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Original Article

Effect of Electron – Phonon Interaction on the Magneto-optical Absorption in Monolayer Phosphorene

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Abstract: In this work, we investigate the magneto-optical absorption in a phosphorene monolayer subjected to a perpendicular static magnetic field. The magneto-optical absorption power is calculated using the projection operator technique taking account of the effect of electron – optical phonon interaction. Numerical results showed that in the case of absence of any interaction, the higher the resonant frequency, the smaller absorbed power was. If the electron - phonon interaction exists, there appear the cyclotron-phonon resonant peaks which show the electron transitions between Landau levels by absorbing a photon accompanied by absorbing/emitting an optical phonon. The obtained results are important for further studies and applications of the phosphorene based structures in optoelectronic devices.

Keywords: Phosphorene; magneto-optical transport; absorption power; electron - phonon interaction; projection operator.

1. Introduction

After the discovery of graphene [1], the family of two-dimensional materials has grown tremendously. Phosphorene with its strongly anisotropic properties makes it an attractive material for applications in deciding the specific direction for different purposes. Black phosphorus is the most stable one among different allotropes of phosphorene. It possesses a nonplanar/puckered honeycomb lattice unlike planar graphene, transition-metal dichalcogenides and hexagonal boron nitride [2]. In addition, black phosphorus shows a highly tunable anisotropic dispersion of fermions with a direct band gap of

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about 1.5–2 eV located at the Γ point of the first Brillouin zone [2–4]. The direct band gap in black phosphorus can be tuned by doping or changing the number of layers [5-7]. Also, researchers have reported a high on-off current ratio and high mobility for charge carriers in field-effect transistors based on black phosphorus [8-10]. All these together lead to tremendous research activities on the electronic and optical properties of black phosphorus [11-13].

Recently, in several theoretical works on phosphorene, the performance under the impurity-electron scattering and metal oxide semiconductor field effect transistors under electron-phonon scattering have been researched [14, 15]. In this work, we focused on the effect of electron-phonon scattering on the magneto-optical properties in monolayer phosphorene subjected to a perpendicular static magnetic field and an electromagnetic wave (optical field). The expression of the magneto-optical absorption power is explicitly calculated using the projection operator technique. The analytical results are numerically calculated with specific parameters to show the dependence of the absorption power on the photon energy with different values of the magnetic field and temperature. This paper has the following structure: After Introduction Section, in Section 2, we introduce the expression of electromagnetic wave absorption power in monolayer phosphorene when placed in a perpendicular magnetic field. The numerical results and discussion are presented in Section 4. Finally, important conclusions are listed in Section 4.

2. Analytic Expression for the Absorption Power in Monolayer Phosphorene

We consider a two-dimensional phosphorene monolayer in which charged carriers move freely in its plane (assumed the $(x-y)$ plane). If a static magnetic field $\vec{B}=(0,0,B)$ is present, the Hamiltonian of the fermions in the system is given by [16]

$$H=\begin{pmatrix} E^e+(\alpha'\Pi_x^2+\beta\Pi_y^2)/2 & 0 \\ 0 & E^h-(\lambda'\Pi_x^2+\eta\Pi_y^2)/2 \end{pmatrix} \quad (1)$$

where $E^e=0.34$ eV ($E^h=-1.18$ eV) is the minimum (maximum) value of conduction (valence) band, $\alpha'=\alpha+\gamma^2/E_g$; $\lambda'=\lambda+\gamma^2/E_g$; $\gamma=8.5*10^5 m/s$; $\alpha=1/m_{ex}=1/1.47m_e$; $\beta=1/m_{ey}=1/0.83m_e$; $\lambda=1/m_{hx}=1/10,66m_e$; $\eta=1/m_{hx}=1/1.12m_e$; $E_g=E^e-E^h=1.52eV$. $\vec{\Pi}=\vec{p}+e\vec{A}$ is the 2D canonical momentum with $\vec{A}$ being the vector potential. The eigenfunctions and eigenvalues corresponding to the Hamiltonian (1) in the gauge $\vec{A}=(0,Bx,0)$, respectively, are

$$\psi_{n,k_y}(\vec{r})\equiv|\alpha\rangle=\frac{e^{ik_y.y}}{\sqrt{L_y}}\begin{pmatrix}\phi_n(u_c^+)\\ \phi_n(u_c^-)\end{pmatrix}, \quad (2)$$

