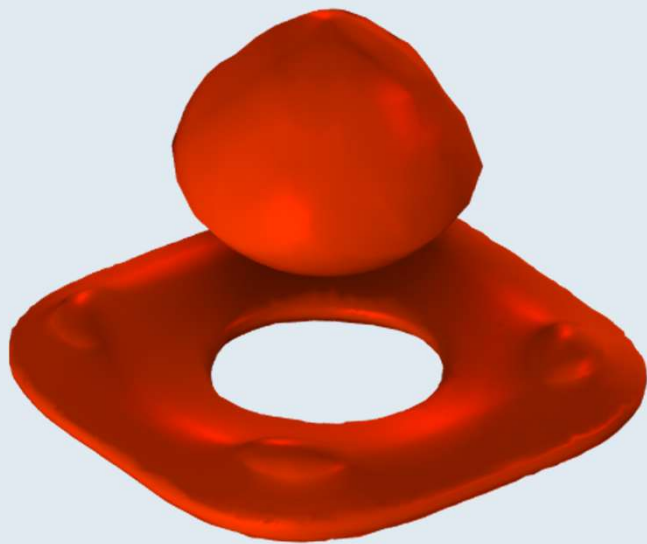




Modeling of Semiconductor Quantum Dots

COMSOL Multiphysics® Mathematics Models couple elasticity and the quantum Schrödinger equation to predict strain, carrier confinement bound-state energies, and wavefunctions in realistic self-assembled semiconductor quantum dots.

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Introduction & Goals

Semiconductor quantum dots provide discrete energy levels and tunable emission for lasers and LEDs. Their electronic states depend on strain, heterostructure geometry, material composition, and quantum confinement, making integrated simulation challenging. This work develops a unified COMSOL Multiphysics® framework to investigate strain effects, quantum-dot/wetting-layer coupling, and carrier bound states with various QD geometries. The simulator supports rapid parametric studies and device-design

iteration.

Goals: Develop a portable COMSOL-based framework to investigate

- strain and piezoelectric effects in semiconductor QDs [1],
- coupling between the quantum dot and wetting layer, and
- carrier bound-state energies and wavefunctions for realistic geometries and material systems [2].

Methodology

The model is implemented in COMSOL Multiphysics® using the Mathematics Module and Coefficient Form PDE interface. Continuum elasticity with three coupled PDEs and piezoelectric equations determine displacement, strain, polarization, and electrostatic fields, which modify the band-edge potential as shown in Figure 1.

Carrier states are then obtained from finite-element eigenvalue calculations. Electrons use an effective-mass model; holes are described by a four-band k·p Hamiltonian including heavy-hole/light-hole mixing. Pyramidal and lens-shaped III-V quantum dots with wetting layers can be modeled.

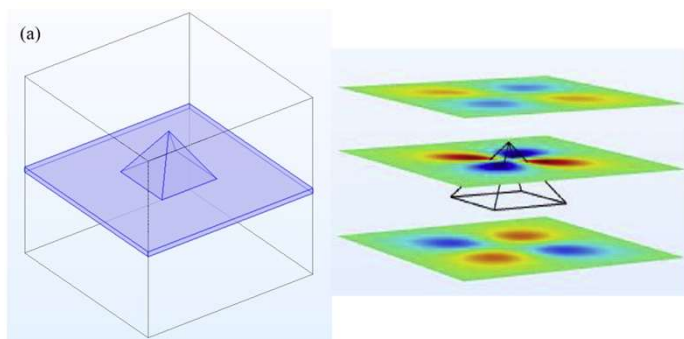


FIGURE 1. (a) A pyramidal InAs quantum dot surrounded by GaAs matrix. Beneath the quantum dot, there is a thin wetting layer. (b) Piezoelectric potential profiles from strain calculations.

Results

The COMSOL framework provides a unified solution for the mechanical and quantum-mechanical behavior of self-assembled semiconductor QDs. Simulations resolve strain-induced changes in the confinement potential and calculate carrier bound-state energies and spatial wavefunctions, including coupling between the QD and wetting layer as shown in Figure 2. The finite-element formulation enables direct investigation of the effects of QD geometry, dimensions, and material composition on carrier localization. The model supports pyramidal and lens-shaped III-V QDs and is designed for rapid parametric studies. Because all physics are implemented within the COMSOL environment, the workflow is portable, reproducible, and readily extendable to additional QD material systems and geometries.

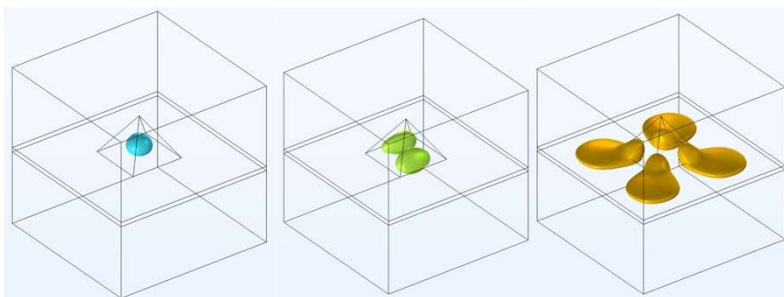


FIGURE 2. The isosurfaces of the wavefunction square for three different energy levels. The isosurface can be interpreted as the carrier distribution in the quantum dot. It is shown that at high energy, carriers leak out of the quantum dot into the wetting layer.

REFERENCES

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2. F. Gerner, E. Steeno, Z. Jensen, and W. Li, "An Efficient and Accurate Semiconductor Quantum Dot Model Implemented by COMSOL," *Phys. Status Solidi A*, vol. 223, no. 7, p. e202501005, 2026, doi: 10.1002/pssa.202501005.

