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Research Article

Theoretical Study on Binding Energy and Optical Properties of GaAs Cubic Quantum Dot under Pressure and Temperature

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Abstract

In this study, the binding energy (E_B) and optical properties, absorption coefficient (AC) and refractive index change (RIC) of a GaAs cubic quantum dot are studied for different pressure and temperature values. Numerical calculations are done by using variational method. The results present that E_B, the linear and nonlinear optical properties are sensitively dependent on the pressure, temperature and quantum dot size. Also, the results indicate that it is possible to modulate the resonant peaks position and magnitude of the AC and RIC with pressure and temperature.

Keywords: Quantum dot, Hydrogenic impurity, Optical properties, Pressure, Temperature

1. INTRODUCTION

Semiconductor quantum nanostructures constitute very attractive objects both for their electronic and optical properties in microelectronics and optoelectronics. Last advancement in growth techniques have allowed to obtain different geometry such as cubical, spherical, cylindrical etc. quantum dots (QDs). These structures exhibit very special properties such as light emitting materials, tunable emission and high photoluminescence quantum yield [1–3] for technological applications. The opto-electronic properties of QDs have been extensively considered in device technology [4–6].

The influence of outside factors, such as electromagnetic field, pressure and temperature on the QDs is one of the attractive subjects both from experimental and theoretical studies. Thus, many studies have been carried out on these factors dependence of opto-electronic properties in different nanostructure such as quantum wire [7,8], spherical QD [9–11], cylindrical QD [12], double quantum wells [13]. It is possible to adjust the transition energy difference between the energy levels of the carriers by applying pressure to quantum nanostructures [14]. Furthermore, Elabsy [15] has presented a study about the effect of temperature on the binding energy of spherical QD. This study shows that temperature changes the electronic structure of the system.

The impurity position causes change the electronic and optical properties in QDs. For example, when the position of the impurity changes from the center to the edge of the QD, the binding energy decreases approximately 35% [16]. It is shown that the energy of an electron in a cubic QD decreases with electric field by Dane et al. [17]. Karabulut et al. calculated optical properties in a cubic QD both with infinite and finite confining potential [18,19]. Moreover, the effects of pressure on the optical properties are investigated for cubic QD by Khordad [20,21].

In the present study, the effects of the temperature and pressure on the E_B and optical properties of cubic QD have been analyzed. In Section 2, theoretical framework is described. Numerical results are presented in Section 3. In last section, a conclusion is given.

2. MATERIAL AND METHODS

We consider an electron and on-center hydrogenic impurity confined in cubic QD under the electric field. Within the effective mass approximation, the Hamiltonian of the structure is given by [22]

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$$H = -\frac{\hbar^2}{2m^*(P,T)}\nabla^2 + |e|Fz + V_c(x,y,z) - \frac{Ze^2}{\varepsilon(P,T)r}. \quad (1)$$

Here, F is the electric field, P is the pressure, $\hbar$ is Planck constant, e is electron charge and T is the temperature. $\varepsilon(P,T)$ and $m^*(P,T)$ are dielectric constant and effective mass, respectively. *Z=1* case indicates the presence of impurity and $r = \sqrt{x^2+y^2+z^2}$. The confining potential $V_c(x,y,z)$ is taken as infinite outside the QD and zero otherwise. $m^*(P,T)$ can be determined [23]

$$m^*(P,T) = m_0\left(1 + E_P^{\Gamma}\left(\frac{2}{E_g^{\Gamma}(P,T)} + \frac{1}{E_g^{\Gamma}(P,T) + \Delta_{SO}}\right)\right)^{-1} \quad (2)$$

where E_P^{Γ} is momentum matrix element, m_0 is the free electron mass, Δ_{SO} is the spin-orbit splitting, $E_g^{\Gamma}(P,T)$ is the energy gap alteration [16,17]

$$E_g^{\Gamma}(P,T) = E_g^{\Gamma}(0) + bP - \frac{\alpha T^2}{T+\beta} \quad (3)$$

where $E_g^{\Gamma}(0)$ is the energy gap at $P = 0$. b, α and β are the characteristic constants for GaAs. $\varepsilon(P,T)$ can be found in literature as [24]

$$\varepsilon(P,T) = \begin{cases} 12.74\, exp(-16.7\times10^{-3}P)\times\, exp(9.4\times10^{-5}(T-75.6)), & T < 200 \\ 13.18\, exp(-17.3\times10^{-3}P)\times\, exp(20.4\times10^{-5}(T-300)), & T \geq 200 \end{cases} \quad (4)$$

