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Semiconductor Nano Materials for Wide Bandgap Photonic and Optoelectronic Device Applications

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Abstract— CdS, CdSe, ZnS, GaAs, InSb, InAs, PbS, PbSe and PbTe Quantum dots (QDs) have been quantitatively studied for wide bandgap device applications using Brus model. The results strongly indicate that absorption and emission bands of QDs broaden with decreasing dot size leading to dramatic increase in energy of band-to-band excitation peaks and photoluminescence spectra compared to the spectrum of the materials in bulk form. These wide bandgap QDs differ significantly from conventional semiconductors as a result of their larger bandgap that is tunable by dimensional constraints due to quantum confinement and therefore exhibit tremendous advantages in terms of power capability, energy conversion efficiency, optical properties, radiation strength, high temperature, and high frequency operation suitable for high frequency fields, power electronics, solid state lightings etc. Wide bandgap semiconductor QDs also play an important role in optical absorption and emission of ultraviolet (UV) light for photonic and optoelectronic devices. Among the QDs, ZnS possesses the largest band gap (~ 8.5 eV) and hence exhibits widest and broadband spectral range and should be studied extensively due to its applicability in transparent electronics.

Keywords— Wide bandgap, semiconductor, Quantum dot, emission and absorption, ultraviolet (UV) light, confinement.

I. INTRODUCTION

Wide bandgap semiconductors have stimulated wide scientific and technological interests as key materials for applications in high-performance photonic and optoelectronic devices operating at higher voltages and power, higher operating temperatures, faster switching and improved efficiencies. Recent technological advancements have allowed traditional semiconductor technology to approach their theoretical limits in that high power device requirements for many utility applications are at a point that the present traditional based devices cannot handle. To overcome these limitations, new semiconductor materials for power device applications are needed. Quantum dots (QDs) with superior optical and electrical properties are likely candidates to replace traditional semiconductors in the near future due to their broadband absorption band emanating from the quantum confinement effect. The quantum confinement effects are directly influenced by the material's composition and physical dimensions and are observed when the size of the semiconductor is smaller than the exciton Bohr's radius. As a result, the charge carriers become spatially confined, and the energy spectrum become discrete.

Wide bandgap semiconductors are electronic materials in which the energy of the band-to-band electronic transitions exceeds approximately 2 eV and differ significantly from conventional semiconductors since they have a larger electronic bandgap [1]. QDs low cost and bandgap tunabilities are some of the basic qualities that enable them to overtake the parental bulk as the dominant wide bandgap semiconductor materials [2]. The physical and electrical properties of QDs determine the functional and application characteristics of the devices built with them. A bandgap refers to the energy difference in semiconductors between the top of the valence band and the bottom of the conduction band [3]. The optical and electronic behaviors of semiconductor materials lie in their fundamental band gap which in turn governs their absorption and emission bands as illustrated in Figure 1 [4]. When an electron in the valence band absorbs a photon with energy equal to, or higher than the bandgap, it becomes excited and makes transitions to the conduction band. Recombination occurs when an electron from a higher energy level relaxes to a lower energy level and recombines with an electron hole. This process is accompanied by the emission of radiation known as fluorescence, which can be measured to give the band gap size of a semiconductor [5].

QDs are semiconductor nano particles that have been reduced below the size of the critical quantum limit, often termed as the exciton Bohr's radius. Quantum confinement is more prominent in semiconductors because they have a bandgap in their electronic band structure [6]. Typically, QDs are composed of groups II-VI, III-V, and IV-VI materials. They have bandgaps that are tunable across a wide range of energy levels by changing their size due to charge carrier confinement, in contrary to

bulk materials whose bandgap is fixed by the choice of material(s) as shown Figure 1 [7]. According to Brus model, the effective bandgap of QDs of a given radius (R) is expressed as [8]

$$E_{g(QD_S)} = E_{g_{(bulk)}} + \frac{h^2}{8\mu R^2} - \frac{1.8\, e^2}{4\pi\varepsilon_0\varepsilon_r R} \quad (1)$$

The model predicts that the band gap energy increases as size of the semiconductor QDs decreases [9]. This potential quantum effect makes them suitable materials for wide bandgap semiconductor device applications.

