Electric- and magnetic-field dependence of the electronic and optical properties of phosphorene quantum dots

L L Li¹,2, D Moldovan¹, W Xu²,3 and F M Peeters¹

¹Department of Physics, University of Antwerp, Groenenborgerlaan 171, B-2020 Antwerpen, Belgium
²Key Laboratory of Materials Physics, Institute of Solid State Physics, Chinese Academy of Sciences, Hefei 230031, People’s Republic of China
³Department of Physics, Yunnan University, Kunming 650091, People’s Republic of China

E-mail: longlong.li@uantwerpen.be, dean.moldovan@uantwerpen.be and francois.peeters@uantwerpen.be

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Abstract
Recently, black phosphorus quantum dots were fabricated experimentally. Motivated by these experiments, we theoretically investigate the electronic and optical properties of rectangular phosphorene quantum dots (RPQDs) in the presence of an in-plane electric field and a perpendicular magnetic field. The energy spectra and wave functions of RPQDs are obtained numerically using the tight-binding approach. We find edge states within the band gap of the RPQD which are well separated from the bulk states. In an undoped RPQD and for in-plane polarized light, due to the presence of well-defined edge states, we find three types of optical transitions which are between the bulk states, between the edge and bulk states, and between the edge states. The electric and magnetic fields influence the bulk-to-bulk, edge-to-bulk, and edge-to-edge transitions differently due to the different responses of bulk and edge states to these fields.

Keywords: phosphorene quantum dots, electronic and optical properties, electric and magnetic fields

(Some figures may appear in colour only in the online journal)

1. Introduction
Recently, two-dimensional (2D) black phosphorus (BP) has drawn a lot of attention from the research community. Bulk BP is a layered material in which the individual layers are stacked via weak van der Waals interactions. Single- and few-layer BP were experimentally fabricated from bulk BP [1, 2]. Inside a single layer, each phosphorus atom is covalently bonded with three nearest phosphorus atoms to form a puckered honeycomb lattice. This unique lattice structure gives rise to anisotropic electronic and optical properties of 2D BP [3, 4]. Furthermore, compared to other known 2D materials such as graphene with zero band gap [5] and transition metal dichalcogenides (TMDs) with low carrier mobility [6], 2D BP has the combined property of finite band gap (∼1 eV) [7] and high carrier mobility (∼1000 cm² V⁻¹ s⁻¹) [1], which is crucial for practical applications in e.g. field-effect transistors.

At present, various interesting properties of 2D BP have been investigated theoretically and experimentally, such as strain-engineered band structure [8], superior mechanical flexibility [9], tunable optical property [10], enhanced thermoelectric efficiency [11], strong excitonic effect [12], nonlinear optical response [13], magneto-optical Hall effect [14], and integer quantum Hall effect [15]. BP nanoribbons (BPNRs) have also been studied, and their electronic, optical, thermal and transport properties were found to depend sensitively on the edge type and ribbon width [16–23]. A very striking property of BPNRs is the presence of topological edge states, which are well separated from the bulk states and can be greatly influenced by an external electric field [20, 22]. However, compared to BP bulk and its nanoribbons, less
attention has been paid to BP quantum dots (QDs). Most recently, BP QDs (BPQDs) have been successfully synthesized through chemical methods [24, 25]. The obtained BPQDs have a lateral size of several nanometers and a thickness of few layers. Theoretical studies have also been carried out to investigate the electronic and optical properties of monolayer BPQDs or phosphorene QDs (PQDs) [26, 27]. Some interesting results were obtained, such as unconventional edge states in PQDs [26] and anomalous size-dependent optical properties of PQDs [27]. In particular, it has been shown [26] that edge states appear stably in the band gap of the PQD regardless of its geometric shape and edge structure due to the anisotropic electron hopping in the system. As is known, from a device-application point of view, it is more convenient and efficient to tune the electronic and optical properties of a QD material by external electric and/or magnetic fields than by its geometric parameters such as size and shape. Based on this viewpoint, in the present work we investigate the electronic and optical properties of PQDs under external electric and magnetic fields. We employ the tight-binding (TB) method to study how these external fields influence the electronic and optical properties of PQDs.

