A Study on Core Shell Quantum Dots NPs

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Abstract

Core/Shell quantum dots are products of further engineering in the structures of quantum dots (QDs). A QD has a high surface area to volume ratio with unsaturated bonds, or dangling bonds, existing on the surface. These under-coordinated atoms make them more active than those in the bulk of the QD materials. Core-shell type nanoparticles are a type of biphasic materials which have an inner core structure and an outer shell made of different components. These particles have been of interest as they can exhibit unique properties arising from the combination of core and shell material, geometry, and design. Core/Shell quantum dots are products of further engineering in the structures of quantum dots (QDs). A QD has a high surface area to volume ratio with unsaturated bonds, or dangling bonds, existing on the surface. These under-coordinated atoms make them more active than those in the bulk of the QD materials.Core-shell nanostructures can be defined as nanoparticles, which are encapsulated and covered by an exterior shell, which provide stability to the core nanoparticles against agglomeration and coalescence, which might happen during any type of reaction.

Keywords: Man-made, Crystal structure, Nanoscale, Core-shell, QDs, NPs

I. Introduction

Core–shell type nanoparticles are a type of biphasic materials which have an inner core structure and an outer shell made of different components. These particles have been of interest as they can exhibit unique properties arising from the combination of core and shell material, geometry, and design [1–2].The so-called quantum size effect describes the physics of electron properties in solids with great reductions in particle size. This effect does not come into play by going from macro to micro dimensions. However, it becomes dominant when the nanometer size range is reached. CdSe quantum dots (QDs) are produced by simultaneously injecting cadmium (Cd) and selenium (Se) precursor solutions into a heated growth solution of octadecene in ambient atmosphere. Once combined, Se and Cd form CdSe clusters that become continually growing QDs as the reaction progresses.Colloidal semiconductor nanocrystals, often referred to as colloidal quantum dots (QDs), have attracted numerous research interests over the past decades [1-3]. Colloidal QDs are nanometer-scale semiconductor crystals (with diameters less than ~20 nm) capped with surfactant molecules (ligands) and dispersed in solution. A critical advantage of colloidal QDs is the quantum confinement effect that is observed when the size of QDs is comparable to the electron wavelength, which leads to discrete energy levels for increased band gap, thus allowing for the size/shape tunable optical and electrical properties [3]. This unique quantum confinement effect triggers research interests in the design and synthesis of colloidal QDs with tunable size, shape, and composition to realize fine-control of the optoelectronic properties [4-6].

However, bare QDs capped with organic ligands are very sensitive to the surface chemical environment and typically exhibit abundant surface-related defect/trap states, which serve as non-radiative recombination center for photo-excited charge carriers, thus reducing the luminescence efficiency and materials stability [7,8]. The growth of core/shell architecture is an efficient approach for QDs' surface passivation. The robust inorganic shell can effectively isolate the core QDs from surrounding environment and suppress the formation of surface defects/traps. Besides, it is possible to modulate the band structure of the core/shell QDs by appropriately selecting the core and shell materials [9]. As depicted in Fig.1, according to the relative position of conduction band (CB) and valence band (VB) edges of core and shell materials, the band structures of core/shell QDs are generally classified as three types: Type I, Type II and quasi-type II. Type I core/shell QDs exhibit band alignment in which the bandgap of the core material is narrower than that of the shell, confining both electrons and holes into the core region and leading to

enhanced photoluminescence quantum yield (PLQY) and photo-/chemical-stability, which is beneficial to the luminescent QD-devices including luminescent solar concentrators (LSCs) and light-emitting diodes (LEDs) [10-12]. Type-II core/shell QDs possess a staggered CB and VB edges of core and shell materials, resulting in a spatial separation of the electrons and holes in different regions of core/shell QDs, and quasi-type II core/shell QDs have either small CB and VB offsets, in which one type of the charge carriers are delocalized into shell region while the other type of charge carrier is still confined in the core region, these efficient charge carriers separation are favorable for the photovoltaic systems such as solar-driven QD-based photoelectrochemical (PEC) cells and QDs-sensitized solar cells (QDSCs) [13]. The rational design of core/shell QDs has demonstrated a powerful platform for the development of various classes of optoelectronic devices [14-15].

II. Methodology

II.A Types of the Quantum Dots

These nano dots can be single component materials with uniform internal compositions, such as chalcogenides (selenides, sulfides or tellurides) of metals like cadmium, lead or zinc, example, CdTe. It is divided in to two parts: such as Core-Shell Quantum Dots and Alloyed Quantum Dots.

II.B What is basic difference between quantum dots and nanoparticles?

Nanoparticles is typically used for particles in the nm size regime, while quantum dots are those nanoparticles that are in "quantum size regime" characterized by the discretization of the energy levels inside the material.

II.C What is quantum dot effect?

