Journal of the Nigerian Association of Mathematical Physics
Volume 29, (*March, 2015*), **pp 303 – 308**

Comparison of the first Optical Transition Probability for Nine Ternary Semiconductor Alloy Spherical Quantum dots

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Abstract

This article focuses on comparing the calculation of the first optical transition probabilities of nine ternary semiconductor alloy quantum dots (artificial atoms) using the Hydrogenic atom model and the Fermi's golden rule of optical transition between levels. The quantum dots is found to respond to colored lights in the Visible region.

The transition probabilities were affected by the size, index of refraction and the effective mass of the semiconductor alloys. Maintaining the same dot radius of 2.50nm, the highest transition probability obtained is for Indium Arsenide (lnAs), while lowests obtained is for Zinc Selenide (ZnSe). The result gives a clue that lnAs quantum dot will more than other alloy best function in Visible light region nanosensors.

1.0 Introduction

Since the 1960's, quantum-size confinement [1]have been observed in three dimensional semiconductor nanocrystals. These confinement have limited the motion of electrons and holes in semiconductor nanocrystals from one to three spatial directions. Nanocrystal that confines the motion of electrons/holes in one spatial direction and allows for free propagation in the other two spatial directions is called quantum wells. Quantum wires are nanocrystals that confine the motion of electrons/holes in two directions and if a nanocrystal confines the electron/holes in three directions it is called a quantum dot [2-5].These quantum size confinement can be due to electrostatic potentials, the presence of an interface between different semiconductor materials, the presence of the semiconductor surface or due to a combination of these.

Quantum dots nanostructures are of particular interest because their optical and electrical properties can be readily modified. For example, the peak emission frequency of a quantum dot is extremely sensitive to the quantum dot's radius and composition[6-9]. This fascinating property gives rise to numerous fabrication techniques[10].

2.0 Theoretical Consideration

$$H = H_0 + H_k^{'} \quad (1)$$

$$H_0 = \frac{p^2}{2m} + V \quad (2)$$

$$H_k^{'} = \frac{h^2 k^2}{2m} + \frac{h\hat{k}.\hat{p}}{m} \quad (3)$$

H_0 is the unperturbed Hamiltonian

$$H = \frac{p^2}{2m} + \frac{\hbar^2 k^2}{2m} + \frac{\hbar\hat{k}.\hat{p}}{m} + V \quad (4)$$

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One get;

$$P_{if} = \frac{m_0}{\hbar}\left\langle i\left|\frac{\partial H}{\partial k}\right|f\right\rangle \qquad (5)$$

The matrix element depends only on the direction £ of light polarization and not amplitude. The matrix element is given by;

$$M_{if}^{£} = \frac{|e|}{m_0}P_{if}£ = \frac{|e|}{\hbar}\left\langle i\left|\frac{\partial H}{\partial k}\right|f\right\rangle \qquad (6)$$

According to the Fermi's golden rule,the transitionfrom an initial state I to the final state f due to the interaction with electromagnetic radiation of angular frequency ω is given by

$$W_{if} = \frac{2®}{\hbar}\left|\left\langle i\left|\hat{H}'\right|f\right\rangle\right|^2 ¢\left(E_f - E_i \pm \hbar´\right) \qquad (7)$$

$$W_{if} = \frac{2®}{\hbar}\left|\left\langle i;0\left|\hat{H}'\right|f;1_{q,\pm}\right\rangle\right|^2 ¢\left(E_f - E_i \pm \hbar µ\right)$$

$M_{if}^{£}.A = \left\langle i\left|\hat{H}'\right|f\right\rangle$, implies that

$$\left|\left\langle i\left|\hat{H}'\right|f\right\rangle\right|^2 = \left|M_{if}^{£}\right|^2.A^2 \qquad (8)$$

A is the operator of the vector potential.

$\hat{H}'$ is the pertubative Hamiltonian operator

$$A = i\sqrt{\frac{\hbar}{2£µV}} \qquad (9)$$

$$|A|^2 = \frac{\hbar}{2£µV}$$

$$\left|\left\langle i\left|\hat{H}'\right|f\right\rangle\right|^2 = \left|M_{if}^{£}\right|^2 \frac{\hbar}{2£µV}$$

$$W_{if} = \frac{2®}{\hbar}\sum_{q,\pm}\frac{\hbar}{2£µV}\left|M_{£\pm}\right|^2 ¢\left(E_f - E_f - \hbar µ\right) \qquad (10)$$

$$W_{if} = \frac{V}{(2®)^3}\int d^3q\,\frac{®}{£µV}¢\left(E_i - E_f - \hbar µ\right)\sum_{\pm}\left|M_{£\pm}\right|^2$$

$$W_{if} = \frac{V}{(2®)^3}\,\frac{2}{3}\int d^3q\,\frac{®}{£µV}¢\left(E_i - E_f - \hbar µ\right)\left(\left|M_{ex}\right|^2 + \left|M_{ey}\right|^2 + \left|M_{ez}\right|^2\right)$$