Like modeling graphene QDs [29], one has to take into account the effects of geometric shape and edge type when modeling PQDs using the TB method. The geometric shapes of experimentally fabricated BPQDs [24] are rectangular-like [27] but there is no experimental identification of the edge types in such nanostructures. Because of this unknown, the authors in previous theoretical works [26, 27] considered regular armchair and zigzag edges in PQDs with rectangular shapes. Although the edge types will probably be more complex in realistic BPQDs, this consideration is reasonable for theoretical modeling since the armchair and zigzag edges have been demonstrated to be chemically stable in BPNRs [28]. Based on the above statements, in the present work we consider rectangular PQDs (RPQDs) with armchair and zigzag terminations.

This paper is organized as follows. In section 2, we present the theoretical model for calculating the electronic and optical properties of RPQDs in the presence of electric and magnetic fields. In section 3, we present and discuss the effects of electric and magnetic fields on the electronic and optical properties of RPQDs. Finally, we conclude our results with a summary in section 4.

2. Model and theory

The lattice structure of phosphorene is shown in figure 1. As can be seen, phosphorene has a puckered honeycomb lattice with unit-cell lengths \((a, b) = (0.443, 0.327) \text{ nm} [20]\), and due to the puckered lattice structure there are four inequivalent phosphorus atoms in a unit cell. The TB Hamiltonian proposed for phosphorene is given by [30]

\[
H = \sum_i \varepsilon_i c_i^\dagger c_i + \sum_{ij} t_{ij} c_i^\dagger c_j,
\]

where the summation runs over the lattice sites of phosphorene, \(\varepsilon_i\) is the on-site energy of the electron at site \(i\), \(t_{ij}\) is the hopping energy between the \(i\)th and \(j\)th sites, and \(c_i^\dagger (c_i)\) is the creation (annihilation) operator of the electron at site \(i\) (j).

In the present work, we employ this TB model to study the electronic and optical properties of RPQDs with armchair and zigzag edges under external electric and magnetic fields.

We consider a RPQD placed in the \((x, y)\) plane (see figure 1), an external electric field applied along one of the in-plane directions (e.g. the \(x\) or \(y\) direction), and an external magnetic field applied perpendicular to the \((x, y)\) plane (i.e. the \(z\) direction). When an in-plane electric field is applied to the RPQD, the on-site energy in the original TB Hamiltonian (1) should be modified by adding the electric potential term \(-e\mathbf{F} \cdot \mathbf{r}_i\) with \(e\) being the elementary charge, \(\mathbf{F} = (F_x, F_y)\) the in-plane electric field vector, and \(\mathbf{r}_i = (x_i, y_i)\) the in-plane position vector at site \(i\). On the other hand, when a perpendicular magnetic field is applied to the system, the hopping energy in the original TB Hamiltonian (1) should be modified by multiplying with a phase factor determined by the magnetic flux, which is achieved via the so-called Peierls substitution:

\[
t_{ij} \rightarrow t_{ij} \exp \left( \frac{2\pi i e}{\hbar} \oint_{\gamma_i} \mathbf{A} \cdot d\mathbf{l} \right),
\]
with $\hbar$ being the Planck constant and $A$ the vector potential induced by the magnetic field. In the Landau gauge, the magnetic vector potential is written as $A = (0, Bx, 0)$ with $B$ being the magnetic field strength. The magnetic flux threading a plaquette is defined as $\Phi = Bab$ in units of the flux quantum $\Phi_0 = \hbar/e$.

The energy levels and wave functions in the RPQD are obtained by diagonalizing the TB Hamiltonian matrix numerically. All numerical TB calculations are performed using the recently developed $Psbinding$ package [31], and the obtained results are then imported into the calculations of the electronic density of states (DOS) and the optical absorption spectrum. The electronic DOS of a QD system is the sum of a series of delta functions, which can be numerically calculated with a Gaussian broadening as

$$D(E) = \frac{1}{\sqrt{2\pi} \Gamma^2} \sum_n \exp \left[ -\frac{(E - E_n)^2}{2\Gamma^2} \right],$$