The variation of QD size by pressure is given by [25]:

$$L(P) = L_0C(P),\ \ C(P) = [1-(S_{11}+2S_{12})P] \quad (5)$$

where L_0 is the original size of cubic QD. S_{11} and S_{21} are the compliance constants. The values of material parameters as follows: $E_g^{\Gamma}(0)$ =1.519eV [26], Δ_{SO} = 341 meV [27], $E_g^{\Gamma}(P,T)$=7.51 eV [20], $\alpha(\times 10^{-4})$ =5.405 eV/K^2 [28], β=204 K [28], b=107.3 meV/GPa [29], $S_{11}(\times 10^{-2})$=1.16 GPa^{-1} [30], $S_{21}(\times 10^{-2})$=0.37 GPa^{-1} [30].

The eigenvalues, also the binding energy (E_B), are obtained numerically by variational method. The linear $\alpha^{(1)}$, the nonlinear $\alpha^{(3)}(w,I)$ and total AC $\alpha(w,I)$ can be obtained as [31,32]

$$\alpha^{(1)}(w) = w\sqrt{\frac{\mu}{\varepsilon_R}}\frac{|M_{21}|^2\sigma_V\hbar\Gamma_{12}}{(E_{21}-\hbar w)^2+(\hbar\Gamma_{12})^2} \quad (6)$$

and

$$\alpha^{(3)}(w,I) = -w\sqrt{\frac{\mu}{\varepsilon_R}}\left(\frac{I}{2\varepsilon_0 n_r c}\right)\frac{|M_{21}|^2\sigma_V\hbar\Gamma_{12}}{[(E_{21}-\hbar w)^2+(\hbar\Gamma_{12})^2]^2} \times\left[4|M_{21}|^2 - \frac{|M_{22}-M_{11}|^2[3E_{21}^2-4E_{21}\hbar w+\hbar^2(w^2-\Gamma_{12}^2)]}{E_{21}^2+(\hbar\Gamma_{12})^2}\right] \quad (7)$$

The linear $\Delta n^{(1)}$, the nonlinear $\Delta n^{(3)}(w,I)$ and total $\Delta n(w,I)$ RIC can be obtained as [31,32]

$$\frac{\Delta n^{(1)}(w)}{n_r} = \frac{\sigma_V}{2n_r^2\epsilon_0}|M_{21}|^2\frac{(E_{21}-\hbar w)}{(E_{21}-\hbar w)^2+(\hbar\Gamma_{12})^2} \quad (8)$$

and

$$\frac{\Delta n^{(3)}(w,I)}{n_r} = -\frac{Ic}{4n_r^3\epsilon_0}|M_{21}|^2\left[\frac{\sigma_V I}{[(E_{21}-\hbar w)^2+(\hbar\Gamma_{12})^2]^2}\right] \times\left[4(E_{21}-\hbar w)|M_{21}|^2 - \frac{(M_{22}-M_{11})^2}{E_{21}^2+(\hbar\Gamma_{12})^2}\{(E_{21}-\hbar w)[E_{21}(E_{21}-\hbar w)-(\hbar\Gamma_{12})^2\,]-(\hbar\Gamma_{12})^2(2E_{21}-\hbar w)\}\right] \quad (9)$$

Here, μ is the magnetic susceptibility, ε_0 is the vacuum dielectric permittivity, σ_V is the electron density, $\hbar w$ is photon energy, c is the speed of light in free space, n_r is the refractive index of the material, E_{ij} is the energy differences, Γ_{12} is the relaxation rate and I is the intensity of light. M_{ij} is the transition matrix element.

3. RESULTS AND DISCUSSION

The calculations were carried out in atomic units and $a^* = \hbar^2\varepsilon/m^*e^2$ is Bohr radius. In Figure 1, E_B is plotted as functions of the quantum dot size (L) and pressure (P) at $F = 20(|e|/2\varepsilon a^*)^2$ and $T = 100K$. As expected, E_B decreases as quantum dot size increase. Moreover, this figure indicates that the E_B increases with pressure which causes additional confinement. This is because the presence of pressure leads to the enhancement in the effective mass and the reduction in the QD size and dielectric constant.

The variation of $E_B$with temperature and cubic QD size for $F = 20(|e|/2\varepsilon a^*)^2$ and pressure $P = 20kbar$ is shown in Figure 2. One can see that from this figure, E_B of the system decreases with temperature due to the augment in the dielectric constant and the decrease in the effective mass. The obtained results in Figure 1 and Figure 2 are in agreement with the results of Liang et al [32].