Using $µ = cq/\overline{n}$

$$W_{if} = \frac{\left(E_i - E_f\right)\overline{n}}{3\hbar^2£_0®c^3}\left(\left|M_{ex}\right|^2 + \left|M_{ey}\right|^2 + \left|M_{ez}\right|^2\right) \qquad (11)$$

Assuming $\left|M_{ex}\right|^2 = \left|M_{ey}\right|^2 = \left|M_{ez}\right|^2 = \left|M_{if}\right|^2 \; and \; E_i - E_f = 2®\hbar f$ (12)

$$W_{if} = \frac{\left(E_i - E_f\right)\overline{n}}{3\hbar^2£_0®c^3}3\left|M_{if}\right|^2 \qquad (13)$$

$$= \frac{2\overline{n}}{\hbar£_0 f^2 a^3}\left|M_{if}\right|^2$$

$M_{if}^{£} = \frac{|e|}{\hbar}\left\langle i\left|\frac{\partial H}{\partial k}\right| f\right\rangle$, from equation (6) were $|e|$ magnitude of electron.

$$W_{if} = \frac{2\bar{n}|e|^2}{\hbar^3 £_0 f^{2} a^{3}}\left|\left\langle i\left|\frac{\partial H}{\partial k}\right| f\right\rangle\right|^2$$

Usihg Eq. (3)

$\frac{\partial H}{\partial k} = \frac{\hbar^2 k}{m}$, $but\ k = \frac{\hat{p}}{\hbar}$, $\hat{p} = i\hbar\,\frac{d}{dr}$, therefore,

$$\left\langle i\left|\frac{\partial H}{\partial k}\right| f\right\rangle = \left\langle i\left|\frac{i\hbar^2}{m}\frac{d}{dr}\right| f\right\rangle \tag{14}$$

We assume the quantum dots to be spherical by using the radial function of the hydrogen atom, we have[11];

$$R_{n,l}(r) = \sqrt{\left(\frac{2z}{na_0}\right)^2 \frac{(n-l-1)!}{2n\{(n+l)!\}^3}}\left(\frac{2zr}{na_0}\right)^l L_{n+1}^{2l+1}\frac{2zr}{na_0}\exp\left(\frac{-2zr}{na_0}\right) \tag{15}$$

Where $a_0 = 4®£_0 h^2 / me^2$ and $L_{n+1}^{2l+1}(r)$ is associated Laguerre polynomial.

For a hydrogen atom for s-state orbital, $l=0, n=1$ and 2 we have that,

For $n = 1$,

$$R_{1,0} = 2\left(\frac{z}{a_0}\right)^{3/2} e^{-}\left(zr/a_0\right) \tag{16}$$

$$R_{2,0} = \frac{1}{2\sqrt{2}}\left(\frac{z}{a_0}\right)^{3/2}\left[2-\frac{zr}{a_0}\right]\exp\left(-\frac{zr}{2a_0}\right) \tag{17}$$

$$\langle 1|H|2\rangle = \left\langle 1\left|\frac{i\hbar^2}{m}\frac{d}{dr}\right|2\right\rangle = \frac{i\hbar^2}{m}\left\langle R_{1,0}\left|\frac{d}{dr}\right|R_{2,0}\right\rangle$$

$$= \frac{i\hbar^2}{m}\int R_{1,0}^{*}\left|\frac{d}{dr}\right| R_{2,0}\,dr \tag{18}$$

Implying that $\frac{d}{dr}R_{2,0} = \frac{1}{2\sqrt{2}}\left(\frac{z}{a_0}\right)^{5/2}\left[-2+\frac{r}{2}\left(\frac{z}{a_0}\right)\right]\exp\left(-\frac{zr}{a_0}\right)$, $R_{1,0}^{*} = R_{1,0}$ (19)

Hence

$$\langle 1|H|2\rangle = \frac{i\hbar^2}{3m\sqrt{2}}\left(\frac{z}{a_0}\right)^4\left[\frac{10}{3}\left(\frac{a_0}{z}\right)-r\right]\exp\left(-\frac{3zr}{2a_0}\right)$$

For $z = 1$, we have,

$$\langle 1|H|2\rangle = \frac{i\hbar^2}{3m\sqrt{2}}\left(\frac{1}{a_0}\right)^4\left[\frac{10a_0}{3}-r\right]\exp\left(-\frac{3r}{2a_0}\right)$$

$$W_{12} = \frac{2\bar{n}|e|^2}{\hbar^3 \text{£}_0 f^2 \text{a}^3} \left| \frac{i\hbar^2}{3m\sqrt{2}} \left(\frac{1}{a_0}\right)^4 \left[\frac{10}{3}\left(\frac{a_0}{z}\right) - r\right] \exp\left(-\frac{3zr}{2a_0}\right) \right|^2$$

$$W_{12} = \frac{2\bar{n}|e|^2}{\hbar^3 \text{£}_0 f^2 \text{a}^3} \left| \frac{i\hbar^2}{3m\sqrt{2}} \left(\frac{z}{a_0}\right)^4 \left[\frac{10}{3}\left(\frac{a_0}{z}\right) - r\right] \exp\left(-\frac{3zr}{2a_0}\right) \right|^2$$

