Introduction

Quantum nanostructured materials have the potential to enact significant change in the most varied areas of research, from biomedical applications to solar cells and luminescent-down shifting [1,2]. Consequently, detailed overviews of their properties are fundamental to create a conducive path for practical implementations. In particular colloidal quantum dots have garnered particular attention for usage in quantum nanostructured applications, being thus a focus point for the authors in this work. Here we used the single band effective mass equation [3] to determine the absorption profile of a PbS quantum dot (QD) in a perovskite host and to study the behaviour of its 3 main parameters (potential barrier, effective mass, size). This approach was chosen due to the inherent simplicity of the employed method coupled with the important information that can be extracted from this analysis. It was thus ascertained that the size has the single biggest effect on the number and energy of the energy levels, while the potential barrier is mostly responsible for shifting these values. The absorption density was determined for QDs with radii of 1.6 and 2.5 nm. Here, the 2.5 nm QD was shown to have a higher absorption density and more allowed transitions. This work constitutes an unprecedented step for the detailed modelling of quantum nanostructures. Besides, the build-up of tools to simulate arbitrary QDs in a host material that opens new pathways to investigate a wide range of other promising material combinations.

Methodology

Effective Mass Equation

\[ -\frac{\hbar^2}{2m^*} \nabla^2 \Phi(r) + \left( E_{e,0} + \mu \right) \Phi(r) = E \Phi(r) \]

Energy Levels

Wavefunctions

Absorption Coefficient

\[ \alpha_{a\rightarrow f} = \frac{2\pi\hbar^2 k_a k_f}{\hbar \epsilon_0 c} \int |\psi_f(r)|^2 |\psi_a(r)|^2 \frac{d^3 r}{r} \]

\[ \delta(E_f - E_e - \hbar\omega) = \frac{1}{\sqrt{2\pi}} \int \frac{e^{i\mathbf{p} \cdot \mathbf{r}}}{\mathbf{p}} \delta(E_f - E_e - \hbar\omega) \frac{d^3 p}{(2\pi)^3} \]

Results

Parameter relations

Parameter Interaction

Absorption Coefficients

Conclusion

- The QD size has the single-most effect on the energy levels and how they are placed;
- The potential barrier is mostly responsible for shifting the energy levels, whereby higher potential barrier values leads to lower energies;
- The number of allowed transitions is mostly governed by the QD size and thus, only small sizes can lead to a minimal number of allowed optical transitions;
- Absorption with z-polarization is favored in detriment of left and right handed polarizations

References


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