$$E_n^s\equiv E_\alpha=E^s+s(n+1/2)\hbar\omega_c^s,\ \ n=0,1,2,3,... \quad (3)$$

Here, $s=+1(-1)$ for electron (hole), $E^s=E^{e/h}$, $\omega_c^s=\omega_c^{e/h}$, where $eB/\sqrt{m_{ex}m_{ey}}=2.696w_c$, $w_c^h=eB/\sqrt{m_{hx}m_{hy}}=2.2076w_c$, $m'_{ex}=1/\alpha'$, $m'_{hx}=1/\lambda'$ and $w_c=eB/m_e$, $u_c^s=(x-x_0)/a_c^s$, $\alpha_c^s=\sqrt{m'_{sx}\omega_c^s/\hbar}$, and $f_n(u)$ is a harmonic oscillation function, centered at $x_0=l_c^2k_x$, with $l_c=\sqrt{\hbar c/eB}$.

Assuming that the system is further stimulated by a time-varying electric field $\vec{E}(t) = \sum_{k=1}^{s} E_0 e^{i\omega t}\vec{e}_k$ with the frequency w and $\vec{e}_k$ being unit vector of external field direction ($k = x, y, z,\ldots$) then the absorption power is proportional to the absorption coefficient and can be given by an expression of the form as reported in [17]:

$$P(w) = \frac{E_0^2}{2}\mathrm{Re}\left[\sigma_{\pm}(w)\right], \tag{4}$$

where the symbol "Re" means "the real part of" and the optical conductivity tensor $\sigma_{\pm}(w)$ is given as [18]:

$$\mathrm{Re}\left[\sigma_{\pm}(\omega)\right] = \frac{1}{\omega}\sum_{\alpha}\frac{\left|j_{\alpha}^{+}\right|^2 (f_{\alpha} - f_{\beta})B_{\alpha}(\omega)}{\left[\hbar\bar{\omega} - (E_{\beta} - E_{\alpha})\right]^2 + B_{\alpha}^2(\omega)}, \tag{5}$$

where the current operator j_{α}^{+} defined as $j_a^{+} = j_x + ij_y$ and $f_a = f(E_n^s) = 1/(1 + e^{b(E_n^s - E_F)})$ is the Fermi-Dirac distribution function for fermions with E_{F} being the Fermi energy level; $\bar{\omega} = \omega - i\Delta, \Delta \to 0^+$. The line-shape function $B_a(w)$ is determined by the scattering mechanism. In the case of electron - phonon interaction, it has a form as follows:

$$\begin{aligned} B_a(w) = \frac{p}{f_a - f_{a+1}}\Bigg[\sum_{q}\sum_{b\neq a+1} g_{qn}\left|J_{a+1,b}(q)\right|^2\left[W_L^{(+)}(a,b) - W_R^{(-)}(b,a) + W_L^{(-)}(a,b) - W_R^{(+)}(b,a)\right] \\ + \sum_{q}\sum_{b\neq a} g_{qn}\left|J_{a,b}(q)\right|^2\left[W_L^{(+)}(b,a+1) - W_R^{(-)}(a+1,b) + W_L^{(-)}(b,a+1) - W_R^{(+)}(a+1,b)\right]\Bigg] \end{aligned} \tag{6}$$

where

$$W_L^{(\pm)}(\alpha,\beta) = \left(N_{qv} + \frac{1}{2} \pm \frac{1}{2}\right) f_{\alpha}(1 - f_{\beta})\delta(\hbar\omega + E_{\alpha} - E_{\beta} \mp \hbar\omega_q)\delta_{k_x, k_x' \pm q_y} g(\theta) g_v g_s, \tag{7}$$

$$W_R^{(\pm)}(\alpha,\beta) = \left(N_{qv} + \frac{1}{2} \pm \frac{1}{2}\right) f_{\alpha}(1 - f_{\beta})\delta(-\hbar\omega + E_{\alpha} - E_{\beta} \mp \hbar\omega_q)\delta_{k_x, k_x' \pm q_y} g(\theta) g_v g_s. \tag{8}$$