$$W_{12} = \frac{2\bar{n}|e|^2}{\hbar^3 \text{£}_0 f^2 \text{a}^3} \left| \frac{i\hbar^2}{3m\sqrt{2}} \left(\frac{z}{a_0}\right)^4 \left[\frac{10a_0}{3} - r\right] \exp\left(-\frac{3r}{2a_0}\right) \right|^2$$

$$W_{12} = \frac{\bar{n}|e|^2 \hbar}{9m^2 \text{£}_0 f^2 \text{a}^3 a_0^{\,8}} \left| \left[\frac{10a_0}{3} - r\right] \exp\left(-\frac{3r}{2a_0}\right) \right|^2 \tag{20}$$

3.0 Results and Discussion

Permittivity of free space $\text{£}_0 = 8.85 \times 10^{-12}\ Fm^{-1}$

Rest mass $m_0 = 9.11 \times 10^{-31} kg$

Charge of an electron $e = -1.602 \times 10^{-19} C$

Angular momentum $\hbar = 1.055 \times 10^{-34}\ Js$

Bohr radius $a_0 = 0.529 \times 10^{-10} m$

Radius of the quantum dot*radius* = 2.50nm.The radius is constant for the dots.

$m = pm_0$, $\bar{n}$ are the effective mass and the refractive index of the various alloys of quantum dots as given in the table below

Table 1: Semiconductor Alloy standard values of refractive index and effective mass [12]

Semiconductor alloy	**Index of refraction**	**Effective mass (pm_0)**
GaAs (Gallium Arsenide)	3.30	*$0.067m_0$*
ZnSe (Zinc Selenide)	2.89	$0.17m_0$
CdTe (Cadmium Telluride)	2.50	$0.14m_0$
InAs (Indium Arsenide)	3.50	$0.027m_0$
GaSb (Gallium Antimonide)	3.80	*$0.05m_0$*
AlSb (Aluminum Antimonide)	3.20	*$0.09m_0$*
InSb (Indium Antimonide)	3.96	$0.013m_0$
InP (Indium Phosphide)	3.10	*$0.077m_0$*
GaP (Gallium Phosphide)	3.20	*$0.35m_0$*

Table 2: Results f0r the first optical transition probability of nine Ternary semiconductor alloy quantum dots

Alloys	**N**	**P**	**violet**	**blue**	**Green**	**Yellow**	**Orange**	**Red**
GaAs	3.3	0.067	0.0186	0.0165	0.0146	0.0136	0.013	0.0113
ZnSe	2.89	0.17	0.00254	0.002247	0.00199	0.00184	0.00177	0.00153
CdTe	2.5	0.04	0.00323	0.00287	0.00254	0.00235	0.00225	0.00195
InAs	3.5	0.027	0.12	0.108	0.0955	0.0885	0.0848	0.0735
GaSb	3.8	0.05	0.0385	0.0342	0.0302	0.028	0.0268	0.0233
AISb	3.2	0.09	0.01	0.008	0.00785	0.00729	0.00697	0.00605
lnSb	3.96	0.013	0.594	0.52	0.466	0.432	0.414	0.359
InP	3.1	0.077	0.0133	0.0117	0.0104	0.00964	0.00923	0.00801
GaP	3.2	0.35	0.000662	0.000587	0.000519	0.000482	0.000461	0.0004

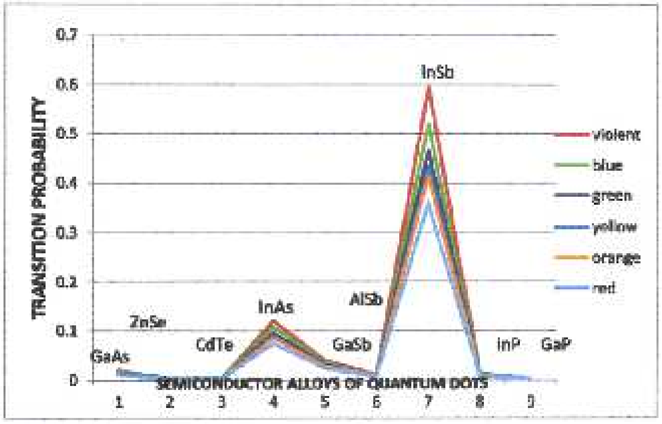

Fig 1: Graph displaying the transition probabilities of nine semiconductor alloy quantum dots.

4.0 Conclusion

The transition probability of the quantum dot is dependent on the size, effective mass and band structure of the quantum dot [4,5,11,13].

However, the overall aim of this project was to discover through the transition probability calculation the quantum dot in the visible light region of an electromagnetic field with the best response performance. Maintaining the same dot radius of 2.50nm, the highest transition probability obtained is for Indium Arsenide (lnAs), while lowest obtained is for Zinc Selenide (ZnSe). This result (fig. 1) clearly gives a clue that lnAs quantum dot will more than other alloy best function in Visible light region nanosensors.

5.0 References

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