Quantum Dot Lab: An Online Platform for Quantum Dot Simulations

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Introduction

Self-assembled quantum dots have improved the performance of many optoelectronic devices such as infrared photodetectors and intermediate band solar cells [1], [2]. They offer the ability to tune device parameters by carefully adjusting device dimensions. Designing an optimal quantum dot for a specific purpose requires intensive simulation beforehand to get an idea on effect of various materials and dimensions on optical properties such as position of eigenstates and absorption spectrum. Quantum Dot Lab deployed on nanoHUB [3] provides such a simulation platform for the research community. The tool has the ability to simulate quantum dots ranging from simplistic particle in a box in effective mass approximation (EMA) till self-assembled quantum dots in 10-band sp3d5s* tight binding (TB) basis.

Tool Description

Quantum Dot Lab provides users the ability to choose between simulating a simple particle in a box problem in EMA, multilayered quantum dots comprising of a substrate, wetting layer, dot and a capping layer topology in both EMA and 10 band sp3d5s* TB basis with spin-orbit coupling. Different dimensions and materials for each region can be chosen as well. The tool solves Schrödinger's equation using the Lanczos method [4] to compute the eigenstates of the system. In multilayered device, in addition to Schrödinger's equation, a valence force field based strain model [5] is solved using PETSc Newton solver [6]. The relaxed atom positions are then calculated and incorporated into the TB Hamiltonian to get a physically reasonable answer for the eigenvalues. With the eigenstates and eigenvalues obtained, the optical absorption spectrum is calculated using Fermi's golden rule. The tool provides users the ability to vary different physical parameters such as temperature, Fermi level and polarization angles which affect the final absorption spectrum. The users can view/download results such as real space eigenfunctions, strain components, eigen energies, local bandstructure and absorption spectrum.

The tool runs within a Rappture interface [7] and uses the NEMO5 [8] simulation tool in the background to perform serial and parallel device calculations. Typical device dimensions that are simulated range from 10nm$\times$10nm$\times$10nm till 50nm$\times$50nm$\times$50nm run on a maximum of 256 cores.

Conclusion

An online platform for simulating quantum dots has been shown. The tool has been deployed on nanoHUB and can simulate quantum dots with varying degrees of complexity acting as a research and learning tool for the scientific community.

Acknowledgement

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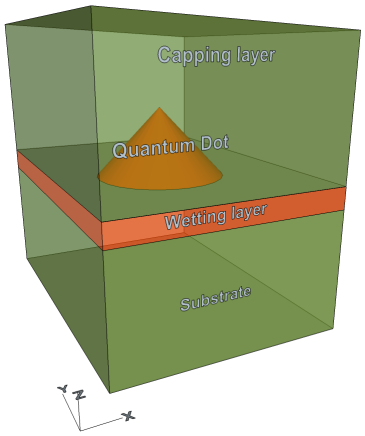

Fig. 1: Typical quantum dot structure simulated with the tool.

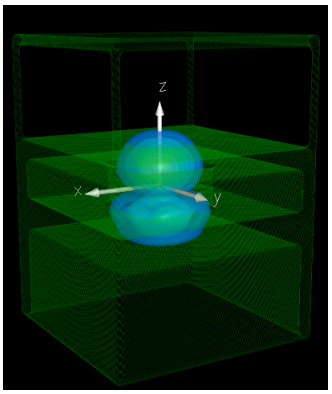

Fig. 2: Visualization of real space electronic wavefunction in the quantum dot structure.

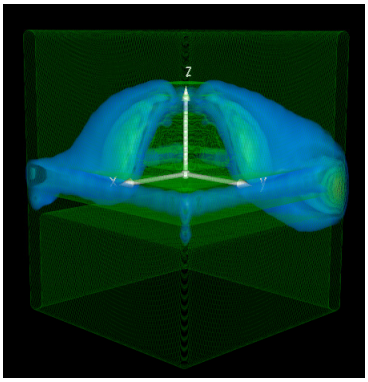

Fig. 3: Visualization of ϵ_{xz} strain component in the quantum dot structure.

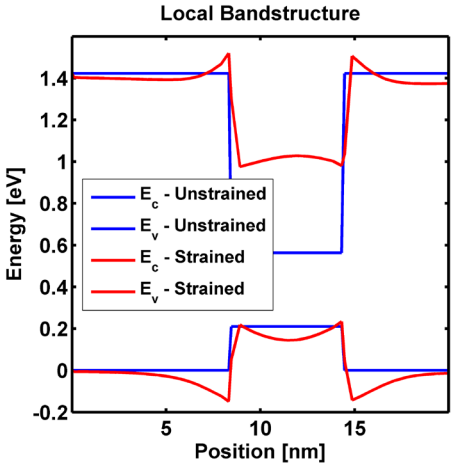

Fig. 4: Local bandstructure output showing the effect of strain on conduction and valence band edges.

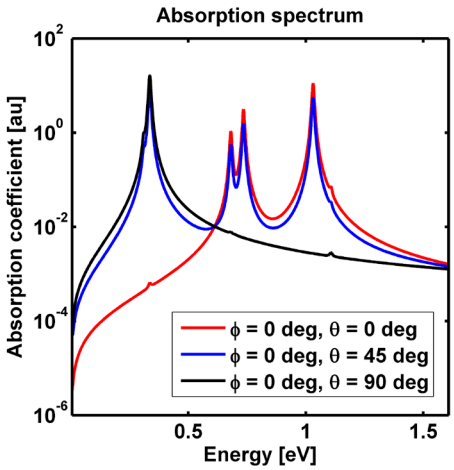

Fig. 5: Absorption spectrum plot. θ and ϕ correspond to the orientation of the polarization vector with respect to the quantum dot structure.

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