Here, N_{qn} is the distribution function of phonons in the state $|q,n\rangle$ with energy $\hbar\omega_q$, $g_n = 2$ and $g_s = 2$ are, respectively, the valley and spin degeneracy, and $g(q) = \cos^2(q/2)$ is the overlap integral of spinor wave functions. The term g_{qn} denotes the square of the electron-phonon interacting matrix element. For the optical phonon scattering, within the deformation potential approximation, it is expressed as [19]:

$$g_{qv} \equiv g_{q(\mathrm{op})} = \Theta_{\mathrm{op}}^2 \hbar / 2\rho V\omega_q, \tag{9}$$

where Θ_{op} is the optical deformation potential constant, ρ is the mass density of the material, and V is the normalization volume. In Eqs. (7) – (14), $\left|J_{a,b}(q)\right|^2$ is called the form factor that is given as

$$\left|J_{ab}(q)\right|^2 = 4e^{-u}u^j \frac{m!}{(m+j)!}\left[L_m^j(u)\right]^2 \delta_{k_y, k_y \pm q_y} \tag{10}$$

where $L_m^j(u)$ is the associated Laguerre polynomial in the case of $u = u_c^e = u_c^s$, $u = q_x^2 l_c^2 / 2$, $m = min(n, n')$, $j = |n' - n|$.

To obtain the explicit expression of $P(\omega)$, one needs to calculate the terms of $B_a(w)$ given in Eq.(6). To do this, we transform the summations over q and α to integrals as $S/(2\pi l_c)^2 \int du \int dq$; and $\sum_{n,s} (L_y/2\pi) \int dk_y = S/(2\pi l_c^2) \sum_{n,s}$, then use the orthogonality of the Laguerre polynomials. We also assume that optical phonons are dispersionless so that we can take the approximation $\hbar\omega_q \approx \hbar\omega_0 =$ constant (subsequently, $N_{qv} = N_0$ = constant) in the following calculations. For instance, the explicit expression of the first term in Eq. (6) after a straightforward calculation, is obtained as:

$$T = \sum_q \sum_{\beta \neq \alpha+1} g_{qv} \left| J_{\alpha+1,\beta}(u) \right|^2 \mathrm{W}_L^{(+)}(\alpha, \beta)$$

$$= \frac{\Theta_{op}^2 S^2 \hbar g_s g_v}{16 V \rho \omega_q \pi^2 l_c^4} \sum_{\substack{n' \neq n+1 \\ s'}} I_{ns}^{n's'} \left(N_0 + 1 \right) f_{ns} (1 - f_{n's'}) \delta(X_{\alpha,\beta}^{(+)}), \quad (11)$$

where

$$I_{ns}^{n's'} = \int \left| J_{a+1,b}(u) \right|^2 du = 4; \; X_{\alpha,\beta}^{(+)} = \hbar\omega + E_\alpha - E_\beta - \hbar\omega_0 \quad (12)$$

To treatment the delta function, following the collision broadening model for the electron-phonon scattering, we can replace the delta function by Lorentz function [20]

$$\delta(X_{\alpha,\beta}^{(\pm)}) = \frac{1}{\pi} \frac{\hbar\gamma_{\alpha,\beta}^{(\pm)}}{(X_{\alpha,\beta}^{(\pm)})^2 + \hbar^2 (\gamma_{\alpha,\beta}^{(\pm)})^2}, \text{ with } (\gamma_{\alpha\beta}^{(\pm)})^2 = \frac{1}{\hbar^2} \sum_q \left[N_0 \pm \frac{1}{2} + \frac{1}{2} \right] g_{qv} \left| J_{\alpha,\beta}(u) \right|^2$$

The rest terms in Eq. (6) can be calculated similarly to obtain the full $B_a(w)$ as well as $P(w)$.

3. Numerical results and discussion

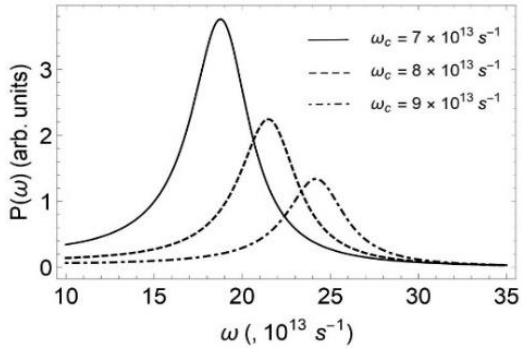

Figure 1. Absorption power (in arbitrary units) as a function of electromagnetic wave frequency at different values of cyclotron frequency. Here, T=200K.