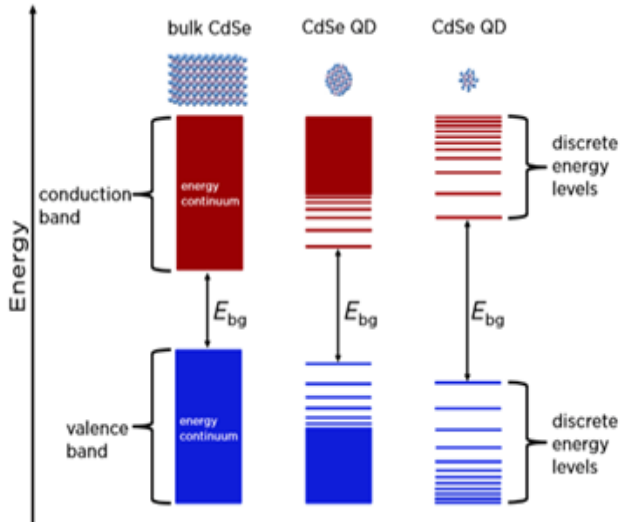

Figure. 1.The Size-Dependent of the Band gap of QDs in relation to Bulk

Higher the bandgap of a semiconductors, the greater the sustainability of the materials operating temperature capabilities and lower their susceptibility to radiation. Thus larger distance between the forbidden region of QDs makes them excellent wide bandgap semiconductor candidates crucial for power devices operating at higher voltages, temperatures, and frequencies [10]. In this paper we used the Brus model for the investigation of QDs for wide bandgap device applications.

II. Materials and Methods

The verified experimental parameters used for this study are: effective masses of electron, M_e^* and hole, M_h^* band gap of bulk semiconductors $E_{g(bulk)}$, specifically for group II-IV (CdSe, CdS and ZnS), group III-V (GaAs, InAs and InSb) and the group IV-VI (PbSe, PbS and PbTe) QDs acquired at Advance Physics Laboratory, Sheda Science and Technology Complex Abuja as shown in the Tables 1, 2 and 3. The variation of optical bandgaps as a function QD sizes were theoretically computed using Brus model to ascertain QDswith the required wide bandgap for device applications. The input parameters used in the quantitative analysis have been listed in Tables 1, 2 and 3.

Table 1.The Group II-IV QDs material parameters used for the study.

Quantum dots	M_e^x	M_h^x	$Eg_{(bulk)}$ at 300k
CdSe	0.13mo	0.45mo	1.74Ev
ZnS	0.34mo	0.23mo	3.68eV
CdS	0.21mo	0.80mo	2.42eV

TABLE 2.The Group III-V QDs experimental parameters used for the study.

Quantum dots	M_e^x	M_h^x	$Eg_{(bulk)}$ at 300k
InAs	$0.02m_o$	$0.40m_o$	0.36eV
InSb	$0.02m_o$	$0.40m_o$	0.17eV
GaAs	$0.06m_o$	$0.51m_o$	1.42eV

TABLE 3.The Group IV-VI QDs experimental parameters used for the study.

Quantum dots	M_e^x	M_h^x	$Eg_{(bulk)}$ at 300k
PbSe	$0.05m_o$	$0.04m_o$	0.27eV
PbS	$0.25m_o$	$0.25m_o$	0.37eV
PbTe	$0.17m_o$	$0.20m_o$	0.32eV

III. Results and Discussion

The optical bandgap (excitation energy) as a function of dot sizes for group II-IV (CdSe, CdS and ZnS), group III-V (GaAs, InAs and InSb) and the group IV-VI (PbSe, PbS and PbTe) QDs using Brus equation are plotted in Figures 3, 4 and 5 respectively. The results show that optical bandgap of QDs exhibits an inverse quadratic correlation with dot size. Thus absorption and emission bands broaden with decreasing dot size leading to significant increase in energy of band-to-band excitation peaks and hence a blueshift in the photoluminescence spectra compared to the spectrum of the material in bulk as shown in Figure 2 below.

This generally indicate substantial increased in the size-dependent optical gap between the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) referred to as bandgap and hence the separation between the valence and conduction bands. These optical characteristics suggest that more excitation energy is needed to elevate electron from valence band to conduction band and also more energy will be released during recombination.

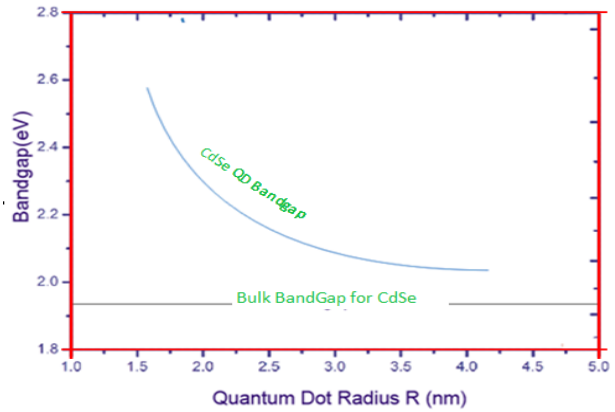

Figure. 2. Showing a Large Optical Blue Shift for CdSe QD

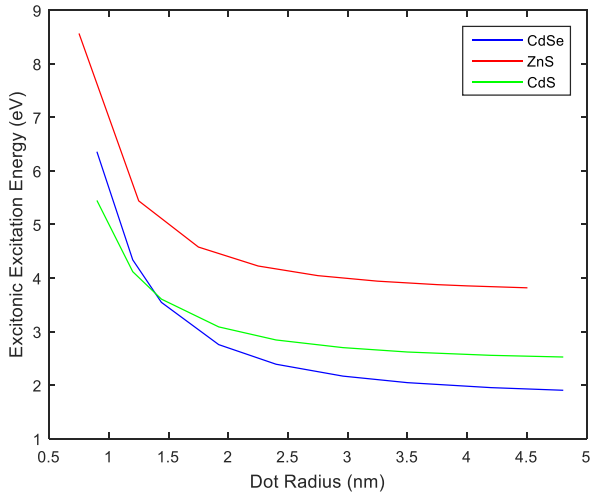

Figure.3. Excitonic Excitation Energy versus Dot Radius for CdSe, ZnS and CdS QDs