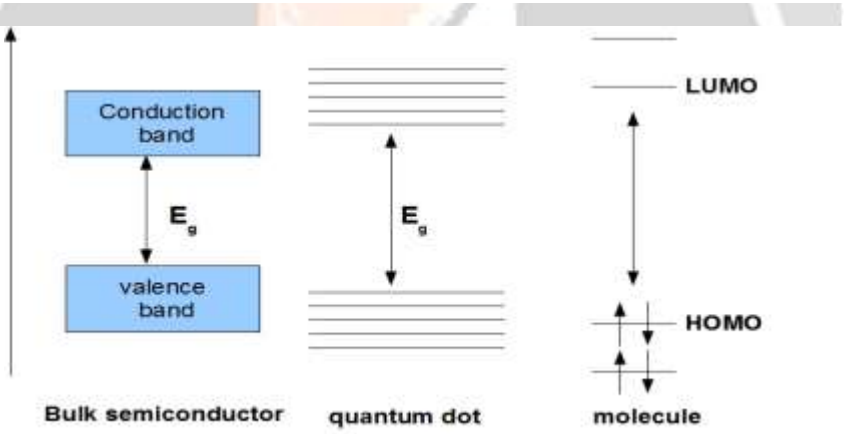

Fig.1 Quantum dots (QDs) are man-made nanoscale crystals

Charge carrier trapping on QDs increases the probability of non-radiative recombination, which reduces the fluorescence quantum yield. Surface-bound organic ligands are typically used to coordinate to surface atoms having reduced coordination number in order to passivate the surface traps. For example, tri-n-octylphosphine oxide (TOPO) and trioctylphospine (TOP) have been used to control the growth conditions and passivate the surface traps of high quality CdSe quantum dots. Although this method provides narrow size distributions and good crystallinity, the quantum yields are ~5–15%.[10] Alkylamines have been incorporated into the TOP/TOPO synthetic method to increase the quantum yields to ~50%[11].
Quantum dots (QDs) are man-made nanoscale crystals that that can transport electrons.If semiconductor particles are made small enough, quantum effects come into play, which limit the energies at which electrons and holes (the absence of an electron) can exist in the particles.

II.D What condition is required for showing quantum size effect by a semiconductor particle?

In a semiconductor crystallite whose size is smaller than twice the size of its exciton Bohr radius, the excitons are squeezed, leading to quantum confinement. The energy levels can then be predicted using the particle in a box model in which the energies of states depend on the length of the box.

II.E What is size quantization?

Due to this confinement the electronic properties of quantum dots depend on their size in the **nanometer** regime [1,2].This effect, now called size-quantization, was first observed in 1926 with CdS colloids[3], but was only properly recognized in the 1980s [4-5].

II.F Why does band gap increase with decrease in size?

The results show that the band gap energy increases with the decreasing particle size. Because of the confinement of the electrons and holes, the band gap energy increases between the valence band and the conduction band with decreasing the particle size.

II.G What is quantum confinement in nanoparticles?

Quantum confinement is change of electronic and optical properties when the material sampled is of sufficiently small size - typically 10 nanometers or less. The bandgap increases as the size of the nanostructure decreases.

II.H How does nano size influence the electron band gap?

Band gap increases with decrease in size due to electron confinement at nano-scale so called "quantum size effect". In a simple words electrons are confined i.e occupied less space than bulk, hence VBM and CBM potentials are shifted more +ve and -Ve respectively, resulting high band gap.

II.I How quantum dots are used in medical field?

Applications for in vivo use of semiconductor quantum dots are imaging of tumor vasculature, imaging of tumor-specific membrane antigens, as well as imaging of sentinel lymph nodes. Multicolor fluorescence imaging of cancer cells can be accomplished by systemic injection of quantum-dot-based multifunctional nanoprobes.

III. Results and Discussion

Quantum dots (QDs) are considered efficient fluorescent labels used in a drug delivery system for monitoring the metabolism process of drugs in the body owing to the unique physicochemical characteristics.Colloidal core/shell quantum dots (QDs) are promising for solar technologies because of their excellent optoelectronic properties including tunable light absorption/emission spectra, high photoluminescence quantum yield (PLQY), suppressed Auger recombination, efficient charge separation/transfer and outstanding photo-, thermal-/chemical stability. In this review, engineered core/shell QDs with various types of band structures and corresponding device performance in luminescent solar concentrators (LSCs),light-emitting diodes (LEDs), solar-driven photoelectrochemical(PEC) devices and QDs-sensitized solar cells (QDSCs) are summarized. In particular, the applications of interfacial layer engineering and eco-friendly, heavy metal-free core/shell QDs in optoelectronic device are highlighted. Finally, strategies towards the developments and practical perspectives of core/shell QDs are briefly mentioned to offer guidelines for achieving prospective high-efficiency and long-term stable QD devices.

IV. Conclussions

The main challenge in using organic ligands for quantum dot surface trap passivation is the difficulty in simultaneously passivating both anionic and cationic surface traps. Steric hindrance between bulky organic ligands results in incomplete surface coverage and unpassivated dangling orbitals.[4] Growing epitaxial inorganic semiconductor shells over quantum dots inhibits photo-oxidation and enables passivation of both anionic and cationic surface trap states.[9] As photogenerated charge carriers are less likely to be trapped, the probability for excitons to decay through the radiative pathway increases. CdSe/CdS and ZnSe/CdSe nanocrystals have been synthesized that exhibit 85% and 80–90% quantum yield, respectively.[12-13]

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