where $\Gamma$ is the broadening factor and $E_n$ is the energy level for the $n$th eigenstate. The dipole matrix element for the transition from the initial state $|i\rangle$ to the final state $|f\rangle$ is given by $M_{ij} = \langle j | r | i\rangle$, where $r$ is the light assumed to be polarized in the $(x, y)$ plane of the RPQD. The optical absorption is then calculated as $A(\hbar \omega) = \sum_{ij} A_{ij}(\hbar \omega)$, where the summation is over all the possible dipole transitions and $A_{ij}(\hbar \omega)$ is given by

$$A_{ij}(\hbar \omega) = (E_i - E_j) \epsilon \cdot M_{ij} \delta(E_i - E_j + \hbar \omega),$$

where $E_i$ ($E_j$) is the energy level for the initial (final) state $|i\rangle$ ($|f\rangle$), $\epsilon$ is the light polarization vector, and $\omega$ is the angular frequency of light. In the numerical calculation of $A(\hbar \omega)$, we use the same Gaussian broadening (equation (3)) for the delta function in equation (4).

### 3. Single-particle spectrum: electric- and magnetic-field dependence

In this part, we present and discuss our numerical results for the electronic and optical properties of RPQDs with armchair and zigzag edges in the presence of electric and magnetic fields. For convenience, we denote $L$ and $W$ as the side lengths of the RPQD along the armchair and zigzag directions, i.e., the $x$ and $y$ directions, respectively. The side lengths considered in the present work are taken as several nanometers which are comparable to those realized experimentally [24, 25].

In figure 2, we show the energy levels, electronic DOS, and wave functions in a RPQD with side lengths $(L, W) = (5.5, 4.1)$ nm. Here, the region between the two red solid lines denotes the band gap of the RPQD. As can be seen, the edge states appear in the band gap of the RPQD and they are well separated from the bulk states (see figure 2(a)). This means that these edge states are well-defined in the RPQD. The electronic DOS exhibits a two-peak structure within the band gap corresponding to the edge states while a many-peak structure outside the band gap to the bulk states (see figure 2(b)). The two-peak structure for the edge states is caused by different sublattice contributions at the zigzag boundaries. The many-peak structure for the bulk states is caused by the discrete energy levels due to the usual quantum confinement effect. Here, we call the edge and bulk states according to their wave-function properties. To show such properties, we take three typical points labeled by the numbers 1, 2, and 3 in figure 2(a) and plot the squared wave functions for such three points in figure 2(c). It is clear that the edge states are only localized at the zigzag boundaries while the bulk states are mainly distributed in the central part of the RPQD. The zigzag edge states obtained here are not peculiar to phosphorene nanostructures, which can also occur in graphene and MoS$_2$ nanostructures as predicted by first-principle calculations [34, 35]. We also note from our numerical calculations that the number of edge states is equal to the number of phosphorus atoms at the zigzag boundaries. The results shown in figure 2 indicate that edge states appear as mid-gap states in a RPQD with armchair and zigzag boundaries.

In figure 3, we show the energy spectra of the same RPQD as in figure 2 in the presence of (a) perpendicular magnetic field and (b) in-plane electric field (applied along the $x$ direction). As can be seen, in the presence of magnetic field and with increasing magnetic flux, a nearly flat band is formed by the mid-gap edge states in the RPQD. The energy levels in this edge band are two-fold degenerate due to the presence of two identical zigzag boundaries. These edge levels are almost unaffected by the magnetic field, which is a consequence of the strong localized nature of edge states. However, the energy levels of the bulk states in the RPQD are non-degenerate due to the intrinsic asymmetry caused by the anisotropic boundaries, i.e., the armchair and zigzag boundaries along the $x$ and $y$ directions, respectively. These bulk levels correspond to the so-called Fock–Darwin states due to the competing geometric and magnetic confinements, and they will eventually approach the Landau levels as the magnetic flux further increases due to the dominant magnetic confinement.

