nextnano³ - A powerful tool for the simulation of 3D nanometer semiconductor structures

T. Andlauer, M. Bayer, S. Birner, T. Kubis, J. A. Majewski, M. Sabathil, A. Trellakis (project leader), C. Uhl, P. Vogl, T. Zibold
Physik Department and Walter Schottky Institut, TU München

Capabilities Overview

- Calculation of electronic structure
- Calculation of current
- Calculation of excitation energies and optical matrix elements
- Magnetic fields and spin effects
- Global strain minimization
- Piezoelectric and pyroelectric charges
- Equilibrium and nonequilibrium systems
- Convenient graphical device editor
- Approx. 50 regular users worldwide

Program Flow

1. Database: material parameters
2. Input: structure, options
3. Deformation, band structure, strain and piezo/pyro
4. Determination of quasi Fermi levels
5. Determination of wave functions and bound states
6. Determination of quasi Fermi levels
7. Determination of optical spectra

Elastic deformations – Quantum wire

InGaAs quantum wire, grown on a patterned (311)-GaAs substrate

Piezoelectric charges and excitons in quantum dots

Self-assembled InAs/GaAs quantum dot, grown on (211)-GaAs substrate

Double-Gate MOSFET – Electronic States

Occupied electron state

Electron tunneling from quantum dots

Comparison experiment vs. theory

Ballistic current through a model resonant tunneling diode

T(E) near peaks converges rapidly
T(E) converges poorly in nonresonant regime, but current is dominated by resonance peaks
Calculation requires ~1-2 h on PC