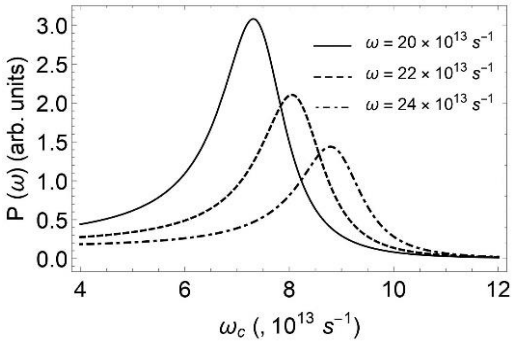

Figure 2. Absorption power (in arbitrary units) as a function of cyclotron frequency at different values of the electromagnetic wave frequency. Here, T= 200K.

In to see clearly the characteristics order of the absorption spectrum, we numerically evaluate the expression of absorption power utilizing specific parameters. The parameters used in the computation are taken from Refs. [2, 5].

We first consider the case of absence of the electron -- phonon interaction, i.e. there are only state transitions of electrons due to excitation by electromagnetic wave photons. Figure 1 shows the dependence of the magneto-optical absorption power on the electromagnetic wave frequency at different values of the cyclotron frequency. It is seen that each absorption curve has a maximum peak for every value of the cyclotron frequency. One can see that these maxima are at $\omega = 18.872 \times 10^{13} s^{-1}$; $\omega = 21.568 \times 10^{13} s^{-1}$; and $w = 24.264 \times 10^{13} s^{-1}$; respectively, for $\omega_c = 7 \times 10^{13} s^{-1}$; $\omega_c = 8 \times 10^{13} s^{-1}$ and $w_c = 9 \times 10^{13} s^{-1}$. It turns out that these maxima are cyclotron resonance peaks which arise from the condition $w_c^e = w$ recall that $w_c^e = 2.696 w_c$ where an electron transits between two Landau energy levels by absorbing a photon of energy $\hbar\omega$. The cyclotron resonance has also been observed in monolayer 2D materials exposed to a perpendicular magnetic field and electromagnetic wave such as graphene [21], silicene [22], and MoS_2 [23]. To confirm this behaviour, in Figure 2 we plot the dependence of the absorption power on the cyclotron frequency at different values of the electromagnetic wave frequency. The dependence of the absorption power on the cyclotron frequency has the same behaviour as shown in Figure 1. In particular, as the cyclotron frequency increases, the absorption peak lowers, namely the absorption power decreases. This can be physically explained that as the cyclotron frequency increases (i.e. the magnetic field gets stronger) the radius of the cyclotron orbits decreases, leading to stronger confinement of electrons by the magnetic field, reducing the probability of electromagnetic wave absorbing due to the increase of selectivity.

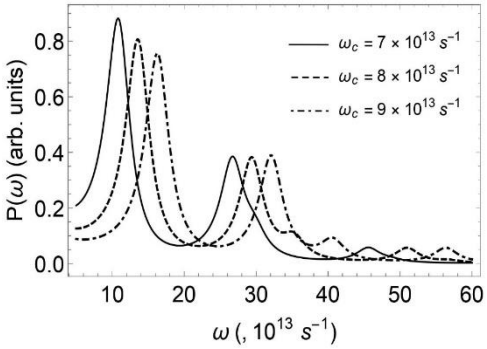

Figure 3. Absorption power (in arbitrary units) as a function of electromagnetic wave frequency at different values of cyclotron frequency. Here, T=200K.

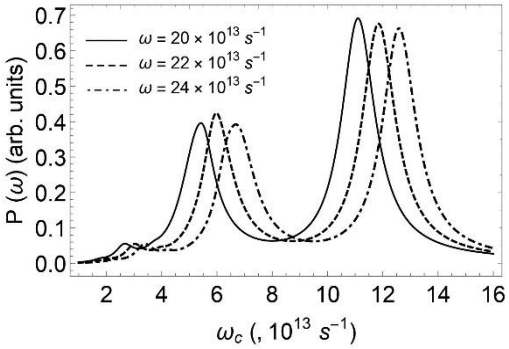

Figure 4. Absorption power (in arbitrary units) as a function of cyclotron frequency at different values of the electromagnetic wave frequency. Here, T=200K.