On the other hand, in the presence of an electric field, the degeneracy of the edge levels is lifted due to the broken spatial inversion symmetry induced by the electric field. As a result, the single edge band at zero electric field is now split into two bands. One of these two bands (labeled as $E_1$) increases with increasing electric field and the other band (labeled as $E_2$) decreases with increasing electric field, which leads to anticrossings of the energy levels in the $E_1$ and $E_2$ bands. This feature can be understood within perturbation theory as follows. We denote the edge-state Hamiltonian in the presence of an electric field applied along the $x$ direction as $H_F = H_0 - eFx$ with $H_0$ being the zero-field Hamiltonian and $F$ being the electric field strength. And the electric-field-induced part is treated as a perturbation. Since the edge levels are two-fold degenerate at zero electric field, we need to apply degenerate perturbation theory. Denoting $E_1$ and $E_2$ ($|1\rangle$ and $|2\rangle$) as two degenerate eigenenergies (corresponding eigenstates) of the unperturbed Hamiltonian $H_0$, we have $H_0 |1\rangle = E_1 |1\rangle$ and $H_0 |2\rangle = E_2 |2\rangle$. Within degenerate
perturbation theory, the matrix elements of the perturbed Hamiltonian $H$ can be obtained in a degenerate basis set composed of unperturbed eigenstates $|1\rangle$, $|2\rangle$ as

$$[H_F] = \begin{bmatrix} E_0 & \Delta \\ \Delta' & E_0 \end{bmatrix}$$

(5)

where $E_0 = E_1 = E_2$ due to the degeneracy and

Figure 2. (a) Energy levels, (b) density of states (DOS), and (c) wave functions of a RPQD with side lengths $(L, W) = (5.3, 4.1)$ nm at zero electric and magnetic fields. The wave functions in (c) are shown for the electronic states labeled by the numbers 1, 2 and 3 in (a). The region between the two red solid lines represents the band gap of the RPQD. In the DOS calculation, a broadening factor is taken of $\Gamma = 0.02$ eV.

Figure 3. Energy spectra of the same RPQD as in figure 2 in the presence of (a) perpendicular magnetic field and (b) in-plane electric field (applied along the x direction). Here, $E_+$ and $E_-$ label the two split edge bands in the presence of an in-plane electric field. The red rectangular region in (b) is enlarged to show the anticrossings between the $E_+$ and $E_-$ bands.
\Delta = -(1/\hbar)\ eFX \sim -eFL. Diagonalizing this Hamiltonian matrix, we find that the energy levels exhibit a Stark shift under the electric-field perturbation as \( E_k = E_0 \pm |\Delta| \). Thus, the \( E_{1+} \) (\( E_1 \)) band increases (decreases) linearly with increasing electric-field strength, as shown in figure 3(b). The up- and down-going behaviors of the \( E_{1+} \) and \( E_1 \) bands initially lead to the crossings of the energy levels but the interactions between the degenerate levels at the crossing points finally give rise to anticrossings, as shown by the zoomed plot in figure 3(b). However, compared to the edge states, the bulk states shown here are almost unaffected by the electric field due to the strong QD confinement.

4. Optical absorption

The optical absorption spectra of RPQDs in the presence of electric and magnetic fields are calculated with a constant broadening factor \( \Gamma = 0.01 \) eV. This is in fact a relatively crude approximation because the realistic value of \( \Gamma \) should be in principle calculated by considering both field-dependent electronic states and various scattering mechanisms. However, the main features of the absorption spectrum with this approximation are maintained and it has been still widely used in the literature [36–38]. Furthermore, in the present work we only consider the optical properties of undoped RPQDs, where the chemical potential is assumed to be \( E_F = 0 \) eV and the temperature is taken as \( T = 0 \) K, which implies that only optical transitions between the occupied states below \( E_F \) and unoccupied states above \( E_F \) are possible.

Now we give a brief analysis on the possible optical transitions from the view point of the energy spectrum. As shown in figure 3, due to the presence of edge states within the band gap of the RPQD, it is expected that optical transitions are possible between the bulk and bulk states, between the edge and bulk states, and between the edge and edge states.

In figure 4, we show the optical absorption spectrum of the same RPQD as in figure 2 in the absence of electric and magnetic fields for different light polarizations as indicated. Here, the green solid line represents the band gap energy of the RPQD, and the characters \( bb \) and \( eb \) denote the bulk-to-bulk and edge-to-bulk transitions, respectively.

