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A comparative study on the edge states in phosphorene quantum dots and rings

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ABSTRACT

Using the tight-binding Hamiltonian approach, we comparatively investigate the energy spectrums of triangular zigzag phosphorene quantum dots (PQDs) and rings (PQRs), as well as their potential applications. In comparison with the outer edge states in the PQD, new extra inner edge states can be produced in the PQR by its internal hole. A transition from the uncoupled to coupled edge states can be induced by decreasing the width between the outer and inner edges of the PQR. Also, the edge states in PQD/PQR are all anisotropically localized in one side, rather than three sides as in triangular graphene quantum dots (QDs) and rings (QRs). Furthermore, the PQD/PQR energy levels can be anisotropically manipulated by the external electric fields and strains, clearly demonstrating their potential applications in field effect transistors or electromechanical devices. In the meanwhile, we also consider the electron probability distributions corresponding to the different energy levels, clearly exposing the characteristics of the PQD/PQR energy levels. The comparison between the asymmetrical triangular PQDs/PQRs and the symmetrical triangular QDs/QRs in graphene should be instructive for understanding the similar triangular QDs/QRs in other two-dimensional layered materials, as well as other types of QDs/QRs of different shapes.

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1. Introduction

Two-dimensional materials ranging from $NbSe_2$ [1], graphene [2], MoS_2 [3], hexagonal boron nitride [4], and transitional-metal dichalcogenides [5] to phosphorene [6] have triggered overwhelming interest in the low-dimensional research field in recent years. Especially, phosphorene, a single layer of black phosphorus, has started to gain more and more attention due to its finite bandgap [6–8], high carrier mobility [9,10], and large on-off current ratios [10–12]. In spite of its difficulty in material fabrication, phosphorene is still looked upon as a promising candidate in the race for the electronic, thermoelectric, and plasmonic applications. As a newcomer of the two-dimensional material family that can be experimentally realized also by exfoliation [6,12], the initial research focus about phosphorene has been concentrated on the determination of its band structure [13–15], as well as the practicable means of band manipulation [15–21]. It has been demonstrated that the bandgap can be adjusted by changing the layer number [8,14,15], applying the external electric field [16], or imposing the strains [17]. In comparison with the planar graphene, phosphorene of the puckered lattice structure is more flexible and durable, and even able to sustain up to about 30% deformation both in zigzag and armchair directions [18].

Up to now, most of the researches were carried out in the ideal single or few layer phosphorene systems of infinite size. However, it is inevitable to constrain phosphorene to form one-dimensional phosphorene nanoribbon or zero-dimensional phosphorene quantum dots (PQDs) so as to design phosphorene-based functional devices for various applications. Very recently, the investigation on the properties of the phosphorene nanoribbons have begun [22–28]. However, to the best of our knowledge, only two research works on the PQDs have been done. One is the experimental synthesis of the few-layer PQDs based on chemical methods by Zhang et al. [29], whereby a flexible memory device was successfully fabricated that exhibits a nonvolatile rewritable memory effect with a high on-off current ratio and good stability. The other is the theoretical study on the five types of the monolayer PQDs, including triangular, rectangular, and hexangular PQDs with armchair or zigzag edges by Zhang et al. [30]. They studied the energy levels and density of states in the different PQDs of different sizes, as well as the influences of the magnetic field. However, the influences of the electric field, the strains, and so on, have not been discussed. On the other hand, it has been demonstrated that holes in graphene quantum rings (GQRs) will produce new edge states in

