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SnO_2 nanoparticles were synthesized by micro wave assisted co-precipitation method. The FTIR spectra, the peak at 640cm^{-1} indicates the presence of SnO_2 .the powder XRD pattern indicates the crystalline nature of the sample. The particle size was determined as 27.4nm from Debye Scherrer formula. The optical band gap was determined to be 3.98eV from absorption spectrum. From the present work it was inferred that microwave assisted co-precipitated method holds good for tin oxide nano particle synthesis.

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Compositional Effects on Enegry of A Nanodot

A.RejoJeice[a], Sr.GerardinJayam[b], K.S.JosephWilson[c*]

[a]Department of Physics, AnnaiVelankannai College, Tholayavattam,kanyakumari dist-629157,India.

[b]Department of Physics, Holy Cross College,Nagercoil,629 002, India.

[c]Departmant of Physics, Arul Anandar College,Karumathur,Madurai-625514,India

Abstract

The compositional effects on theground and excited states energies of a nanodot are theoretically investigated within the effective mass approximation. The results are presented for the nano dot with different composition of x. Our results demonstrate that i) the energies decreases as the dot size increases ii) It approaches to zero as the dot size tends to infinity and iii) The composition value increases as the binding energy increases.

Key Words: Nano Dot; confined energy

Corresponding author: E-mail address:rejojeice@gmail.com

1. Introduction

The interest in low dimensional semiconductor system (LDSS) found wider applications in nanotechnology and nanostructures. There has been a tremendous improvement in research activities on the LDSS due to the invention of molecular-beam

epitaxy, atomic layer epitaxy, metal-organic chemical vapour deposition and advanced electron lithography. Lithography have made possible to manufacture different sizes and shapes of semiconductor quantum dots (QD), Quantum wires and Quantum well [1]. In these quasi-zero dimensional system (QD) in which the carrier motion is restricted to a narrow region of a few nanometers in dimension hence the study of confinement is interesting.Quantum dots are semiconductor nanostructures where charge carriers are confined in all three spatial dimensions. The energy levels of a nanodot are discrete and atomic like hence QD are also called as artificial atoms. The energy levels of the nanodot are 1s, 1p, 1d, 2s,etc.,

In the present work, we have considered a GaAsnanodot embedded in a $Ga_{1-x}Al_xAs$ matrix with finite barriers. The barrier height depends on the composistion of x. When an electron is introduced into the dot, we estimate the total energy of the system, by assuming nanodot potential confinement for the barrier heights. The plan of the presentation of the present work is as follows. In Section 2 we present the mathematical models and the details of calculations. The results obtained are presented in Section 3 with a detailed discussion of the results. Conclusions are presented in Section 4.

2. Model and Theory

2.1. Single electron in a spherical quantum dot

We consider a single electron in a spherical quantum dot (nanodot) in the finite barrier model. In the absence of impurity, within the effective mass approximation, the Hamiltonian is given by

$$H_1 = -\frac{\hbar^2}{2m^*}\nabla^2 + V_D(r) \qquad (1)$$

where m* is the effective mass of the electron at the conduction band minimum, which is $0.067m_0$ for GaAs [1], where m_0 is the free electron mass. In our numerical calculations we use atomic units in which $m_0 = e^2 = \hbar^2 = 1$. The confining potential $V_D(r)$ is given by [2],

$$V_D(r,T) = \begin{cases} 0 & r \le R \\ V_0 = Q_C \Delta E_g^{\Gamma}(x,T) & r \ge R \end{cases} \qquad (2)$$

where V_o is the barrier height, Q_c is the conduction band offset parameter which is taken to be 0.6 [1]. The band gap difference depends of the concentration of Al. In our case $Ga_{1-x}Al_xAs$ is the barrier medium in which GaAs dot is embedded. The total energy difference [3] between the dot and barrier media, as a function of x, is given by

$$\Delta E_g^{\Gamma}(x) = 1.155x + 0.37x^2 eV \qquad (3)$$

In the present work we have chosen x=0.2 and 0.4 and the value of V_0 turns to be 147.48and 312.72 meV respectively. The lowest lying three bound states are given by

$$\psi_{1s}(\vec{r}) = \begin{cases} N_1 \frac{\sin(\alpha_1 r)}{\alpha_1 r} r \le R \\ A_1 \frac{e^{-\beta_1 r}}{\beta_1 r} r \ge R \end{cases} \quad (4)$$

$$\psi_{1p}(\vec{r}) = \begin{cases} N_2 \left(\frac{\sin(\alpha_1 r)}{(\alpha_2 r)^2} - \frac{\cos(\alpha_2 r)}{\alpha_2 r}\right)\cos\theta r \le R \\ N_2 \left(\frac{\sin(\alpha_1 r)}{(\alpha_2 r)^2} - \frac{\cos(\alpha_2 r)}{\alpha_2 r}\right)\cos\theta r \le R \end{cases} \quad (5)$$

$$\psi_{1d}(\vec{r}) = \begin{cases} N_3 \left(\left(\frac{3}{(\alpha_3 r)^3} - \frac{1}{\alpha_3 r}\right)\sin(\alpha_3 r) - \frac{3}{(\alpha_3 r)^2}\cos(\alpha_3 r)\right)(3\cos^2\theta - 1) r \le R \\ A_3 \left(\frac{1}{\beta_3 r} + \frac{1}{(\beta_3 r)^2} + \frac{1}{(\beta_3 r)^3}\right) e^{-\beta_3 r}(\cos^2\theta - 1) \qquad r \ge R \end{cases} \quad (6)$$

where N_1 ,N_2 ,N_3,A_1,A_2 and A_3 are normalization constants and α_1 and β_1 are given by $\alpha_1 = \sqrt{2m^* E}$ and $\beta_1 = \sqrt{2m^*(V_o - E)}$.