As mentioned above, there are possibly three types of optical transitions in the RPQD. In the following, we will examine these possible optical transitions under electric and/or magnetic fields. To proceed, we define an averaged optical absorption \( A_{ave}(\hbar \omega) = [A_{ac}(\hbar \omega) + A_{zz}(\hbar \omega)]/2 \) with \( A_{ac}(\hbar \omega) \) and \( A_{zz}(\hbar \omega) \) being the optical absorptions induced by light polarized along the armchair and zigzag directions, respectively.

In figure 5, we show the contour plots of \( A_{ave}(\hbar \omega) \) of the same RPQD as in figure 2 in the presence of (a) perpendicular magnetic field and (b) in-plane electric field (applied along the \( x \) direction). Here, the optical absorption intensity is normalized with respect to its maximum value. The green solid line in each panel represents the optical gap which is defined as the photon energy that is equal to the global energy gap of the system. This global gap changes with electric and magnetic fields significantly (see figure 3), and it becomes the band gap of the RPQD at zero electric and magnetic fields, as shown in figure 4. As can be seen, the absorption lines exist with the magnetic and electric fields in different ways. For example, they vary linearly with electric field but nonlinearly with magnetic field. Such a difference is mainly caused by the different responses of bulk and edge states to the electric and magnetic fields, as manifested in the corresponding energy spectra shown in figure 3. We observe two (three) types of optical transitions under magnetic (electric) fields: the first comes from the bulk-to-bulk transitions above the optical gap (labeled by \( bb \) in the figure); the second from the edge-to-bulk transitions below the optical gap (labeled by \( eb \)
in the figure); and the third from the edge states themselves (the edge-to-edge transitions labeled by ee in the figure) which is far below the optical gap. This peculiar optical absorption is due to the presence of edge states within the band gap of the RPQD (see the energy spectra shown in figure 3). The strong absorption lines above the optical gap are mainly induced by the bulk-to-bulk transitions for light polarization along the armchair direction, while the weak absorption lines below the optical gap are mainly induced by the edge-to-bulk transitions for the same light polarization. This is because the bulk and edge states are spatially separated: the former are mainly located around the center of the RPQD while the latter are mainly localized at the boundaries of the RPQD. When the electric field strength exceeds a critical value \( F_c \approx 0.001 \, \text{V nm}^{-1} \), addition absorption lines emerge far below the optical gap (at photon energies around 0.1 eV), which are mainly induced by the edge-to-edge transitions for light polarization along the zigzag direction. This is because the electric field splits the single edge band into the two bands, in which some energy levels are above the Fermi energy while others are below the Fermi energy (see figure 3(b)). Moreover, the absorption intensity induced by the edge-to-edge transitions increases with increasing electric field because more transition channels can be opened as the electric field increases (see figure 3(b)). The distinct optical-absorption features induced by the bulk-to-bulk and edge-to-bulk transitions can be used to determine the band gap of the RPQD.

We also examine how the electric and magnetic fields interplay and influence the optical absorption of the RPQD. In figure 6, we show the contour plot of \( A_{\text{opt}}(h\omega) \) of the same RPQD as in figure 2 in the presence of both perpendicular magnetic field and in-plane electric field (applied along the \( x \) direction). Here, we sweep the magnetic field strength and fix the electric field strength \( F = 0.03 \, \text{V nm}^{-1} \) which is chosen above the critical value \( F_c \approx 0.001 \, \text{V nm}^{-1} \) in order to make the edge-to-edge transitions observable. The green solid line represents the optical gap of the RPQD. The white and black colors stand for the lowest and highest absorption intensities, respectively.

Figure 5. Contour plots of the normalized optical absorption spectra of the same RPQD as in figure 2 in the presence of (a) perpendicular magnetic field and (b) in-plane electric field (applied along the \( x \) direction). Here, the green solid line represents the optical gap of the RPQD, the characters bb, eb, and ee denote the bulk-to-bulk, edge-to-bulk, and edge-to-edge transitions, respectively, \( F_c \approx 0.001 \, \text{V nm}^{-1} \) is a critical electric field, and for an electric field of \( F > F_c \), the edge-to-edge transitions are activated. The white and black colors stand for the lowest and highest absorption intensities, respectively.