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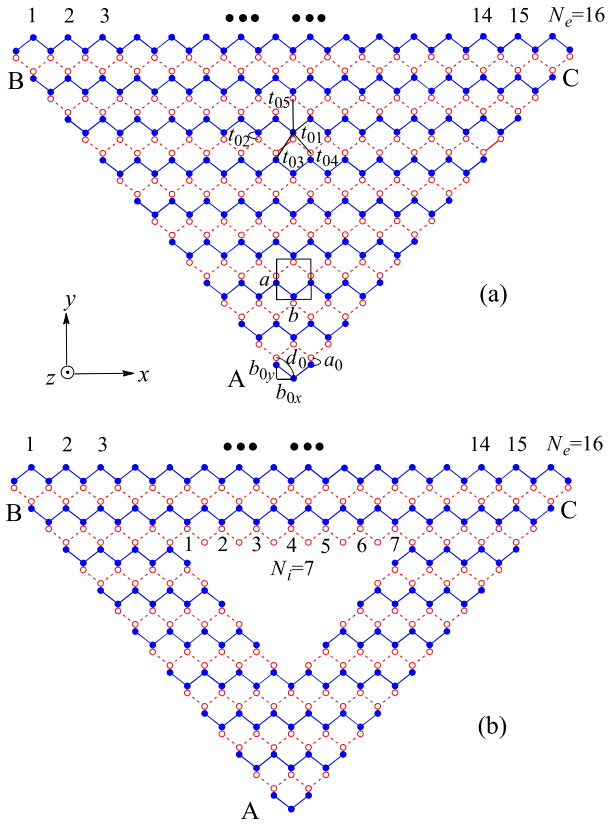

Fig. 1. (Color online.) Top views of the triangular zigzag PQD (a) and PQR (b). The solid and open circles represent phosphorus atoms in the up and down sublayers, respectively. x (y) axis is along the zigzag (armchair) direction. Schematically shown are the five coupling terms t_{0i} ($i = 1, 2, \ldots, 5$), the basis vector lengths a and b of the primitive cell, and the other related in-plane geometry parameters a_0, b_{0x}, b_{0y}, and d_0. Also the size of the PQD or PQR is denoted by N_e and the hole size in PQR is by N_i.

the GQRs [31–33], different from those in graphene quantum dots (GQDs) [34–36]. One may naturally wonder whether there are similar new edge states appearing in PQRs in comparison with the corresponding PQDs. In addition, the electron probability distributions are symmetrically localized on three sides for the triangular GQDs or GQRs. Geometrically, the triangular GQDs or GQRs can be readily designed with the three sides having the same edges. However, there is no way to make the triangular PQDs/PQRs have three completely same sides due to the phosphorene anisotropy. Therefore, it should be instructive to investigate, between the asymmetrical PQDs/PQRs and symmetrical GQDs/GQRs, what kind of differences exist in the aspects such as the energy levels, the edge states, the effect of the hole in PQRs, as well as their potential application in device designing.

Motivated by these researches, in this paper we design one kind of triangular zigzag PQDs and PQRs, as shown in Fig. 1, to carry out a comparative study on their energy spectrums. It is found that the energy levels of the triangular zigzag PQDs/PQRs are assembled in the full-filled band (FB), the zero-energy band (ZB), and the unoccupied band (UB), and further ZB are found to be edge states while FB and UB are not according to the electron probability distributions. It is demonstrated that the holes can produce new edge states in the PQRs, making serious influences on the energy spectrum in relative to those of the PQDs. Both the electric field and mechanical strains can make the anisotropic influences on their spectrums of the PQDs/PQRs, demonstrating the potential applications in designing the electronic or electromechanical devices. Moreover, the specific distributions of the electron probabilities are selectively presented to deepen the understanding about the FB, ZB, and UB. In the meanwhile, the necessary comparisons between PQDs/PQRs and GQDs/GQRs are made, and the applicability of the PQD/PQR-based devices and the universality of the conclusion drawn from the triangular PQDs/PQRs are discussed.

This paper is organized as follows. In Sec. 2, we present the tight-binding Hamiltonian of the PQD and PQR. A complete numerical investigation into the PQD/PQR energy levels, as well as the influences of the electric field and the strain, is carried out in Sec. 3. Finally, a brief conclusion is given in Sec. 4.

