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Original Article

Investigation of Electronic and Optical Properties of PbTe, PbSe, PbS Semiconductor Quantum Dots For Device Applications Using The Brus Equation

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Abstract *- Group IV–VI semiconductor Quantum Dots (QDs), particularly lead chalcogenides such as PbS, PbSe, and PbTe, have gained significant attention for next-generation optoelectronic and electronic devices due to their size-dependent band gap tunability and pronounced quantum confinement effects. In this study, the Brus equation is applied to theoretically examine how the energy band gap varies with quantum dot radius for PbS, PbSe, and PbTe. The analysis shows that as the dot radius decreases, the band gap increases owing to confinement of charge carriers, with the extent of tunability determined by each material's intrinsic exciton Bohr radius and effective Mass. PbS QDs display the strongest quantum confinement, allowing band gap tuning from the Near-Infrared (NIR) to the visible range, making them ideal for solar cells, Light-Emitting Diodes (LEDs), and photodetectors. PbSe QDs, with moderate confinement, reach into the Mid-Infrared (MIR) region and are suitable for telecommunications, optical modulators, and infrared sensors. PbTe QDs exhibit weaker confinement due to their larger exciton Bohr radius, retaining narrow band gaps that are advantageous for thermoelectric devices, far-infrared detectors, and low-temperature infrared lasers. These findings underscore the critical role of particle size in tailoring the optical and electronic properties of PbS, PbSe, and PbTe QDs, providing valuable guidance for their optimized deployment in photovoltaic, optoelectronic, and thermoelectric applications.*

Keywords *- Band gap tunability, Exciton Bohr radius, Infrared sensors, Quantum confinement, Semiconductor quantum dots.*

1. Introduction

Quantum Dots (QDs) are semiconductor nanocrystals whose electronic and optical properties are governed by quantum confinement when one or more dimensions approach the exciton Bohr radius. This confinement induces discrete electronic structures, more akin to the quantized energy levels observed in single atoms and size-dependent blue shift in optical absorption and emission with decreasing dot sizes, as shown in Figure 1, enabling continuous tuning of the band gap through precise control of particle size, an effect central to many emerging optoelectronic applications.

The Effective-Mass Approximation (EMA) form of the Brus equation [1] offers a simple and widely used analytical framework to relate quantum dot radius to the optical gap, combining a kinetic (confinement) term with an electron–hole Coulomb correction. Among colloidal QDs, lead chalcogenides (PbS, PbSe, PbTe) stand out for their narrow bulk band gaps, large exciton Bohr radii, and strong infrared absorption cross-sections [2]. These intrinsic properties make PbX QDs highly tunable across the Near- to Mid-Infrared (NIR–MIR) spectral regions for nanocrystal sizes typically ranging from 2 to 20 nm [3], driving intense interest for infrared photodetection, IR photovoltaics, and related optoelectronic applications [4].

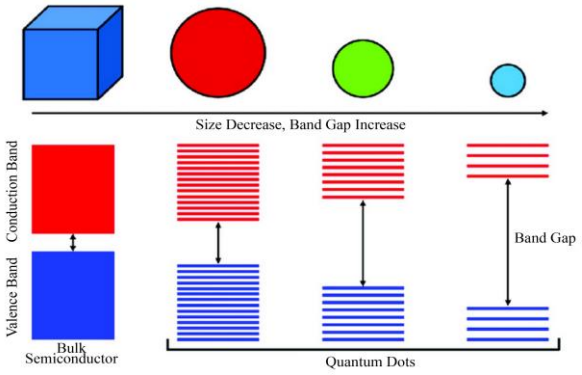

Fig. 1 Quantum confinement effect on the band gap of general semiconductors

Material-specific band-structure parameters dictate the magnitude of quantum confinement in each lead chalcogenide [5]. For instance, PbSe possesses a particularly large exciton Bohr radius (tens of nanometres), resulting in significant confinement even for relatively large nanocrystals. PbS, in contrast, exhibits strong tunability from the visible to Near-Infrared (NIR) range with modest size reduction. PbTe generally shows smaller blue shifts at comparable radii due to its large Bohr radius, distinctive effective masses, and dielectric screening, maintaining a narrow-gap character over a wider size range. These intrinsic differences directly determine which material and size regimes are best suited for specific device spectral windows [6].

