In this section of Resonance, we invite readers to pose questions likely to be raised in a classroom situation. We may suggest strategies for dealing with them, or invite responses, or both. “Classroom” is equally a forum for raising broader issues and sharing personal experiences and viewpoints on matters related to teaching and learning science.

Various Quantum Mechanical Concepts for Confinements in Semiconductor Nanocrystals

Semiconductor nanocrystals or quantum dots (QDs) are nanometer-scale materials which have attracted the attention of researchers in various branches of science and technology because of their peculiar characteristics as compared to their bulk counterpart. Optical, electronic and optoelectronic properties of semiconductors are greatly influenced when the crystallite size is in the quantum confinement regime. Various quantum mechanical concepts are being used to predict the quantum confinement regime. Here, an attempt has been made to compare and evaluate the consistency of various concepts.

1. Introduction

Quantum-size effect for semiconductor nanocrystals has become a subject of interest due to the effect of confinement on electrons, holes and excitons [1-4] which leads to changes in the optical properties of nanocrystallites significantly as compared to those of the bulk counterpart [5]. Size-dependent luminescence of CdTe nanoparticles [6] is shown in Figure 1. Many of the interesting and potentially useful properties of nanocrystals

Jayakrishna Khateti\(^1\) and Karuna Kar Nanda\(^2\)
Materials Research Centre
Indian Institute of Science
Bangalore 560 012, India.
Email: \(^1\) khateti@gmail.com
\(^2\) nanda@mrc.iisc.ernet.in

Keywords
Quantum confinement, quantum mechanics, semiconductor nanostructures, Bohr radius.

Figure 1. The size dependent emission color of the thiol-capped CdTe quantum dots.
can be understood at the level of undergraduate quantum mechanics. In a bulk semiconductor, the conduction electrons are free to move around in the solid; so their energy spectrum is almost continuous. However, in semiconductor nanocrystals the electron in the conduction band or hole in the valence band is confined due to quantum size effects. As a consequence, the continuous band appears to be discrete.

Various quantum mechanical concepts including infinite square-well potential model, de Broglie wavelength, and Bohr radius are being used to predict the quantum confinement regime. Here, we address these concepts to evaluate the quantum size effect and the relation between them in various semiconductor nanoparticles. We have used room temperature thermal energy as a measurement ruler to the excitonic binding energy to calculate the strong quantum confinement limit in various well-known semiconductor systems. The confinement size limits depend on the effective mass of the electron/hole and the dielectric constant.

2. Quantum Mechanical Concepts for Semiconductor Nanocrystals

Concept 1. Bohr radius formalism

Quantum size effect is described as the phenomenon resulting from electrons and electron holes being squeezed into a dimension that approaches a critical quantum measurement, called the exciton Bohr radius. An exciton is composed of an electron and a hole. The distance between an electron and a hole in the exciton is known as exciton Bohr radius. Electron, hole and exciton Bohr radius are given by

\[ a_e = \frac{0.0529\varepsilon}{m^*_e/m_0} \text{ (nm)}, \quad \text{electron Bohr radius,} \quad (1) \]

\[ a_h = \frac{0.0529\varepsilon}{m^*_h/m_0} \text{ (nm)}, \quad \text{hole Bohr radius,} \quad (2) \]