Table 1
Coefficients $\alpha_{ix,y,z}$ for different interatom couplings.

	t_1	t_2	t_3	t_4	t_5
α_{ix}	$b_{0x}^2 r_{01}^{-2}$	0	$b_{0x}^2 r_{03}^{-2}$	$d_{0x}^2 r_{04}^{-2}$	0
α_{iy}	$b_{0y}^2 r_{01}^{-2}$	$a_0^2 r_{02}^{-2}$	$(d_{0y}+a_0)^2 r_{03}^{-2}$	$d_{0y}^2 r_{04}^{-2}$	$(d_{0y}+b_{0y})^2 r_{05}^{-2}$
α_{iz}	0	$l_0^2 r_{02}^{-2}$	0	$l_0^2 r_{04}^{-2}$	$l_0^2 r_{05}^{-2}$

2. Model

The structures of the triangular zigzag PQD and PQR considered in this paper are schematically shown in Figs. 1(a) and 1(b), respectively. The PQD is composed of one normal zigzag side BC and two skewed zigzag sides AB and AC, and the PQR can be viewed as a PQD with a central hole. Obviously, along BC direction the up and down sublayer atoms separately constitute one-dimensional horizontal zigzag atom chains represented by the solid blue circles and the open red ones, respectively. For each zigzag atom chain, they can be viewed as a compound lattice including two types of atoms localized on the down-sawtooth (A-type atoms) and up-sawtooth (B-type atoms) terminal positions. The size of the triangular PQD is described by its side length N_e (the number of the atoms in side BC), which indicates that the total number of the phosphorus atoms in the PQD is $N_e^2 + 4N_e + 1$. Since there are $N_i^2 - 2N_i + 1$ atoms in the hole of size length N_i for the triangular PQR in Fig. 1(b), the total number of the phosphorus atoms left in the PQR is equal to $N_e^2 - N_i^2 + 2(2N_e + N_i)$. The tight-binding Hamiltonian of the PQD or PQR can be written as [14,15]

$$H = \sum_i \epsilon_i c_i^\dagger c_i + \sum_{i \neq j} t_{ij} c_i^\dagger c_j, \tag{1}$$

where $c_i^\dagger$ (c_i) is the creation (annihilation) operator of the electron at atom i , ϵ_i the on-site energy of atom i, and t_{ij} the hopping coupling between atoms i and j. According to Ref. [14], it is a good approximation to take into account the five hopping couplings t_{01}, t_{02}, t_{03}, t_{04}, and t_{05}, which are -1.22 eV, 3.665 eV, -0.205 eV, -0.105 eV, and -0.055 eV, respectively, as shown in Fig. 1(a). Correspondingly, the interatom distances are denoted by r_{01}, r_{02}, r_{03}, r_{04}, and r_{05}, which can be expressed by using the parameters a_0, $b_{0x,y}$, $d_{0x,y}$, and l_0. Note that $d_{0x,y}$ are the x, y-direction components of d_0, and l_0 the vertical distance between the two sublayers. When the PQD/PQR structure is deformed by a strain, the hopping coupling t_i will be modulated as [37]

$$t_i/t_{0i} \approx 1 - 2(\alpha_{ix}\varepsilon_{ix} + \alpha_{iy}\varepsilon_{iy} + \alpha_{iz}\varepsilon_{iz}). \tag{2}$$

Here $\varepsilon_{ix,y,z}$ denote the strain indices applied along the x, y, z-directions with the coefficients $\alpha_{ix}(= x_{0i}^2 r_{0i}^{-2})$, $\alpha_{iy}(= y_{0i}^2 r_{0i}^{-2})$, and $\alpha_{iz}(= z_{0i}^2 r_{0i}^{-2})$ listed in Table 1. Moreover, the related geometry parameters in Fig. 1 are $a_0 = 0.7054$ Å, $b_{0x} = 1.6570$ Å, $b_{0y} = 1.4826$ Å, $d_{0x} = 1.6570$ Å, $d_{0y} = 2.1880$ Å, and $l_0 = 2.1312$ Å.

3. Results and discussion

In this section, we will carry out a numerical study on the energy levels of the triangular zigzag PQDs and PQRs. We consider

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