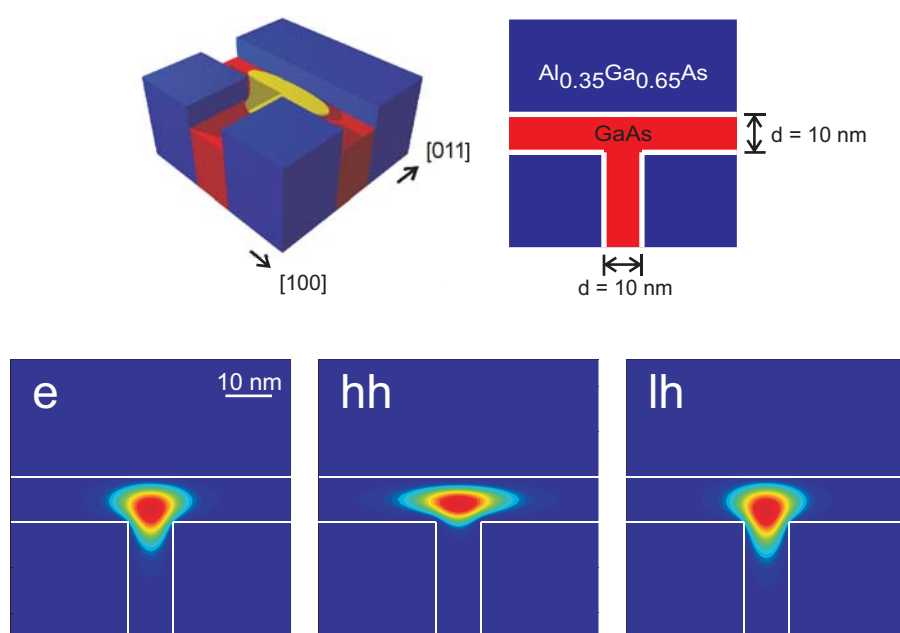


a powerful tool for the simulation of semiconductor nanostructures

## Quantum Wires

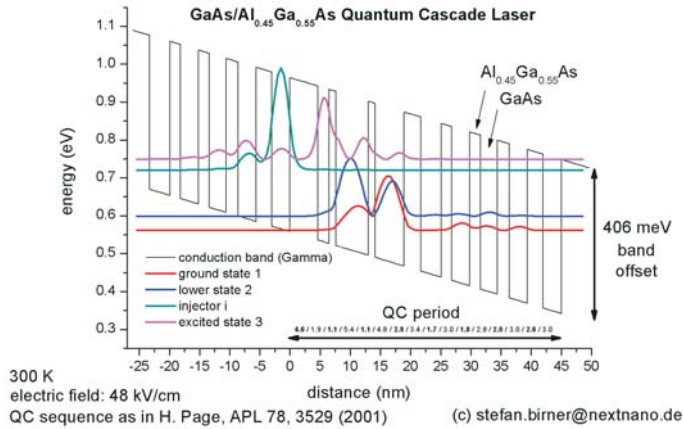


Calculated wavefunctions ( $\psi^2$ ) of the electron (e), heavy hole (hh) and light hole (lh) of a T-shaped quantum wire structure. One can clearly see the effect of the different effective-mass tensors that were used. The heavy hole wavefunction shows a strong anisotropy. It is possible to calculate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

# Quantum Cascade Lasers

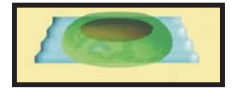
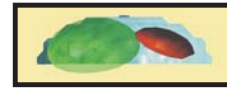
In quantum cascade lasers, strain can be used to alter the band offsets and thus the lasing wavelength. *nextnano*<sup>3</sup> automatically determines the band offsets taking into account strain and deformation potentials and calculates the corresponding wavefunctions. The selection rules for intraband 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 ( $\psi^2$ ).



