the absence of band gap [7–10]. As a member of TMD family, unlike graphene, monolayer MoS₂ is a semiconductor with a large band gap (~1.8 eV) and relatively high on/off ratio exceeding 10⁸ [11–13]. However, the carrier mobility of MoS₂ was previously reported to be approximately 200 cm² V⁻¹ s⁻¹ and may be further improved to 500 cm² V⁻¹ s⁻¹, which is still not suitable for applications [13].

Very recently, as a new 2D compound, few-layer black phosphorus or phosphorene has been successfully exfoliated and attracted a great deal of attention [14–26]. The few-layered phosphorene-based FET exhibits ambipolar with drain current modulation up to ~10⁵ and a carrier mobility up to 1000 cm² V⁻¹ s⁻¹ at room temperature [14]. Moreover, it was reported that the p-type phosphorene transistor can be integrated with the n-type MoS₂ tran-

sistor to make a 2D Complementary Metal Oxide Semiconductor (CMOS) inverter [15]. In addition, phosphorene also shows some unique features, such as anisotropic electric conductance and optical responses, which are distinguishing from other 2D materials [27]. And the anisotropic electrical conductance can be engineered by applying appropriate strain [28].

The layered structures can be etched or patterned along a specific lattice direction, forming one-dimensional (1D) strips. Because of peculiar quantum confinement and edge effects, nanoribbons exhibit many exploitable electrical, optical, and magnetic properties [29–31]. The carrier mobility of pristine armchair PNRs is quite low [32], therefore tailoring transport property of PNRs is crucial for their applications in nanoelectronic devices. Peng et al. [33] studied the edge passivation effect on the electronic properties of PNRs. Han et al. [34] thought the effective masses of H passivated PNRs could be tuned under the strain, therefore, they concluded that the carrier mobility of H passivated PNRs could be modulated by the strain effect. As well known, the carrier mobility mainly depends on three factors which are the stretching modulus, deformation potential (DP) constant and effective mass. Therefore, our main concerns are as follows: Whether there is a close relationship between the carrier mobility of PNRs and different passivation groups? Whether the anisotropic carrier transport property of passivated PNRs can be modulated significantly by an external strain?

Based on first-principle calculations and deformation potential theory we perform systematic calculations in the carrier mobil-

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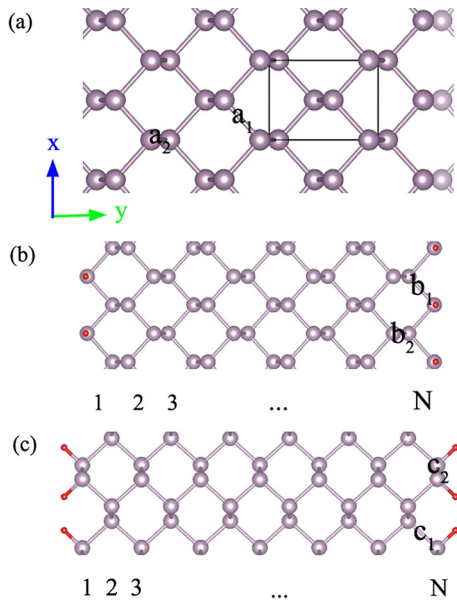


Fig. 1. Structure model of phosphorene sheet and nanoribbons with structural parameters (a_1 , a_2 , b_1 , b_2 , c_1 , and c_2). (a) Structure of monolayer phosphorene, the straight lines represent the primitive cell. (b) The ZPNR and (c) APNR are truncated from phosphorene along the x - and y -directions, respectively. The edge dangling bonds of PNR are passivated by H, F, and Cl (red-colored) atoms. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

ity of passivated PNRs and find that the carrier mobility is not very sensitive to different saturation groups (such as H, F and Cl), but strongly associated with the orientation of nanoribbons. The carrier mobility of H passivated armchair-PNR (H-APNR) is much larger than that of H passivated zigzag-PNR (H-ZPNR) such as the electron mobility in H-APNR is two orders of magnitude larger than that in H-ZPNR for a width of ~ 20 Å. The electron mobility in H-APNR can reach up to $4353 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ at the ribbon width of 22.04 Å. We have also investigated the effect of tensile strain on the transport property of H-PNR and find that is similar to the monolayer case, [28] the anisotropy of electron transport in H-PNR along each direction will be reversed by applying appropriate tensile strain.

