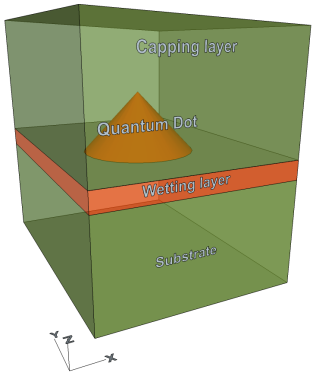
Quantum Dot Lab on nanoHUB

Motivation

Self-assembled QDs offer ability to optimize performance by changing device dimensions

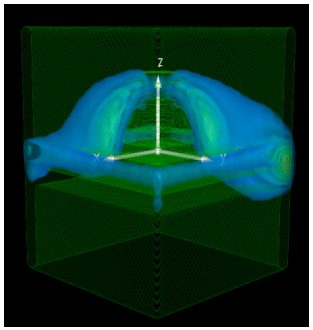
QD lab deployed on nanoHUB offers such a simulation platform

Simulations range from simplistic particle in a box problem to realistic structures in 10 band tight binding model



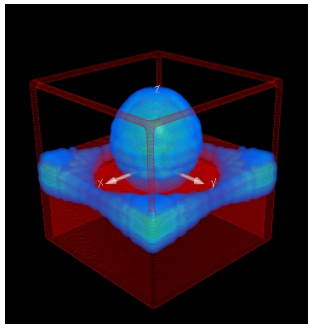
Strain Calculation

- Multilayer QD composed of different materials => Lattice mismatch and strain
- Alters the electron and hole energy levels
- Valence Force Field (VFF) based strain model with Keating potential used to solve for the relaxed atom positions

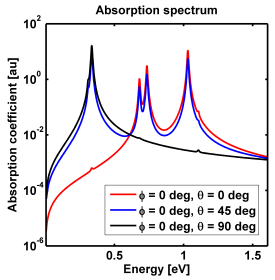


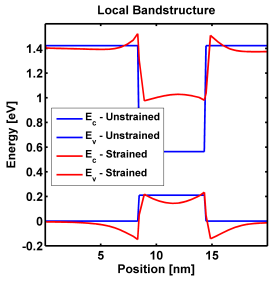
Confined states Calculation

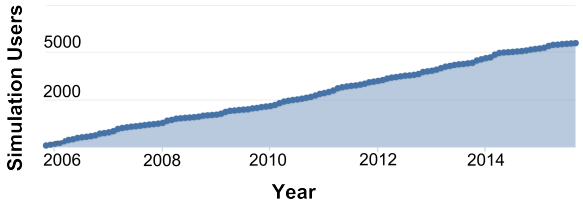
- Schrodinger's equation solved on the relaxed QD structure
- Can simulate both simplistic EM based model or a 10 band Tight Binding (TB) model in sp3d5s* basis (with SO coupling)
- Visualize the spatial distribution of electronic/hole wave functions



Output visualization and Usage







- Can obtain relevant outputs such as optical absorption spectrum, strain components and local bandstructure
- Used by 300+ users worldwide till date. More than 5000+ users since deployment of first version of tool in 2005.

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