Synthesis and surface chemistry critically influence measured optical gaps and device performance, so theoretical predictions must be interpreted in the context of ligand effects, surface traps, and the surrounding dielectric environment [7]. Colloidal synthetic approaches produce ligand-capped PbX QDs, where surface ligands strongly affect dielectric screening, trap densities, and inter-dot coupling. Therefore, controlled ligand exchange and inorganic passivation strategies are essential to translate size-predicted band gaps into high-performance devices [8]. Empirical studies consistently demonstrate that ligand engineering and film processing can govern photocarrier extraction, recombination dynamics, and device stability as much as the QD core size itself [9].

Despite significant experimental progress, important gaps remain that motivate a careful theoretical comparison using the Brus formalism. First, published device studies employ varying synthesis and ligand conditions, which shift optical features relative to idealized core-size predictions [10]. Second, material parameters in the Brus model, such as effective masses, dielectric constants, and Coulomb correction prefactors, differ across literature sources, leading to variations in predicted size–gap relationships. Third, PbTe has received comparatively less systematic modeling relative to PbS and PbSe using consistent parameter sets [11]. A unified, parameter-explicit Brus-equation analysis therefore enables (i) prediction of target QD radii for specific device spectral windows, (ii) identification of parameter sensitivities to determine which material constants most affect tunability, and (iii) assessment of how experimental surface and dielectric effects shift device performance relative to idealized predictions [12,13].

The present study aims to compute and compare the size-dependent optical gaps of PbS, PbSe, and PbTe quantum dots over a representative range of radii, and interpret these results in the context of practical device applications, including photodetectors, photovoltaics, infrared sensors, and thermoelectrics, thereby providing guidance for QD synthesis and device optimization.

2. Theoretical Framework

The size dependence of the Quantum Dot (QD) band gap is commonly described using the effective-mass approximation (EMA) form of the Brus equation. In its basic form, the Brus relation expresses the QD optical gap as the bulk band gap plus a positive confinement (kinetic) term, which scales approximately as $1/R^2$, and a negative Coulomb (electron–hole) interaction term, which scales roughly as 1/R. This simple analytical model captures the primary trend of a blue shift with decreasing radius and is widely employed to interpret experimental absorption and photoluminescence energies. For quantitative applications, the model parameters, including effective masses, dielectric constant, and exciton correction factor, must be selected specifically for each material. By balancing the quantum confinement-induced increase in band gap with the Coulombic attraction-induced reduction, the Brus equation provides a reliable estimation of semiconductor QD band gaps as a function of particle size, expressed as [14]:

$$E(R) = E_g^{bulk} + \frac{h^2\pi^2}{2R^2}\left(\frac{1}{m_e^*} + \frac{1}{m_h^*}\right) - \frac{1.8e^2}{4\pi\epsilon_0\epsilon_r R} \quad (1)$$

Where: E_g^{bulk}: bulk bandgap (eV), R: quantum dot radius (nm), m_e^* and m_h^*: effective masses of electron and hole ϵ_r: relative dielectric constant. The second term: quantum confinement contribution. The third term: Coulomb interaction correction

3. Materials and Methods

3.1. Materials

This study is entirely theoretical and simulation-based, utilizing experimentally reported material parameters for PbS, PbSe, and PbTe Quantum Dots (QDs). The key parameters required for the Brus equation were obtained from literature sources and are summarized in Table 1.

Table 1 The Group IV-VI QDs experimental parameters used for the study

Material	Bulk Band Gap (eV)	Electron Effective Mass (m_e)	Hole Effective Mass (m_h)	Relative Dielectric Constant (ε_r)	Exciton Bohr Radius (nm)
PbS	0.41	0.09 m_0	0.09 m_0	17.2	18–20
PbSe	0.27	0.08 m_0	0.07 m_0	23	46
PbTe	0.31	0.038 m_0	0.038 m_0	32	150

3.2. Methods

Quantum dot radii were varied from 2 nm to 10 nm to capture both strong quantum confinement at small radii and near-bulk behavior at larger radii.

This range was selected based on experimental synthesis reports, which indicate that stable colloidal QDs can be reliably produced within these dimensions. The Brus equation was then applied to model the size-dependent band gap for each quantum dot.

4. Results and Discussion

As shown in Figure 2, the band gaps of PbS, PbSe, and PbTe quantum dots exhibit a clear inverse relationship with particle radius, consistent with predictions from the Brus equation. Decreasing the radius enhances the quantum confinement of charge carriers, increasing the effective band gap. Conversely, as the radius increases, the band gap approaches the bulk value of each material. The magnitude of this size-dependent effect varies among the materials due to differences in effective masses, dielectric constants, and exciton Bohr radii.