The energy eigen values are determined by imposing the Ben Daniel and Duke boundary condition that the normal particle velocity is continuous across the interface

$$-\frac{i\hbar}{m_1^*}\frac{\partial\psi}{\partial r}(r \le R)|_{r=R} = -\frac{i\hbar}{m_2^*}\frac{\partial\psi}{\partial r}(r \ge R)|_{r=R} \quad (7)$$

We obtain $\alpha_1 R + \beta_1 R\tan(\alpha_1 R) = 0$ s-states (8)

$$\frac{\cot(\alpha_2 R)}{\alpha_2 R} - \frac{1}{(\alpha_2 R)^2} = \frac{1}{\beta_2 R} + \frac{1}{(\beta_2 R)^2} \quad \text{p-states} \quad (9)$$

$$(9\alpha_3 R - ((\alpha_3 R)^3) + (4(\alpha_3 R)^2 - 9)\tan(\alpha_3 R) = -[(3 - (\alpha_3 R)^2 \tan(\alpha_3 R) - 3(\alpha_3 R)] * \left[\frac{(\beta_3 R)^3 + 4(\beta_3 R)^2 + 9(\beta_3 R) + 9}{(\beta_3 R)^2 + 3(\beta_3 R) + 3}\right]$$

d-states (10)

If$m_1^* = m_2^* = m^*$, solving these transcendental equations numerically, the confined energies E_l^n (n= 1,2,3…;*l*=0,1,3) are obtained. For other excited states similar equations may be obtained when *l*=3,4,…

3. Results and Discussion

The results obtained are shown in Fig.1 and Tables 1. Fig.1 shows the variation of confined energy of the nanodot as a function of dot radius for x = 0.2 . We observe that as the energy shifted to lower values for exicted states.The variation of confined energies with dot radius for the barrier concentration x= 0.2 and 0.4 for E_{1s}, E_{1p} and E_{1d} states are given in table 1. From the table 1we find that the confined energy decreases as the nanodot radius increases as we expected.

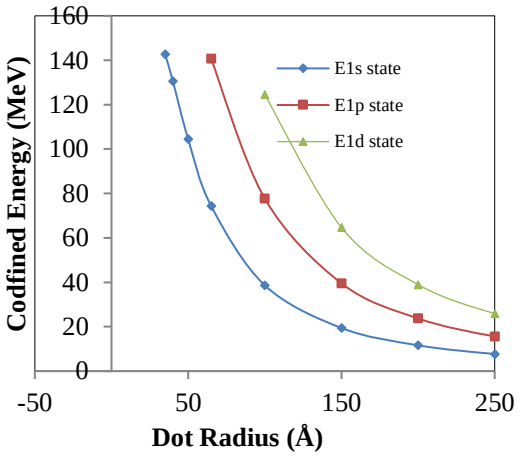

Fig1: Varation of confined energy with dot radius for concentration x = 0.2

For a given dot radius when the composition increases the energy also increases and which is shifted to lower dot radii in the excited state.For smaller dot sizes less than 3Å we notice there is no confinement energy for 1s-state (when x=0.4) since there is no bound state. These results contrast for the quantum well case where in there is a bound state for every well size. Another observation from the tables that we have not considered the value of x beyond x=0.4.Since the directto indirect band gap transition of GaAstakes place. The important conclusion that emerges from the result of Tables 1 is that for smaller dots compositional should be consider in the studies of low dimensional semiconductor systems.

Table 1: Confined energies (meV) under temperature in the finite barrier model for E_{1s},E_{1p}andE_{1d}state

Dot Radii(Å)	E_{1s}		E_{1p}		E_{1d}	
	x =0.2	x =0.4	x =0.2	x =0.4	x =0.2	x =0.4
35	142.74	216.07	-	-	-	-
40	130.69	183.47	-	-	-	287.79
50	104.53	134.32	-	261.17	-	233.13
65	74.39	96.43	140.75	179.56	-	145.65
100	38.66	43.43	77.73	88.35	124.58	71.13
150	19.44	21.02	39.57	42.9	64.71	41.85
200	11.64	12.34	23.75	25.22	38.98	27.51
250	7.73	8.1	15.64	16.56	25.95	19.45
300	5.5	5.72	11.15	11.7	18.5	19.45

(Dashes represent the absence of unbound state)

Like other systems when GaAs dot is embedded in $Ga_{1-x}Al_xAs$ matrix, the dielectric mismatch becomes insignificant, especially when x is small. When we compared the value of confined energy of aluminumconcentration 0.2 with 0.4 we found that x=0.4 have larger confined energy. Thus aluminum concentrations are also important of the nanodot.We can also tune the band gap of the nanodot using concentration of the barriermaterials with temperature, electric field, magnetic field,etc. Here, we had tuned the band gap by using aluminium concentration. Tunability of the band gap of thenanodotplays an important role in luminescent and photo voltaicdevices.