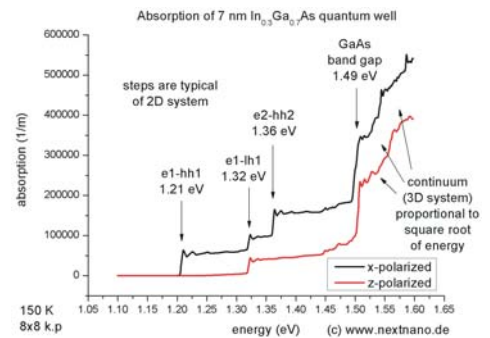
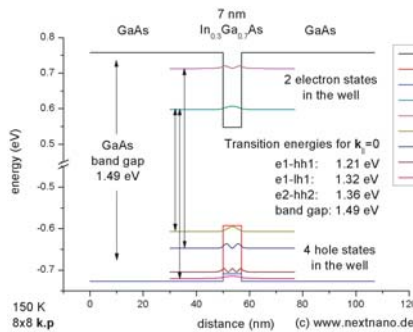
# Quantum Dots

Pyramidal, hexagonal or lens shaped 3D quantum dots: Calculation of strain, piezo- and pyroelectric charges, self-consistent Schrödinger-Poisson equation for zincblende and wurtzite materials. The figures show the electron and hole wavefunctions. 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 *nextnano*<sup>3</sup> 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).

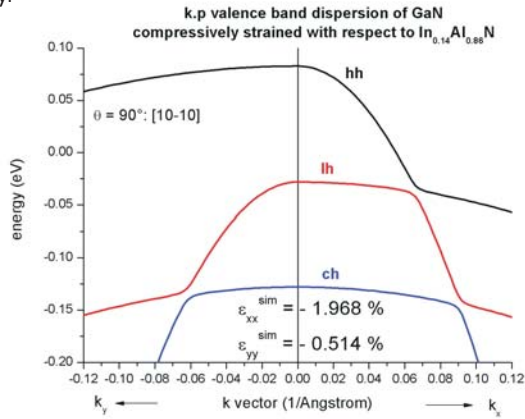
Effects of strain and confinement on the emission wavelength of InAs quantum dots due to a GaAs<sub>1-x</sub>N<sub>x</sub> capping layer  
 O. Schumann, S. Birner, M. Baudach, L. Geelhaar, H. Eisele, L. Ivanova, R. Timm, A. Lenz, S.K. Becker, M. Povolotsky, M. Dähne, G. Abstreiter, H. Riecher  
 Physical Review B **71**, 245316 (2005) & Virtual Journal of Nanoscale Science Technology **12** (1) (2005)

Excited states and band offsets in InGaAs(N) quantum wells determined by surface photovoltage measurements  
 M. Galluppi, L. Geelhaar, H. Riecher, M. Hetterich, A. Grau, S. Birner, W. Stolz  
 accepted for publication in Physical Review B

Si, Ge, Si<sub>1-x</sub>Ge<sub>x</sub>, GaN, AlN, InN, Al<sub>x</sub>Ga<sub>1-x</sub>N, Al<sub>x</sub>Ga<sub>1-x</sub>In<sub>1-x-y</sub>N,...

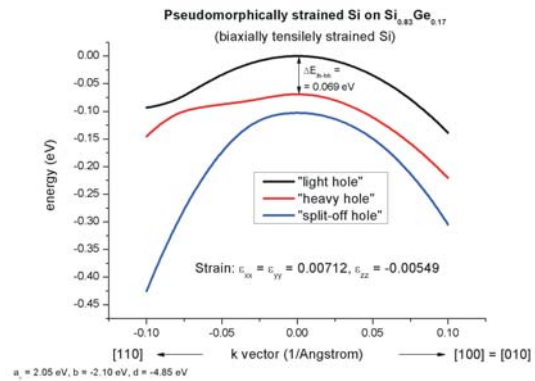
## Energy Dispersion

Calculation of the energy dispersion  $E(\mathbf{k})$  of both zincblende and wurtzite materials including strain and arbitrary crystallographic growth directions within  $8 \times 8$   $\mathbf{k}, \mathbf{p}$  theory.