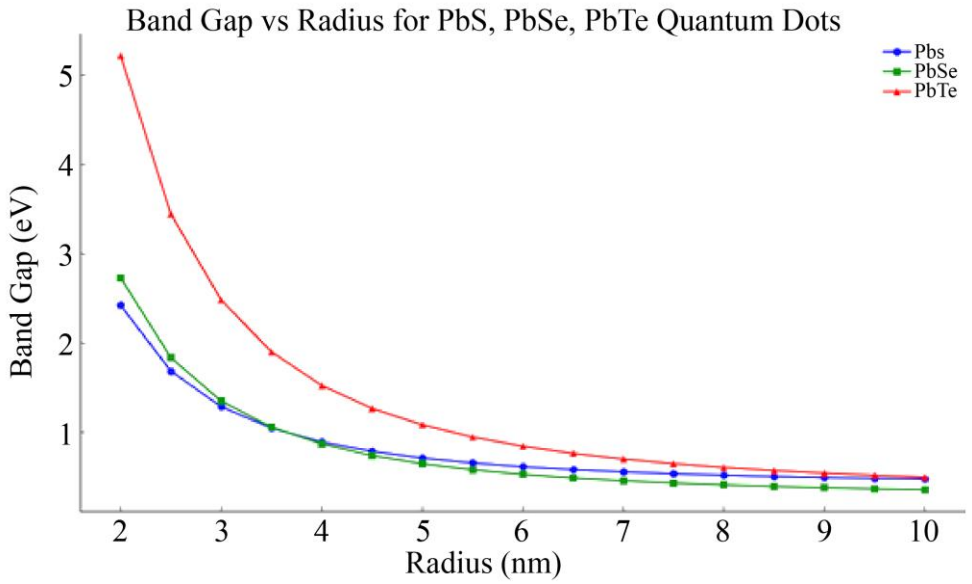

Fig. 2 Band gap of PbS, PbSe, and PbTe quantum dots versus radius

PbS quantum dots exhibit a steep increase in band gap as the radius decreases from ~10 nm to ~2 nm. At very small radii, the band gap shifts from the bulk value (~0.41 eV) into the visible–Near Infrared (NIR) range (>1 eV). This pronounced tunability makes PbS QDs highly suitable for third-generation solar cells, enabling efficient harvesting of both visible and NIR photons. They are also widely employed in NIR photodetectors and Light-Emitting Diodes (LEDs). The steep slope of the size–band gap curve reflects high sensitivity to small size changes, allowing precise band gap engineering for various optoelectronic applications.

PbSe QDs show a more moderate slope compared to PbS, with confinement effects still evident but less pronounced. The bulk band gap (~0.27 eV) can be tuned toward ~1 eV for small radii (≈2–3 nm). This tunability extends PbSe QDs deep into the Mid-Infrared (MIR) region, making them ideal for telecommunications detectors (1.3–1.55 μm), infrared imaging systems, and optical modulators. PbSe's intermediate slope in the graph highlights its versatility for devices requiring MIR sensitivity while still allowing integration into near-IR applications.

PbTe QDs exhibit the least variation in band gap with decreasing radius. Even at very small radii, the band gap remains relatively narrow (near the bulk value of ~0.31 eV). The comparatively flatter slope of PbTe's size–band gap curve reflects weaker quantum confinement. This persistence of narrow band gaps renders PbTe QDs particularly suitable for far-infrared detectors, thermoelectric generators, and low-temperature infrared lasers. The flatter slope indicates that PbTe's optimal device applications lie in niche infrared and energy-conversion technologies, where narrow gaps and strong phonon–electron interactions are advantageous.

5. Conclusion

The theoretical analysis of PbS, PbSe, and PbTe quantum dots using the Brus equation demonstrates the strong dependence of their electronic and optical properties on particle size. Band gaps increase significantly with decreasing radius due to quantum confinement. PbS QDs show the most pronounced tunability, making them ideal for visible-to-near-infrared applications such as solar cells, LEDs, and photodetectors. PbSe QDs exhibit intermediate behavior,

extending into the mid-infrared, and are well-suited for infrared sensors, modulators, and telecommunications devices. PbTe QDs maintain narrow band gaps even at small radii, highlighting their suitability for far-infrared detectors, thermoelectric devices, and specialized laser applications. Overall, this comparative study underscores the versatility of Group IV–VI lead chalcogenide QDs. By carefully controlling particle size, band gaps can be engineered to meet specific device requirements. These findings provide a theoretical foundation for optimizing PbS, PbSe, and PbTe QDs in practical optoelectronic, photonic, and energy-conversion technologies, bridging quantum size effects with real-world device performance.

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