

Progress Report: Numerical Modeling of Truncated Conical Quantum Dot Intermediate Band Solar Cells

1 Project Motivation and Objective

The objective of this project is to numerically investigate the role of **truncated conical quantum dot (QD) geometry** in enhancing the performance of **intermediate band solar cells (IBSCs)**. IBSCs aim to overcome the Shockley–Queisser limit by introducing an intermediate energy band within the host semiconductor bandgap, enabling sub-bandgap photon absorption via two-step optical transitions.

In this work, truncated conical quantum dots embedded in a III–V semiconductor host are studied as a practical and physically realizable approach to forming intermediate bands. **The study is strictly restricted to a single truncated conical quantum dot geometry.** Variations are introduced *only* through geometric parameters such as quantum dot height and barrier width, while the geometry type itself is kept fixed throughout the project.

It is explicitly emphasized that this work does **not** compare different quantum dot geometries (e.g., spherical, pyramidal, or cylindrical quantum dots). All simulations are performed within a unified truncated conical quantum dot framework, ensuring physical consistency and direct comparability with the reference literature.

2 Scientific Basis and Reference Framework

The modeling strategy and physical assumptions of this project are grounded in established IBSC theory and recent peer-reviewed literature, including:

- The detailed balance theory and intermediate band formalism developed by Martí and Ramiro [1].
- Drift–diffusion based semiconductor device modeling approaches for solar cells [2].
- Geometry-dependent quantum confinement effects in truncated conical quantum dots [3, 4].

- Numerical modeling of truncated conical QD-IBSCs using COMSOL Multiphysics [5].

The present project closely follows the physical model, truncated conical quantum dot geometry, and simulation strategy reported in [5]. The aim is to reproduce, numerically stabilize, and systematically extend those results through controlled parametric studies within the same geometry.

3 Physical Model

3.1 Quantum Mechanical Description

The electronic states inside the truncated conical quantum dots are described using the time-independent Schrödinger equation under the effective mass approximation:

$$\left[-\frac{\hbar^2}{2m^*} \nabla^2 + V(\mathbf{r}) \right] \psi(\mathbf{r}) = E\psi(\mathbf{r}), \quad (1)$$

where m^* is the carrier effective mass and $V(\mathbf{r})$ represents the confinement potential defined by the truncated conical quantum dot geometry.

The geometric parameters of the truncated cone (height, top radius, bottom radius, and barrier width) directly determine the intermediate band energy levels and wavefunction localization.

3.2 Carrier Transport Model

Carrier transport within the device is modeled using the coupled Poisson and drift-diffusion equations:

$$\nabla \cdot (\varepsilon \nabla \phi) = q(p - n + N_D - N_A), \quad (2)$$

$$\mathbf{J}_n = q\mu_n n \nabla \phi + qD_n \nabla n, \quad (3)$$

$$\mathbf{J}_p = q\mu_p p \nabla \phi - qD_p \nabla p. \quad (4)$$

Recombination mechanisms include Shockley–Read–Hall and Auger recombination, consistent with intermediate band solar cell theory.

4 Simulation Methodology

4.1 Numerical Platform

All simulations are performed using **COMSOL Multiphysics**, employing:

- The Semiconductor Module
- Stationary studies for DC bias analysis
- Physics-controlled solver settings for numerical robustness

Ohmic contacts are defined at the top and bottom of the device to allow carrier injection and extraction under applied bias conditions.

4.2 Baseline Device Structure

The baseline device structure consists of:

- A III–V semiconductor absorber layer
- Embedded truncated conical quantum dots acting as intermediate band states
- Barrier and wetting layers consistent with experimentally reported structures

The geometry is intentionally simplified to ensure numerical convergence while preserving all physically relevant material interfaces and confinement effects.

5 Current Progress

At the current stage of the project, the following milestones have been achieved:

- Construction of a stable baseline truncated conical QD-IBSC model.
- Successful numerical convergence under applied DC bias using stationary analysis.
- Extraction of initial current–voltage (J–V) characteristics.
- Establishment of a reproducible and robust numerical framework.

This corresponds to approximately **40% completion** of the overall project.

6 Ongoing and Planned Extensions

The next phase of the project focuses on systematic parametric studies **within the same truncated conical quantum dot geometry**, including:

- Parametric variation of truncated quantum dot height and its effect on short-circuit current density.
- Parametric variation of barrier width between truncated quantum dots to study carrier coupling and transport.

- Visualization of carrier concentration and electrostatic potential profiles under applied bias.

These studies will provide quantitative insight into geometry-induced performance optimization while maintaining a fixed quantum dot geometry type.

7 Conclusion

This project establishes a robust and physically consistent numerical framework for studying truncated conical quantum dot intermediate band solar cells. All results are obtained within a unified truncated conical quantum dot geometry, ensuring direct alignment with existing literature. The current findings validate the modeling approach and provide a solid foundation for systematic geometry-parameter optimization and further academic dissemination.

References

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