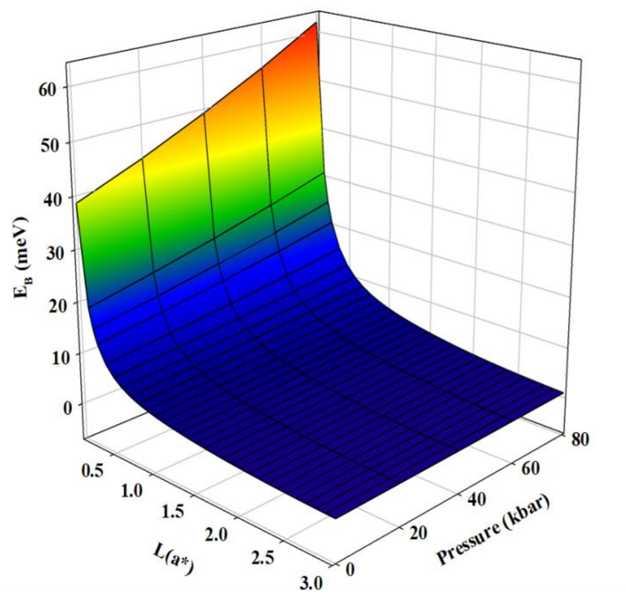

Figure 1. The E_B of cubic QD vs edge length and pressure for T = 100K

To see the influence of the pressure and temperature effects more clearly, we have drawn the graph E_B as functions of P and T for given quantum dot size $L = 1.0a^*$ and electric field strengths $F = 20(|e|/2\varepsilon a^*)^2$ in Figure 3. When comparing the effect of pressure on the E_B with that of temperature, the pressure effect is more apparent than that of the temperature.

In Figure 4, we present the variations of the AC (Figure 4a) and RIC (Figure 4b) versus the photon energy and cubic dot size (L) for $P = 20kbar$, $T = 100K$ and $F = 20(|e|/2\varepsilon a^*)^2$. The energy difference decreases as the cubic dot size increases. Thus, the AC and RIC can move toward smaller energies (red shift). We can explain this evolution by the fact that the energy splitting decreases with increasing cubic dot size. Also, we clearly observe that the AC and RIC of smaller cubic dot radius are stronger than that of the larger cubic dot size due to the absorption spectrum depends on the QD volume.

Figure 5 indicates the AC and RIC as functions of the photon energy and pressure with $T = 100K$, $F = 20(|e|/2\varepsilon a^*)^2$and $L = 0.25a^*$. As can be seen from the figure, the magnitudes of the AC and RIC resonant peaks increase and shift to the higher energy region with increasing the hydrostatic pressure. This can be explained that the increment in pressure causes extra spatial confinement, namely less volume, the difference between energy levels increases by Coulomb interaction energy.

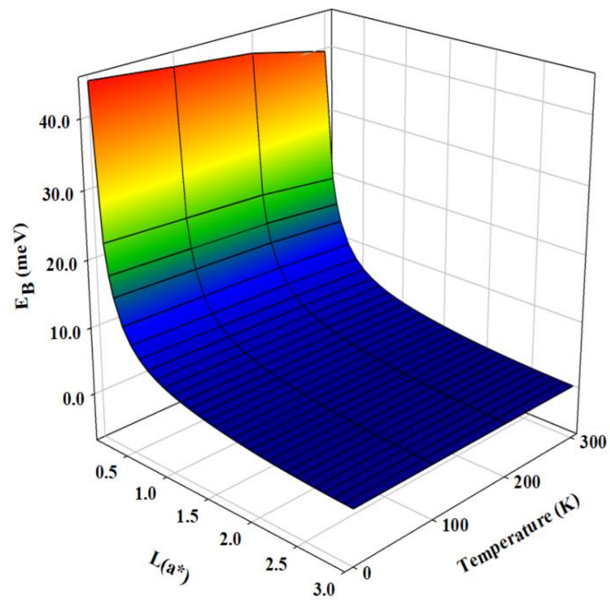

Figure 2. The E_B of cubic QD vs edge length and temperature for $\mathrm{P} = 20\mathrm{kbar}$