4. Conclusion

A systematic investigation of a single electron nonodotsconfined energies has been presented. We found that the confinement is important in nanosystems of smaller dot radius and it approaches to zero as the dot size approaches infinity.

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Thermal Analysis Cost effective smoke as solar selective coating

J.Packiam Juluis[1], T.K.Jayaleka[1],B.Usha[2]

[1]Department of Physics,Pioneer Kumaraswamy College,Nagercoil
[2]Women's Christian College
[Affiliated to Manonmaniam Sundaranar University,Abishekappathi, Tirunelveli]

Abstract

Effective attempts had been made to analyse the thermal properties of smoke coated on Stainless steel absorber. When compared with the other commercially available selective coating materials, the readily available,cost effective smoke showed better results. Stainless steel absorber coated with smoke has been utilized for this investigation. The locally available, cheap smoke was proved to be one of the best solar selective coatings.

Key words : Selective coating, Pyranometer thermal parameters

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Correspending auther:E-mail address:dr.j.pjuluis@gmail.com

MUSLIM ARTS COLLEGE

Affiliated to Manonmaniam Sundaranar University
Thiruvithancode – 629174
Kanyakumari District, Tamil Nadu, India

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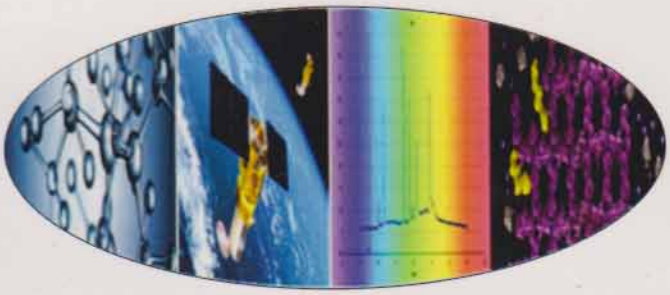

ABSTRACTS

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MOLECULAR STRUCTURAL AND VIBRATIONAL INVESTIGATIONS OF PHENOTHIAZINE

M. Latha Beatrice[a], M. Amalanathan[b] S.Mary Delphine[c]*

[a]Reg.No.12600., Associate Professor, Department of Physics , Annai Velankanni College, Tholayavaattam , Kanyakumari District, Tamil Nadu-629157.
[b]Assistant Professor, Department of Physics, Nanjil Catholic College of Arts and Science Kaliyakkavilai- 629153, Tamil Nadu
[C]Associate Professor,Department of Physics. Holy cross College(Autonomous), Nagercoil-629004
[a,b,c.] Manonmaniam Sundaranar University, Abishekapatti, Tirunelveli-627 012

Abstract

Fourier transform Raman and Fourier transform infrared spectra of Phenothiazine is recorded in the regions 4000–100 cm^{-1} and 4000–400 cm^{-1} respectively in the solid phase. The equilibrium geometry harmonic vibrational frequencies, infrared intensities and Raman scattering activities were calculated by density functional B3LYP/6-31G(d,p) method. A detailed interpretation of the vibrational spectra of this compound has been made on the basis of the calculated Potential energy distribution (PED). A detailed interpretation of the infrared and Raman spectra of Phenothiazine is reported. Stability of the molecule arising from hyper conjugative interactions, charge delocalization has been analyzed using natural bond orbital (NBO) analysis. The calculated HOMO and LUMO energies show that charge transfer occurs within the molecule. The observed and calculated wave numbers are found to be in good agreement. The PED calculation regarding the normal modes of vibration provides a strong support for the frequency assignment. NBO result of Phenothiazine reflects the charge transfer mainly due to C-C group. HOMO and LUMO energy gap explains the eventual charge transfer interactions taking place within the molecule. The calculated atomic charges for the Phenothiazine using Mulliken population analysis in all cases are different by values.

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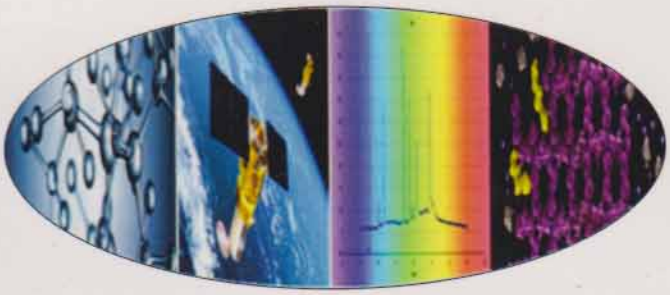

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[b]Assistant Professor, Department of Physics, Nanjil Catholic College of Arts and Science Kaliyakkavilai- 629153, Tamil Nadu
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