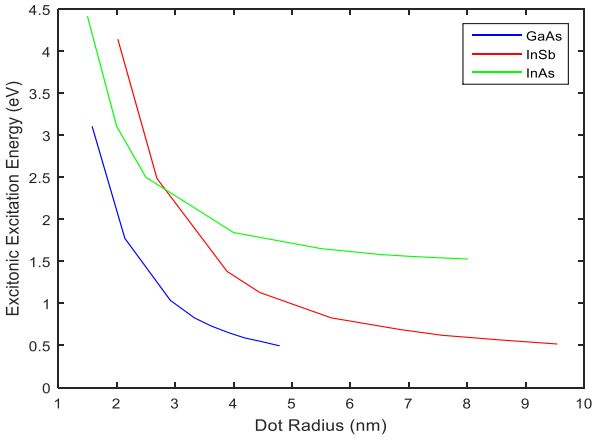

Figure. 4. Excitonic Excitation Energy versus Dot Radius for GaAs, InSb and InAs QDs

From the observed spectra we found that CdS, CdSe, ZnS, GaAs, InSb, InAs, PbS, PbSe and PbTe QDs display exceptional wide bandgap with maximum bandgap of 5.50, 6.20, 8.50, 3.10, 4.20, 4.40, 3.60, 3.80 and 3.70eV respectively to be considered as alternative for wide bandgap semiconductor applications. Wide bandgap semiconductor materials such as mentioned above offer numerous advantages over traditional semiconductor materials. Consider the fact that a fundamental bandgap shrinks as temperatures rise but with wide bandgap materials, rising temperatures will have far less effect on their functionalities.

Thus components made with wide bandgap semiconductors QDs operate significantly at higher voltages, higher power levels, higher frequencies, higher operating speeds, higher operating temperature, faster switching, improved efficiencies and smaller form factor. These properties make them optimal materials for applications in which the required frequencies, voltages, speeds and temperatures are very high. Such as radio frequency communications and power electronics with high current and voltage values.

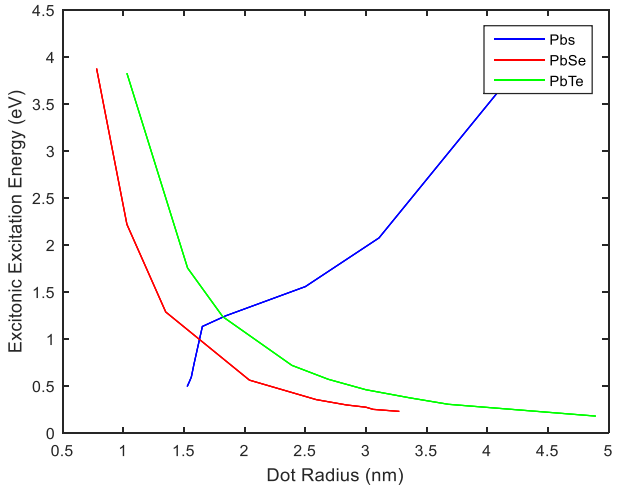

Figure.5. Excitonic Excitation Energy versus Dot Radius for PbS, PbSe and PbSe QDs

The wide bandgap materials also possess many vital implications for optoelectronic and electronic applications due to their large bandgap energies suitable for absorbption and emission ultraviolet (UV) light vital for applications in sustainable energy and solid-state lighting devices. For photovoltaics applications wide-band-gap materialsare proposed to act as a window material for cascade thin-film solar cell to improve quantum efficiency in the UV region. Among other wide bandgap materials, ZnS QD possesses the largest band gap (~ 8.5 eV) and hence exhibits the widest tunable spectral range and has been studied extensively due to its applicability in transparent electronics.

IV. CONCLUSION

Wide-bandgap semiconductors have been studies for CdS, CdSe, ZnS, GaAs, InSb, InAs, PbS, PbSe and PbTe Quantum dots (QDs) using Brus model. These wide bandgap semiconductors possess critical advantages, including the ability to handle higher voltages and power, faster switching, better efficiency, higher operating temperatures, and a significantly smaller form factor. Among QDs materials considered ZnS possesses the widest bandgap energy and hence the largest tunable spectra range which plays a vital role for absorption and emission of high energy ultraviolet (UV) crucial for applications in photonic and optoelectronic devices and will be also relevant in high optical transmittance specifically in the range of visible to infra red (IR) spectral regions.

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