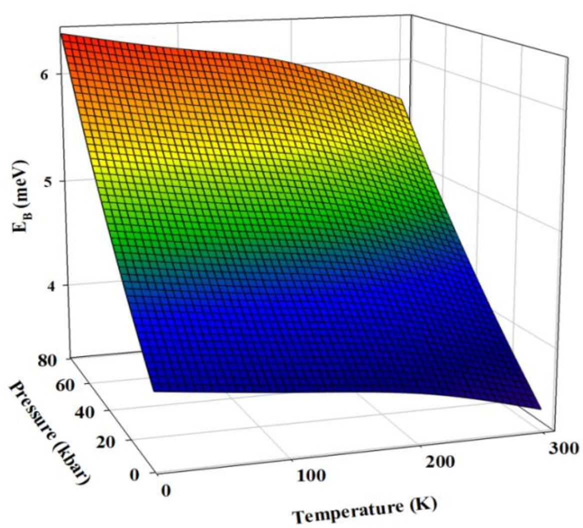

Figure 3. The $\mathrm{E_B}$ of cubic QD vs temperature and pressure for $\mathrm{L} = 1.0\mathrm{a}^*$

In Figure 6, the behavior of AC and RIC as functions of the photon energy and temperature is plotted for $P = 20kbar$, $F = 20(|e|/2\varepsilon a^*)^2$ and $L = 0.2a^*$. This figure displays that the magnitudes of the AC and RIC peaks increase with increasing temperature. Moreover, in contrast of pressure, the peaks of ACs and RIC move to the lower photon energies. This is due to the reduction of the energy splitting when the temperature increases. When the literature is examined, it can be seen that the behavior of the ACs with is in agreement with Ref. [33], and the pressure-dependent change of ACs is in agreement with Ref. [34].