We now consider the effect of electron-phonon interaction on the absorption spectrum. Like Fig. 1, Fig. 3 depicts the dependence of the absorption power on the electromagnetic wave frequency at different values of the cyclotron frequency. There appear more absorption maxima in this case. By positioning the peaks in the figure, one can conclude that they are cyclotron-phonon resonance peaks. For instance, for the case of $w_c = 7 \times 10^{13} s^{-1}$ (the solid curve in Fig. 3), the peaks from left to right, respectively, locate at $w = 10.11 \times 10^{13} s^{-1}$; $26.75 \times 10^{13} s^{-1}$; $29.87 \times 10^{13} s^{-1}$; $45.62 \times 10^{13} s^{-1}$ corresponding to the conditions

$$\omega = (1-0)\omega_c^e - \omega_0, \tag{13}$$

$$\omega = (1-0)\omega_c^e + \omega_0, \tag{14}$$

$$\omega = (2-0)\omega_c^e - \omega_0, \tag{15}$$

$$\omega = (2-0)\omega_c^e + \omega_0. \tag{16}$$

The condition (13)/(14) implies that an electron moves from the Landau level $n = 0$ to the level $n = 1$ by absorbing a photon accompanied by the emission/absorption of an optical phonon. The conditions (15) and (16) can be explained similarly but for the electron transition from $n = 0$ to $n = 2$. We can conclude that under certain conditions, the presence of electron-phonon interaction results in the appearance of more resonance peaks in the absorption spectrum. This is because, with the assistance of phonon absorption or emission there are more values of photon energy/frequency satisfying the selection rules $\omega = (n' - n)\omega_c^e \pm \omega_0$ that an electron can be absorbed during its transition between two specific Landau levels.

4. Conclusion

So far, we have calculated the absorption power of an electromagnetic wave in a phosphorene monolayer subjected to a perpendicular magnetic field using the projection operator technique. The effect of electron - optical phonon interaction has been taken into account. In the case of absence of any interaction, the cyclotron resonance is observed and the stronger the magnetic field, the smaller the absorption power. If the electron - phonon interaction is present, there appear the cyclotron-phonon resonant peaks showing the electron transitions between Landau levels due to absorbing photon and absorbing/emitting an optical phonon under the conditions $\omega = (n' - n)\omega_c^e \pm \omega_0$. In general, for a specific couple of the Landau levels the photon frequency at the resonant peaks is larger than that at the corresponding ones in graphene, silicene and monolayer MoS_2. This is because the electron cyclotron frequency in monolayer phosphorene in this work is larger than it is in those references.

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References

[1] K. S. Novoselov et al., Electric Field Effect in Atomically Thin Carbon Films, Science, Vol. 306, 2004, pp. 666-669, https://doi.org/10.1126/science.1102896.

[2] J. Ribeiro-Soares, R. M. Almeida, L. G. Cançado, M. S. Dresselhaus, A. Jorio, Group Theory for Structural Analysis and Lattice Vibrations in Phosphorene Systems, Physical Review B, Vol. 91, 2015, pp. 205421-205431, https://doi.org/10.1103/PhysR evB.91.205421.

[3] A.S. Rodin, A. Carvalho, A. H. C. Neto, Strain-Induced Gap Modification in Black Phosphorus, Physical Review Letters, Vol. 112, 2014, pp. 176801-176805, https://doi.org/10.1103/PhysR evLet t.112.176801.

[4] H. Asahina, A. Morita, Band Structure and Optical Properties of Black Phosphorus, Journal of Physics C: Solid State Physics, Vol. 17, 1984, pp. 1839-1852, https://doi.org/10.1088/0022-3719/17/11/006.

[5] J. Kim et al., Observation of Tunable Band Gap and Anisotropic Dirac Semimetal State in Black Phosphorus, Science, Vol. 349, 2015, pp. 723-726, https://doi.org/10.1126/scien ce.aaa6486.

[6] J. Kim et al., Two-dimensional Dirac Fermions Protected by Space-time Inversion Symmetry in black phosphorus, Physical Review Letters, Vol. 119, 2017, pp. 226801-226805, https://doi.org/10.1103/PhysRevLett.119.226801.

[7] J. Jang, S. Ahn, H. Min, Optical Conductivity of Black Phosphorus with a Tunable Electronic Structure, 2D Materials, Vol. 6, 2019, pp. 025029-025043, https://doi.org/10.1088/2053-1583/ab075b

[8] H. Liu, A. T. Neal, Z. Zhu, Z. Luo, X. Xu, D. Tomanek, P. D. Ye, Phosphorene: An Unexplored 2D semiconductor with a High Hole Mobility, ACS Nano, Vol. 8, 2014, pp. 4033-4041, https://doi.org/10.1021/nn501226z.