Figure 6. Contour plot of the normalized optical absorption spectrum of the same RPQD as in figure 2 in the presence of both perpendicular magnetic field and in-plane electric field (applied along the \( x \) direction). Here, we sweep the magnetic field strength and fix the electric field strength \( F = 0.03 \, \text{V nm}^{-1} \) which is chosen above the critical value \( F_c \approx 0.001 \, \text{V nm}^{-1} \) in order to make the edge-to-edge transitions observable. The green solid line represents the optical gap of the RPQD. The white and black colors stand for the lowest and highest absorption intensities, respectively.
optical absorption intensity is normalized with respect to its maximum value. As can be seen, unlike that induced by the edge-to-bulk and bulk-to-bulk transitions, the optical absorption induced by the edge-to-edge transitions is almost unaffected by the magnetic field due to the strong localized nature of the edge states. It should be noted that free-carrier absorption in semiconductor systems also occurs at lower photon energies, which is similar to the edge-to-edge absorption considered here. However, free-carrier absorption normally occurs in doped systems, and more importantly it changes significantly with the magnetic field due to the intra-Landau-level transitions. The robust optical absorption induced by the edge-to-edge transitions can be utilized to identify the edge states in the RPQD.

As mentioned previously, the polarization sensitive absorption can be induced by the edge-to-bulk and bulk-to-bulk transitions in the RPQD at zero electric field (see figure 4). In that case, the optical absorption induced by the edge-to-bulk and bulk-to-bulk transitions is much larger for light polarization along the armchair direction than for light polarization along the zigzag direction. However, we find that at nonzero electric field there is additional polarization sensitive absorption induced by the edge-to-edge transitions. But in this case, the optical absorption induced by the edge-to-edge transitions is much smaller for light polarization along the armchair direction than for light polarization along the zigzag edge. We show these results in figure 7 at finite electric field ($F = 0.03$ V nm$^{-1}$). As can be seen clearly, in addition to the edge-to-bulk and bulk-to-bulk absorptions (labeled by $eb$ and $bb$ in the figure), the edge-to-edge absorption (labeled by $ee$ in the figure) is also polarization sensitive but it is almost zero for light polarization along the armchair direction. Again, this absorption feature can be understood by looking to the squared dipole matrix element $\langle f | y \times i \rangle^2$ or $\langle f | y \times i \rangle^2$ for light polarization along the armchair (zigzag) direction, where $|i\rangle$ and $|f\rangle$ are the initial and final edge states, respectively. Our numerical results indicate that at nonzero electric field $\langle f | y \times i \rangle^2$ is much larger than $\langle f | x \times i \rangle^2$ (almost vanishing) for the edge-to-edge transitions.

5. Concluding remarks

We have investigated the electronic and optical properties of RPQDs with armchair and zigzag edges under in-plane electric field and perpendicular magnetic field. The energy spectra and wave functions of RPQDs are obtained by solving the tight-binding model numerically. The corresponding optical absorption spectra of RPQDs are then calculated using the energy spectra and wave functions. In our calculation, we ignore the excitonic Coulomb interaction. Our results show that edge states are formed within the band gap of the RPQD which are mainly localized at the zigzag boundaries and are well separated from the bulk states above and below the band gap. The edge and bulk states have different responses to the electric and magnetic fields, leading to distinct electric- and magnetic-field dependencies of their energy spectra, i.e., the bulk states are more affected by magnetic field while the edge states are more influenced by electric field.

When applying normal incident light, we find that the PRQD can absorb (transmit) light polarized along the armchair (zigzag) direction and a large linear dichroism is observed. In an undoped RPQD and for in-plane polarized light, due to the presence of well-defined edge states, three types of optical transitions are observed under electric and magnetic fields: the first comes from the bulk-to-bulk transitions; the second from the edge-to-bulk transitions; and the third from the edge-to-edge transitions. The electric and magnetic fields influence these three types of optical transitions differently due to the different responses of bulk and edge states to these fields. Particularly, we find that the electric field can activate the edge-to-edge transitions while the magnetic field can not. The absorption intensity induced by such transitions increases with increasing electric field, while it is almost unaffected by the magnetic field. An important result obtained in the present work is that the optical absorption spectra of RPQDs under electric and magnetic fields can be utilized to determine their band gaps and to identify their edge states.

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