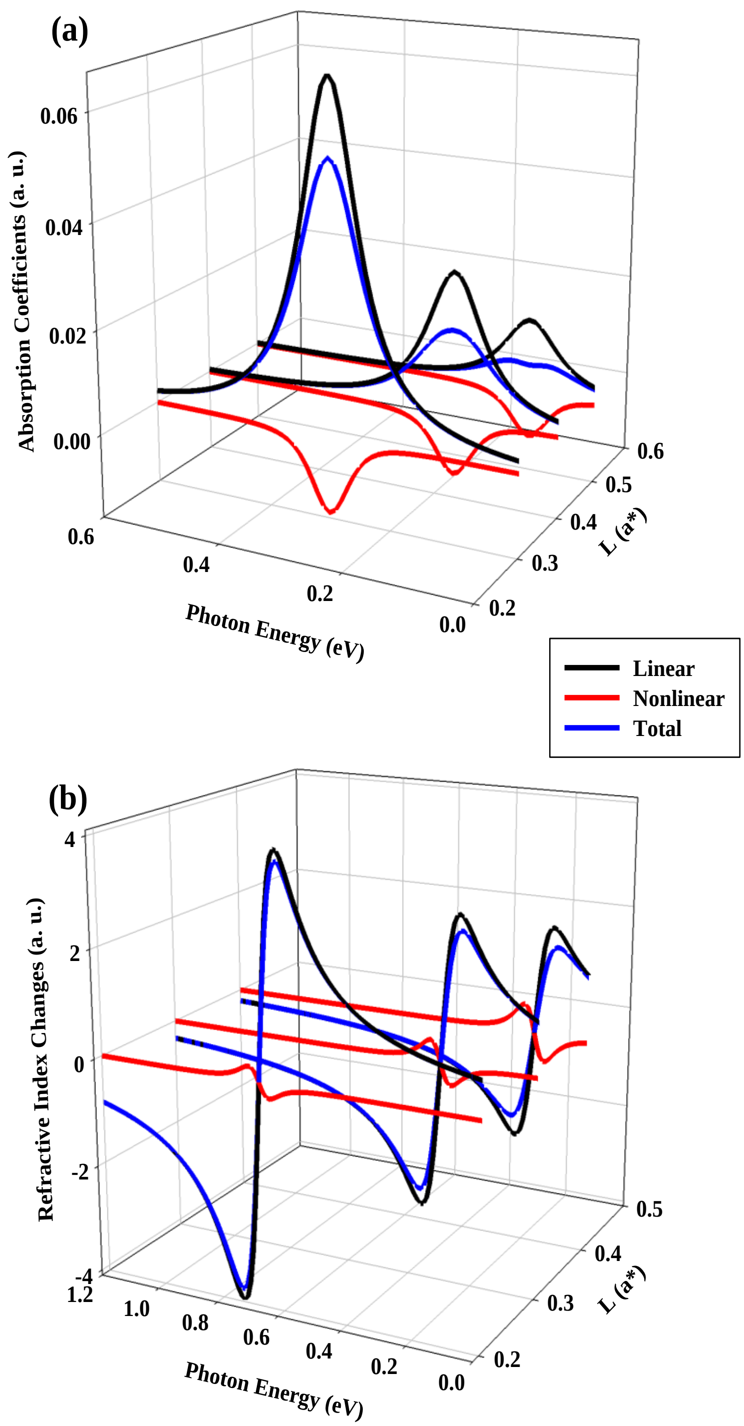

Figure 4. **(a)** The ACs of cubic QD vs photon energy and edge length for $P = 20kbar$ and $T = 100K$ **(b)** The RICs of cubic quantum dot vs photon energy and edge length for $P = 20kbar$ and $T = 100K$

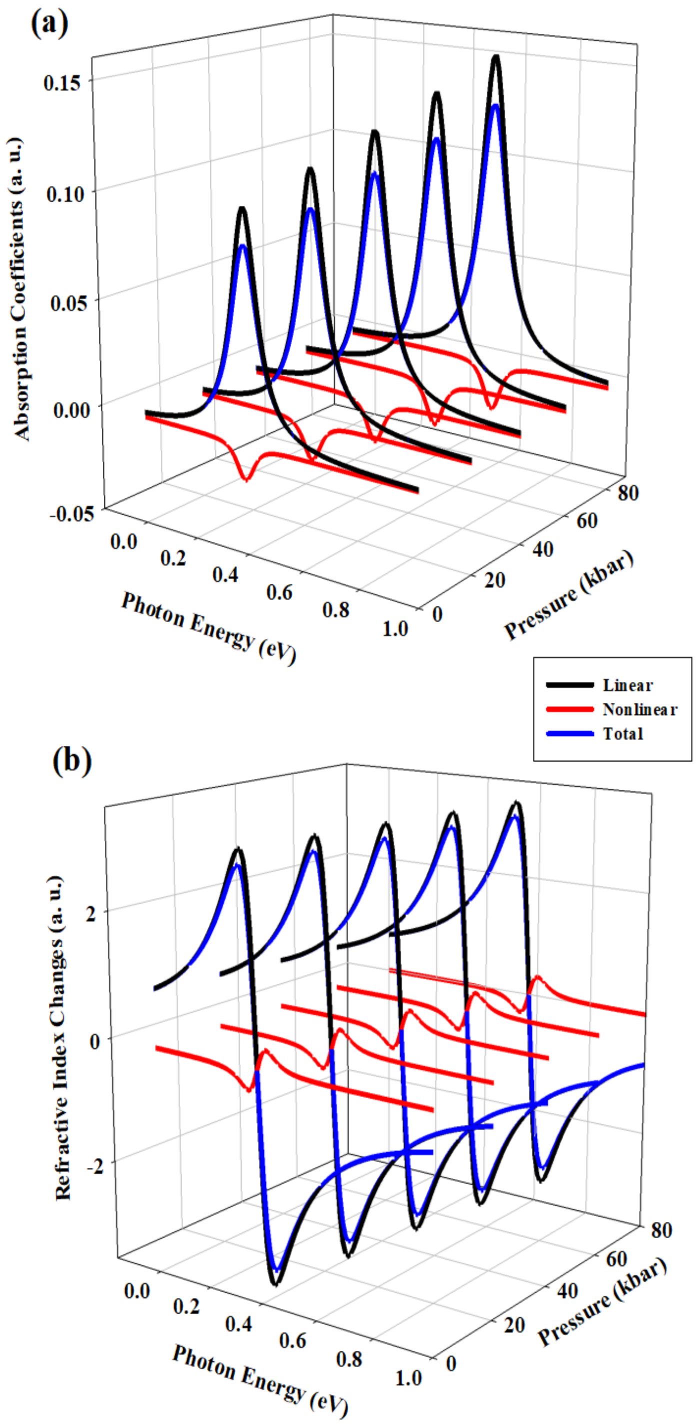

Figure 5. **(a)** The ACs of cubic QD vs photon energy and pressure for $T = 100K$ and $L = 0.25a^*$ **(b)** The RICs of cubic quantum dot vs photon energy and pressure for $T = 100K$ and $L = 0.25a^*$

