International Journal For Technological Research In Engineering
Volume 6, Issue 11, July-2019 *ISSN (Online): 2347 - 4718*

A REVIEW ON VARIATION IN BAND GAP ENERGY OF QUANTUM DOT WITH ITS SIZE

Kirti Vishwakarma
Principal, Gyan Ganga college of Excellence, Jabalpur, India

ABSTRACT: ***Nanotechnology is the coming revolution in molecular engineering, and therefore, it is curiosity-driven and promising area of technology. The field of nano-science and nanotechnology is interdisciplinary in nature and being studied by physicists, chemists, material scientists, biologists, engineers, computer scientists, etc. Research in the field of nano-particles has been triggered by the recent availability of revolutionary instruments and approaches that allow the investigation of material properties with a resolution close to the atomic level. The quantum confinement effect is observed when the size of the particle is too small to be comparable to the wavelength of the electron. Quantum confinement effect modifies the electronic structure of nano-particles when their sizes become comparable to that of their Bohr excitonic radius. When the particle radius falls below the excitonic Bohr radius, the band gap energy is broadened, leading to a blue shift in the band gap emission spectra, etc.***

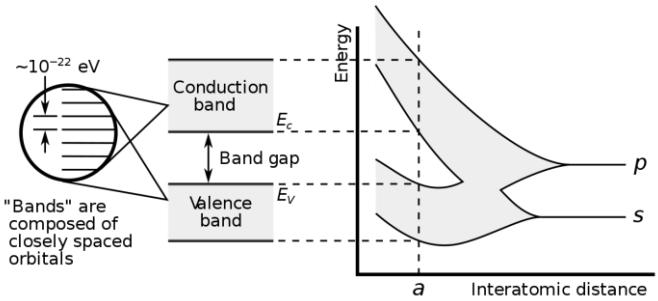
KEYWORDS: ***Nano-particles, quantum dot, Energy band gap, quantum confinement***

I. INTRODUCTION

The most popular term in the nano world is quantum confinement effect which is essentially due to changes in the atomic structure as a result of direct influence of ultra-small length scale on the energy band structure. The length scale corresponds to the regime of quantum confinement ranges from 1 to 25 nm for typical semiconductor groups of IV, III-V and II-VI. In which the spatial extent of the electronic wave function is comparable with the particle size. As a result of these "geometrical" constraints, electrons "feel" the presence of the particle boundaries and respond to changes in particle size by adjusting their energy. This phenomenon is known as the quantum-size effect. Quantization effects become most important when the particle dimension of a semiconductor near to and below the bulk semiconductor Bohr exciton radius which makes materials properties size dependent.

II. REVIEW ON BAND GAP

Quantum dots are semiconductor nanoparticle whose excitons are confined in all three spatial dimensions. [1] It is often called artificial atom because of its quantum properties and interactions similar to bulk semiconductor materials. Generally, the smaller the size of the crystal, the larger the band gap energy; the greater the difference in energy between the highest valence band and the lowest conduction band becomes, therefore, more energy is needed to excite the dot, and the crystal returns to its ground state. [2] Quantum dot structures are widely used as gain material for semiconductor lasers. Quantum-confined semiconductor structures, including quantum wells, quantum rods, and quantum dots, have been extensively investigated in the past few years. One of the most interesting effects of low-dimensional semiconductor structures is the size-dependent band gap. [3-5] The exciton Bohr radius is a threshold value, and the confinement effect becomes important when the quantum dot radius is smaller. For small quantum dots, the exciton binding energy and biexciton binding energy (exciton-exciton interaction energy) is much larger than that for bulk materials. [6]. To understand this effect we break the words like quantum and confinement, the word confinement means to confine the motion of randomly moving electron to restrict its motion in specific energy levels and quantum reflects the atomic realm of particle. So as the size of a particle decrease till we reach a nano scale the decrease in confining dimension makes the energy levels discrete and this increases or widens up the band gap and ultimately the band gap energy also increases. The quantum dot is an assembly of atoms of specific material that has few nanometer dimensions. It is termed as a virtual atom. Because of this microscopic size the electrons are confined inside the dot. This is the same for the electrons in an atom they are confined and localized in the atomic space. In order to obtain the possible energy levels in the atom or in the dot because of the space confinement one has to use quantum mechanical laws. That is one has to solve the Schrodinger equation with relevant boundary condition. The motion of electrons in the confined space can be modeled by the motion of a particle in a potential well with infinite walls. While the atom is modeled by one well with infinite wall with size of the atom, the electrons in the quantum dot can be modeled by a potential well with infinite walls with the minimum energy level is that of the conduction band. So, the picture is now is that we have electrons confined in the conduction band and holes in the valence band. If there is no confinement as in big crystal, there will be no confinement and the electrons in the conduction band will occupy the bottom of the conduction band and the holes will reside at the top of the valence band.
When we solve Schrodinger equation in potential well with infinite wall we find that the electrons will have only discrete energy levels in the valence band. The energy level diagram in the conduction band will be similar to that of an atom and so the energy levels of the holes in the valence band will have also discrete energy levels as the shown in the energy level diagram . [7]



The energy levels above the conduction band has an energy measured from the conduction band edge

$E_{ne} = n^2h^2 / 8\pi^2 m_e d^2$,

Where h is the Planck constant, n the order of the level, m_e is the effective mass of electrons in the quantum dot and d is the width of the dot.

