Quantum Wires

Calculated wave functions ($\psi^2$) of the electron (e), heavy hole (hh) and light hole (lh) of a T-shaped quantum wire structure. One can clearly see the effect of the different effective-mass tensors that were used. The heavy hole wavefunction shows a strong anisotropy. It is possible to calculate the spatial overlap integral of the electron – heavy hole and electron – light hole envelope wave functions which is an important quantity to describe interband transitions.
Quantum Cascade Lasers

In quantum cascade lasers, strain can be used to alter the band offsets and thus the lasing wavelength. The nextnano software automatically determines the band offsets taking into account strain and deformation potentials and calculates the corresponding wave functions. The selection rules for intraband transitions are governed by the dipole matrix element between envelope functions.

The figure on the left shows the conduction band structure of a quantum cascade laser including the most important electron wave functions ($\psi^2$).

Quantum Dots

Pyramidal, hexagonal or lens shaped 3D quantum dots: Calculation of strain, piezo- and pyroelectric charges, self-consistent Schrödinger–Poisson equation for zinc blende and wurtzite materials. The figures show the electron and hole wave functions. An applied electric field leads to the separation of the electron and the hole (Quantum Confined Stark Effect).

The exciton correction in 1D quantum wells, 2D quantum wires and 3D quantum dots can be calculated.

Optical Absorption in Quantum Wells

The figures show the electron and hole eigenstates of a quantum well and the resulting absorption spectrum. The most prominent interband transitions are indicated. Excellent agreement with experiment has been achieved.

New Materials

New materials like GaAsN and InGaAsN that are obtained by introducing tiny amounts of nitrogen into the material systems GaAs and InGaAs show very interesting and unexpected properties. We successfully applied the nextnano software to systematically study quantum wells and quantum dots that are based on these materials. These efforts resulted in two publications in collaboration with the Corporate Research Division “Photonics” of Infineon Technologies AG (Munich, Germany).

Effects of strain and confinement on the emission wavelength of InAs quantum dots due to a GaAs$_{1-x}$N$_x$ capping layer

Bound-to-bound and bound-to-free transitions in surface photovoltage spectra: Determination of the band offsets for In$_{2-y}$Ga$_y$As and In$_{2-y}$Ga$_y$As$_x$N$_{1-x}$ quantum wells
M. Galluppi, L. Geelhaar, H. Riechert, M. Hetterich, A. Grau, S. Biner, W. Stolz
Physical Review B 72, 155324 (2005)
Energy Dispersion

Calculation of the energy dispersion \( E(k) \) of both zinc blende and wurtzite materials including strain and arbitrary crystallographic growth directions within 8x8 \( k \cdot p \) theory.

![Energy Dispersion Graph]

Strained Silicon / SiGe

Calculation of biaxial tensile and compressive strain and its effect on the energy dispersion \( E(k) \) of electrons and holes within 8x8 \( k \cdot p \) theory. It is also possible to read in arbitrary strain tensors (e.g. uniaxial strain along \([100]\) direction).

![Strained Silicon Graph]

Double Gate MOSFETs

Together with the Corporate Research Division “Nano Devices” of Infineon Technologies AG (Munich, Germany) we performed simulations on two- and three-dimensional MOSFETs (metal-oxide semiconductor field effect transistors). We successfully reproduced the current–voltage characteristics of commercial 2D device simulators.

![Double Gate MOSFET Diagram]

Superlattices

Calculation of miniband dispersions in superlattices in one, two and three dimensions.

![Superlattices Graph]

Bio Chips

Possible applications of semiconductor–electrolyte systems, so-called ISFETs (Ion-Sensitive Field Effect Transistor) are:
- Electrolyte Gate AlGaN/GaN Field Effect Transistor as pH sensor
- Detection of proteins with SOI (silicon-on-insulator) electrolyte sensor

Features
- Site-binding model to describe surface charges at semiconductor–electrolyte interfaces
- Self-consistent Poisson–Boltzmann equation to calculate the ion distribution in electrolytes

AIAs, GaAs, InAs, AlP, GaP, InP, AlSb, GaSb, InSb, AlGaAs, AlGaInP, ...
Business idea
Software for the simulation of electronic and optoelectronic semiconductor nanodevices and materials

Vision
“To establish the nextnano software as the de facto standard simulator for the next generation of semiconductor nanodevices and materials.”

Founder
Dr. Stefan Birner studied Physics at the universities of Bayreuth (Germany), Exeter (UK), Ohio State (USA) and the Technische Universität München (Germany). During his studies, he gained experience through internships at companies such as Infineon Technologies and Genius CAD-Software.

Stefan holds a Master of Physics degree from the University of Exeter and a PhD in Physics from the Technische Universität München where he worked at the Walter Schottky Institute in the field of Theoretical Semiconductor Physics under the supervision of Prof. Peter Vogl. He has several years of international experience in the field of semiconductor simulation. Through competent partners at universities he has access to a large network of know-how in this field.

After having received financial support through the EXIST-SEED program “University-based start-ups” of the German Federal Ministry of Education and Research (BMBF), Stefan founded in October 2012 the nextnano GmbH where he serves as the CEO since November 2012.

Applications
Quantum cascade lasers, quantum dots, nano-MOSFETs, strained silicon, LEDs, nitride materials, infrared detectors, biosensors, …

Disruptive technologies
The nextnano GmbH acts in new markets: nanowires, biochips, efficient solar cells, organic semiconductors, nanocrystals, gas sensors, spintronics, quantum computing, …

Executive Summary
The business idea of the nextnano GmbH is the development of software for the simulation of electronic and optoelectronic semiconductor nanodevices and materials (e.g., transistors, resonant tunneling diodes, quantum dots, quantum wires, quantum cascade lasers). Due to the continuing scaling of semiconductor electronics, quantum physical effects are gaining importance and confront the industry with fundamental challenges with respect to simulation and design.

Our unique selling proposition is an advanced physical method for the calculation of the quantum mechanical properties of an arbitrary combination of geometries and materials. The nextnano software is not limited to certain types of devices and thus perfectly suited for both, currently existing devices and novel devices, like for instance protein sensors (biochips). Our customers benefit from faster (time-to-market) and cheaper development of devices.

The nextnano GmbH is a spin-off from the Walter Schottky Institute of the Technische Universität München, Germany (Chair for Theoretical Semiconductor Physics, Prof. Peter Vogl).

Customers
Our customers are the research labs of the leading semiconductor companies. Numerous top-notch universities are among our customers.

Customers’ benefits
• better understanding of device physics
• systematically improve and optimize devices
• less redesign cycles (optimum prototype)

Customer feedback
“One reason that the nextnano software is so good at nanoelectronics is that it was not designed for nanoelectronics. It was designed to do physics.”