Non-linear optical properties of a donor hydrogenic impurity in a group II-VI nano-dot

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ARTICLE INFO
Article history:
Received: 1 August 2012;
Received in revised form: 31 August 2012;
Accepted: 20 September 2012;

Keywords
Binding energy; Exciton;
Optical properties; Quantum dot.

ABSTRACT
Binding energy of a donor hydrogenic impurity is computed in a Cd based II-VI semiconducting material taking into account both the effects of phonon and geometrical confinement effects. The former effect is considered with the inclusion of Fröhlich interaction Hamiltonian whereas the latter effect is considered by varying the dot radius. Moreover, lowest binding energy and the donor binding energy are obtained using internal built-in electric fields. All the computations are carried out using Bessel function as an orthonormal basis for different confinement potentials of barrier height considering the spontaneous and piezoelectric polarizations. Since the optical properties of hydrogenic impurity in a quantum dot are strongly affected by the confining potential and the quantum size effect on the changes of refractive index is brought out. It is also observed that the magnitude of the refractive index changes enhances with the inclusion of phonon and geometrical effects.

Introduction
Optical properties are given due interest in low dimensional semiconductor systems such as quantum wells, quantum well wires and quantum dots because they have potential applications in device fabrications [1]. The absorption coefficients and changes of refractive index are some nonlinear optical properties which are given attention in quantum dots [2].

Model and calculations
A hydrogenic impurity is being considered as at the centre of a ZnCdTe spherical dot confined by a spherical potential barrier (ZnTe). The confining potential is assumed to be zero inside and V outside. Within the framework of single band effective mass approximation, the Fröhlich interaction Hamiltonian of the system, a ZnCdTe/ZnTe quantum dot with the radius $R$, can be written as,

$$H = H_e + H_{ph} + H_{e-ph}$$  

where

$$H_e = -\frac{\hbar^2}{2m_e} \nabla^2 + V(r) + V(r)$$

with $V(r)$ is the strain induced confinement potential of the form

$$V(r) = \sum_q (V_q e^{iqr} a_q + V_q^* e^{-iqr} a_q^+)$$

and

$$a_q^+$$ and $$a_q$$ are the creation and annihilation operators for the LO phonon respectively.

$$H_{e-ph} = \sum_q (V_q e^{iqr} a_q + V_q^* e^{-iqr} a_{q}^+)$$

With the inclusion of impurity, the variation trial wave function is given by

$$\psi(r) = \begin{cases} N e^{i\pi/2} e^{i\theta} J_r(r, R) \exp(-\eta r) & \text{if } r < R \\ N \frac{J_r(r, R)}{K_r(b_{\pi} R)} e^{i\pi/2} J_r(b_{\pi} r) \exp(-\eta r) & \text{if } r \geq R \end{cases}$$

where $N_\eta$ is the normalization constant and $\eta$ is the variational parameter. We calculate the ground state energy $E$ by finding out the expectation value of the energy of the Hamiltonian and the donor binding energy is obtained as

$$E_{\eta} = E_{sub} - \langle H_{mn} \rangle$$

where $E_{sub}$ is the lowest binding energy without the impurity.

Results and discussion
The ground state binding energies of a hydrogenic donor impurity located at the centre of is investigated in a II-VI quantum dot with the inclusion of phonon effect and thereby a nonlinear optical property, the changes of refractive index is discussed. Computations are performed using Bessel function as an orthonormal basis for different confinement potentials of barrier height. The atomic units have been followed in the determination of electronic charges and wave functions in which the electronic charge and the Planck's constant have been assumed as unity.

Fig.1 shows the variation of changes of refractive index for a hydrogenic impurity in the strained Zn$_{0.5}$Cd$_{0.5}$Te/ZnTe quantum dot with the radius $40\,Å$, as a function of photon energy and intensity. It is observed that as the Zn incorporation increases, the total refractive index changes shift towards the higher values and the magnitude of total refractive index increases. This is

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because the increase in hydrogenic impurity binding energy occurs with the Zn-composition.

![Graph](image1)

**Fig.1 Variation of changes of refractive index for a hydrogenic impurity in the strained Zn$_x$Cd$_{1-x}$Te/ZnTe quantum dot with the radius 40Å, as a function of photon energy and $I=10$MW/m$^2$ for three different Zn concentration.**

We present the variation of changes of refractive index as a function of photon energy with and without the polaronic effect for a constant Zn content ($x=0.2$) in Fig.2. It is noticed that the changes of refractive index moves with the higher energy when the polaronic effect is included, this is because the enhancement of the binding energy occurs due to the inclusion of polaronic effect. Also, it is noticed from the Eq.(6) that the linear relative change in refractive index depends on the intensity and the third order relative change in refractive index changes with photon intensity and it varies quadratically with the matrix element of the electric dipole moment of the transition. The nonlinear term must be considered when calculating the refractive index changes of low dimensional semiconductor systems in which the incident light propagates along the $z$-axis [3]. Hence, the nonlinear term must be considered when calculating the refractive index changes in low dimensional semiconductor systems.

![Graph](image2)

**Fig.2 Variation of changes of refractive index as a function of photon energy with and without the polaronic effect for a constant Zn content ($x=0.2$).**

**Conclusion**

It is investigated that the potential with the inclusion of phonon will make the hydrogenic binding energies more than the obtained results using a Coulomb potential screened by a bare static dielectric constant and the optical properties of hydrogenic impurity in a quantum dot are strongly affected by the confining potential, dot radii and the Zn composition. We hope that our results would explore new findings in experimental sides on electro-optical devices.

**References**