The same equation holds for the holes energy E_{nh} in the valence band with m_h the hole effective mass instead of m_e. So, the energy gap for the quantum dot becomes

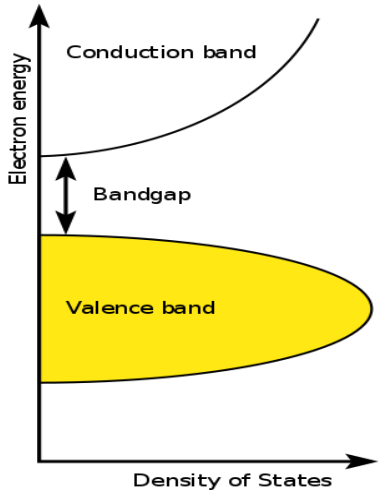
$Eg^{qd} = Eg + E_{1e} + E_{1h}$,

E_{1e} is the excess energy of the first level in the quantum dot and E_{1h} is that corresponding level for the holes. It is clear that one can tune the effective energy gap in the quantum dot by changing its size d.

When the separation of two confining surfaces is less than de broglie wavelength of the electron then electron energy is quantized which is the 2D quantum confinement effect. Such a confinement can be realized in 3-D leading to quantum box or dot. The physical properties of a quantum dot are not affected quantum confinement; however, their optical absorption and emission can be tuned via the quantum size effect. A useful model for this is the particle in a sphere.

In metals and semiconductors the electronic wave functions of conduction electrons are delocalized over the entire particle. These electrons can, therefore, be described qualitatively as particles in a dot. Thus the densities of states and the energies of the particles depend crucially on the size of the dot which leads to some extent to a smooth size dependence. E.g. ionization energies and electron affinities are tuned between the atomic values and the work function of the bulk material by variation of the cluster size. However, there are also discontinuities which are due to filled shell structures leading e.g. to extra stability of such clusters (‘pseudo-atoms’).

The variation of nanoparticle size generates novel properties that can hardly be seen in the bulk, such as the conduction-insulator and nonmagnetic-magnetic transition of noble metals (e.g. Au at ~2-3nm) at the nanoscale. We know that one electron energy level of atoms is split into two levels, when a two-atom molecule is formed. With an increase in the number of atoms in the nanoparticle, the energy level continues to split and finally, merge into quasi–continuous band structure in the bulk solid. However, for small particles with dimension in the nanometer regime, the electron states are not continuous but discrete, due to the confinement of the electron wave function. A semiconductor is a material with an intermediate sized but non-zero band gap that behaves as an insulator at absolute zero but allows thermal excitation of electrons into its conduction band at temperatures that are below its melting point. In contrast, a material with a large band gap is an insulator. In conductors the valence and conduction bands may overlap, so they may not have a band gap. The conductivity of intrinsic semiconductor is strongly dependent on the band gap. The only available charge carriers for conduction are the electrons that have enough thermal energy to be excited across the band gap and the electron hole that are left off when such an excitation occurs.



III. CONCLUSIONS

Electronic states of an atom are typically characterized by discrete energy levels that are often separated by electron volts. The band gap energy of the quantum dot increases with the reduction of its size because of the quantum confinement The spatial distribution of these states is highly localized. At the nanoscale, the dimension of energy states resides between these limits. In the nanoscale phenomena, the energy level spacing of electronic states of atom increases with reduction in dimensionality of particle and is called Quantum Confinement. The QC phenomena can be readily understood from the well-known Heisenberg’s uncertainty principle. Since the uncertainty in momentum cannot exceed the momentum. If one tries to localize the position of an electron by reducing the box size, its energy must increases and diverges as the confining region vanishes. Hence, depending on the dimensions in which the length scale is nanometers, they can be classified into: (a) nanoparticles (0-D), (b) lamellar structure (1-D), (c) filamentary structure (2-D), and (d) bulk nanostructured (3-D) materials. The densities of states and the energies of the particles depend crucially on the size of the dot which leads to some extent to a smooth size dependence.

REFERENCES

[1] M. A. Reed, E. S. Hornbeck,et.al., “Quantum Dots,” Scientific American, 268, 1, 118-123 (1993).
[2] R. D Schaller and V. I. Klimov, Physical Review Letters, 92, 18 (2004)
[3] E.O. Chukwuocha, M.C. Onyeaju and T. T. Harry, World Journal of Condensed Matter Physics, 2, 96-100, (2012).
[4] H. Yu, J. Li, R. A. Loomis, P. C. Gibbons, L. W. Wang and W. E. Buhro, J. Am. Chem. Soc., 125,

16168, (2003).
[5] L. L. Li, J. Hu, W. Yang and A. P. Alivisatos, Nano Lett., 1, 349, (2001).
[6] V.I. Klimov, J. Phys. Chem. B, 110, 16827–16845 (2006).
[7] L.E.Brus, J. Chem. Phys., 79, 5566–5571 (1983).