[9] J. Qiao, X. Kong, Z. X. Hu, F. Yang, W. Ji, High-mobility Transport Anisotropy and Linear Dichroism in Few-layer Black Phos-phorus, Nature Communications, Vol. 5, 2014, pp. 4475-4482, https://doi.org/10.1038/ncomms5475.

[10] A. C. Gomez et al., Isolation and Characterization of Few-layer Black Phosphorus, 2D Materials, Vol. 1, 2014, pp. 025001-025019, https://doi.org/10.1088/2053-1583/1/2/025001.

[11] N. Gillgren et al., Gate Tunable Quantum Oscillations in Air-stable and High Mobility Few-layer Phosphorene Heterostructures, 2D Materials, Vol. 2, 2014, pp. 011001-011007, https://doi.org/10.1088/2053-1583/2/1/011001.

[12] S. P. Koenig, R. A. Doganov, H. Schmidt, A. H. C. Neto, B. Özyilmaz, Electric Field Effect in Ultrathin Black Phosphorus, Applied Physics Letters, Vol. 104, 2014, pp. 103106-103110, https://doi.org/10.1063/1.4868132.

[13] L. Li et al., Black Phosphorus Field-effect Transistors, Nature Nanotechnology, Vol. 9, 2014, pp. 372-377, https://doi.org/10.1038/nnano .2014.35.

[14] A. Szabo, R. Rhyner, H. C. Nunez, M. Luisier, Phonon-limited Performance of Single-layer, Single-gate Black Phosphorus n-and p-type Field-effect Transistors. IEEE International Electron Devices Meeting (IEDM), Washington, DC, USA, 2015, pp. 12.1.1-12.1.4, https://doi.org/10.1109/iedm.2015.7409680.

[15] M. Luisier et al., First-principles Simulations of 2-D Semiconductor Devices: Mobility, I-V Characteristics, and Contact Resistance, IEEE International Electron Devices Meeting (IEDM), San Francisco, CA, USA, 2016, pp. 541-544, https://doi.org/10.1109/IEDM.2016.7838353.

[16] M. Tahir, P. Vasilopoulos, F. M. Peeters, Magneto-optical Transport Properties of Monolayer Phosphorene, Physical Review B, Vol. 92, 2015, pp. 045420-045427, https://doi.org/10.1103/PhysRevB.92.045420.

[17] A. Kawabata, Theory of Cyclotron Resonance Line Width, Journal of the Physical Society of Japan, Vol. 23, No. 5, 1967, pp. 999-1006, https://doi.org/10.1143/JPSJ.23.999.

[18] S. D. Choi, O. H. Chung, Theory of Cyclotron Resonance Lineshape for Electron-Phonon Systems in Two Coupling Schemes, Solid State Communications, Vol. 46, No. 9, 1983, pp. 717-720, https://doi.org/10.1016/0038-1098(83)90514-8.

[19] M. Brahma, A. Kabiraj, M. Bescond, S. Mahapatra, Phonon Limited Anisotropic Quantum Transport in Phosphorene Field Effect Transistors, Journal of Applied Physics, Vol. 126, 2019, pp. 114502-114510, https://doi.org/10.1063/1.5109057.

[20] M. P. Chaubey, C. M. Van Vliet, Transverse Magnetoconductivity of Quasi-two-dimensional Semiconductor Layers in the Presence of Phonon Scattering, Physical Review B, Vol. 33, 1986, pp. 5617-5622, https://doi.org/10.1103/PhysRevB.33.5617.

[21] B. D. Hoi, L. T. T. Phuong, T. C. Phong, Magneto-optical Absorption and Cyclotron–phonon Resonance in Graphene Monolayer, Journal of Applied Physics, Vol. 123, No. 9, 2018, pp. 094303-094306, https://doi.org/10.1063/1.5020746.

[22] N. V. Q. Binh, N. N. Hieu, C. V. Nguyen, H. V. Phuc, B. D. Hoi, L. T. T. Phuong, T. C. Phong, Nonlinear Optical Absorption and Cyclotron–impurity Resonance in Monolayer Silicene, Physica E, Vol. 105, 2019, pp. 168-173, https://doi.org/10.1016/j.physe.2018.09.014.

[23] N. V. Q. Binh et al., Investigation of Cyclotron-phonon Resonance in Monolayer Molybdenum Disulfide, Journal of Physics and Chemistry of Solids, Vol. 125, 2019, pp. 74-79, https://doi.org/10.1016/j.jpcs.2018.10.007