Our theoretical calculations are carried out by first-principle calculations based on the density functional theory (DFT) formalism as implemented in Vienna Ab-initio Simulation Package (VASP) [35]. The generated gradient approximation (GGA) formulated by the Perdew–Bruke–Ernzerh (PBE) functional [36] and the projector-augmented plane wave (PAW) potentials [37] are used. The kinetic energy cutoff for the plane wave set is 500 eV in all computations and the convergence threshold for energy is 10^{-5} eV. A $15 \times 11 \times 1$ k -mesh is used for phosphorene. The k -meshes of $15 \times 1 \times 1$ and $1 \times 11 \times 1$ are adopted for the ZPNRs and APNRs, respectively. A vacuum space of 40 Å is large enough to safely avoid the interaction between nanoribbon and its periodic images. All atoms are relaxed and the final force exerted on each P atom is less than 0.01 eV/Å. To obtain the value of the stretching modulus and the DP constant, we calculated the band structures of unit cells under the uniaxial stress applied along the periodic direction, allowing a unitary deformation in the range of $\pm 1\%$.

We first optimize the geometric and electronic structures of phosphorene. Our calculated results indicate that phosphorene is a direct semiconductor with a gap of 0.90 eV at the Γ point. As displayed in Fig. 1(a), the nearest neighbor P–P bond lengths in phosphorene are $a_1 = 2.22$ Å, and $a_2 = 2.25$ Å, respectively. Our computational results are in good agreement with previous studies [34]. Considering the characteristic structure of phospho-

Table 1

Number of P zigzag lines (dimer lines), nanoribbon width, and energy gap for all phosphorene nanoribbons with H, F and Cl passivations.

ZPNR	H-ZPNR	F-ZPNR	Cl-ZPNR
Width (N)	Width (Å)	Gap (eV)	Gap (eV)
9	20.12	1.45	1.39
10	22.42	1.38	1.33
11	24.73	1.32	1.28
12	27.05	1.27	1.24
13	29.35	1.23	1.20
14	31.67	1.20	1.18
15	33.98	1.17	1.15
APNR	H-APNR	F-APNR	Cl-APNR
Width (N)	Width (Å)	Gap (eV)	Gap (eV)
9	13.19	1.03	1.05
10	14.84	1.00	1.02
11	16.48	0.99	0.99
12	18.14	0.97	0.98
13	19.78	0.96	0.97
14	21.43	0.95	0.96
15	22.04	0.94	0.95

rene, there are two obvious orientations to form nanoribbons: the ZPNR and APNR truncated from monolayer phosphorene along the x - and y -directions, respectively, as shown in Fig. 1. The width of a nanoribbon N is referred according to the number N of zigzag lines (dimer lines) across the ZPNR (APNR) width as indicated in Fig. 1. The formation of each nanoribbon results in the breaking of P–P bonds of edge P atoms. Consequently, these edge P atoms are highly active and may easily bond with impurities, therefore, which could be H, F, and Cl atoms as in our present model.

Secondly, we systematically investigate electronic and transport properties of the H-PNR. After fully geometric relaxation, the P–P bond lengths at the edge of H-ZPNR are $b_1 = 2.23$ Å and $b_2 = 2.24$ Å, while $c_1 = 2.22$ Å and $c_2 = 2.25$ Å at the edge of H-APNR, respectively (Fig. 1). We find these bond lengths at the edge remain almost unchanged, compared to those in phosphorene. Based on the optimized structure, we calculate a series of H-PNRs with ribbon widths ranging from $9 \leq N \leq 15$. We find that the band gap of either H-ZPNR or H-APNR reduces during increasing ribbon width, and converges gradually to phosphorene as shown in Table 1. This behavior can be contributed to the quantum confinement of electrons [2]. The effect of quantum confinement on H-ZPNR is considerably larger than H-APNR, for example, 9-H-ZPNR of 20.12 Å width has a band gap of 1.45 eV, while 13-H-APNR of 19.78 Å width has only a band gap of 0.96 eV. The behavior is derived from the fact that the edge states of phosphorene propagate primarily along armchair direction, which is in line with previous DFT report [34]. In order to discuss the effect of the orientation on the electronic property of H-PNR, we present the band structures of 9-H-ZPNR and 13-H-APNR which have the similar ribbon width (Fig. 2). It is found that 9-H-ZPNR is an indirect band gap semiconductor, whose valence band maximum (VBM) is slightly away from Γ point and conduction band minimum (CBM) is located at Γ point, while 13-H-APNR shows a direct band gap at Γ point.

Next, we calculate the carrier mobility of H-PNRs along armchair and zigzag directions. The carrier mobility of 1D materials usually estimated according to the formula [38–41],

$$\mu = \frac{e\tau}{m^*} = \frac{e\hbar^2 C}{(2\pi k_B T)^{1/2} |m^*|^{3/2} E_1^2}, \quad (1)$$

where m^* is the effective mass of electron and hole, T is the temperature, C is defined as the stretching modulus and simulate the lattice distortion activated by the strain, and the term E_1 is the Deformation Potential (DP) constant representing the scattering of

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