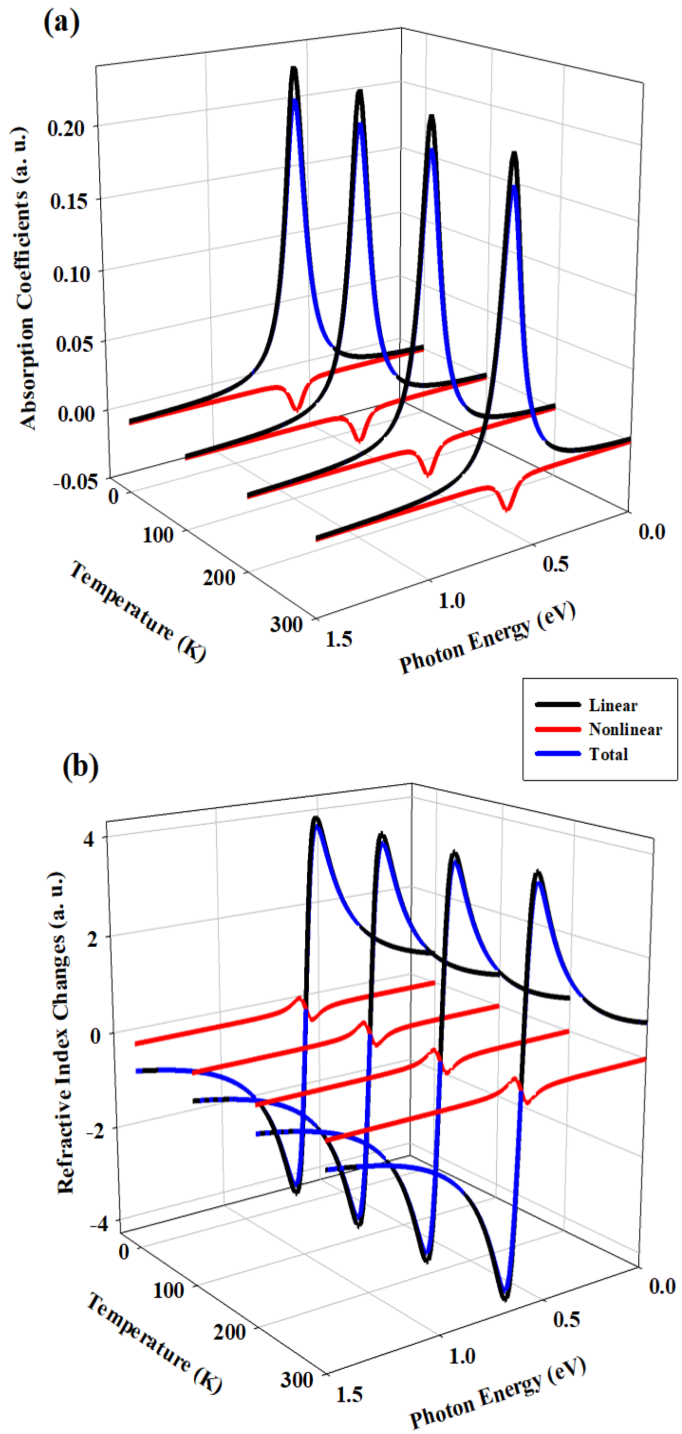

Figure 6. **(a)** The ACs of cubic QD vs photon energy and temperature for $P = 20kbar$ and $L = 0.2a^{*}$ **(b)** The RICs of cubic quantum dots vs photon energy and temperature for $P = 20kbar$ and $L = 0.2a^{*}$

4. CONCLUSIONS

In the present study, we have performed the variational technique to study the influences of the temperature and hydrostatic pressure on the E_B and optical properties for cubic QD under electric field. The considered QD size and outside factors have a remarkable impact on the E_B energy and the optical properties of the system. We found that the donor E_B decreases (increases) as temperature (pressure) increases. Moreover, our computed results show that the effect of pressure on E_B is more apparent than that of the temperature. The increasing of cubic QD size leads to a reduction of the AC and RIC and they exhibit red shift. Also, the results show that optical absorption exhibits blue shift with increasing (decreasing) pressure (temperature). We believe that this study will stimulate researchers to carry out experimental studies of the electronic and optical properties of quantum nanostructures.

AUTHOR'S CONTRIBUTIONS

The authors contributed equally.

CONFLICTS OF INTEREST

Authors have declared no conflict of interest.

RESEARCH AND PUBLICATION ETHICS

The author declares that this study complies with Research and Publication Ethics.

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