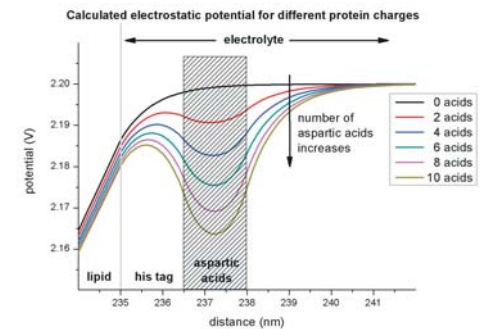
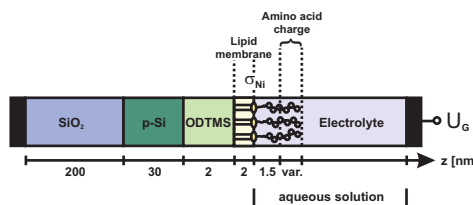
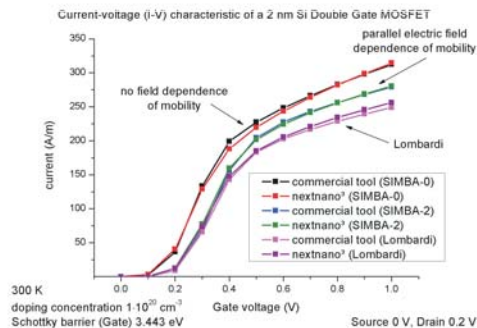
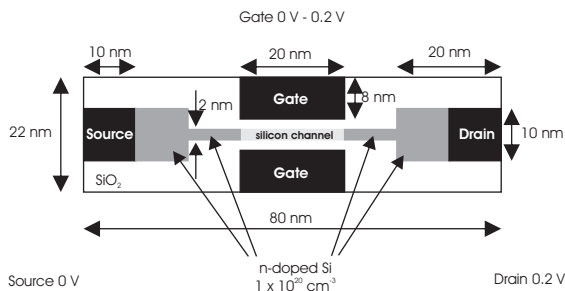
## Strained Silicon / SiGe

Calculation of biaxial tensile and compressive strain and its effect on the energy dispersion  $E(\mathbf{k})$  of electrons and holes within  $8 \times 8$   $\mathbf{k}, \mathbf{p}$  theory. It is also possible to read in arbitrary strain tensors (e.g. uniaxial strain along  $[110]$  direction).



## 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 transistor). We successfully reproduced the current-voltage characteristics of commercial 2D device simulators.



## Superlattices

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

## Bio Chips

Possible applications of semiconductor/electrolyte systems, so-called ISFETs (Ion-Sensitive Field Effect Transistor) are:

- Electrolyte Gate AlGaIn/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 nano devices and materials

**Vision**

"To establish nextnano<sup>3</sup> as the de facto standard simulator for the next generation of electronic and optoelectronic semiconductor nano devices and materials."

**Founder**

Stefan Birner, MPhys, has several years of international experience in the field of semiconductor simulation. Through competent partners at universities and industry he has access to a large network of know-how in this field.

**Partner**

Prof. Dr. Peter Vogl  
Chair for Theoretical Semiconductor Physics  
Walter Schottky Institute  
Physics Department  
Technische Universität München  
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**Project support**

nextnano<sup>3</sup> receives financial support from the German Federal Ministry of Education and Research (BMBF).

**Milestones**

- 2004: Spin-off Walter Schottky Institute
- 2004: Projects with Infineon Technologies
- 2005: Bio chips
- 2006: Expansion

**Market**

The annual, worldwide revenue in the TCAD (Technology CAD) market is about €100 million.

- Growth EDA (2004) 0 %
- Growth TCAD 10 %
- Growth Emerging Devices 50 %

**Executive Summary**

The business idea of nextnano<sup>3</sup> is the development of software for the simulation of electronic and optoelectronic semiconductor nano devices and materials (e.g. transistors, resonant tunneling diodes, quantum dots, quantum wires, quantum cascade lasers). Due to the continuing downscaling of semiconductor electronics, quantum physical effects are gaining importance and confront the industry with fundamental challenges with respect to simulation and design. Existing tools cannot cope with these challenges and alternatives are not in sight.

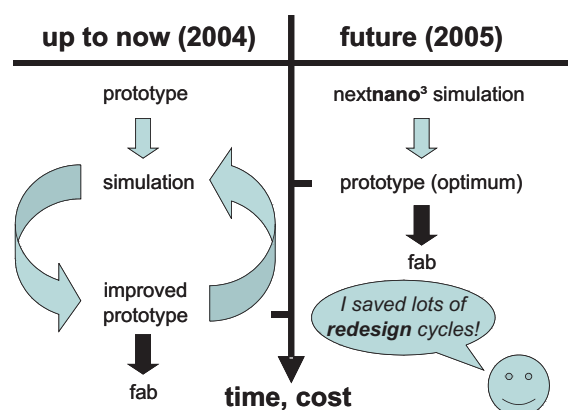
Our unique selling proposition is a better physical method for the calculation of the **quantum mechanical properties** of an arbitrary combination of geometries and materials, i.e. nextnano<sup>3</sup> is not limited to certain types of devices and thus perfectly suited for both, currently existing devices and novel devices, like for instance protein sensors (bio chips).

**Customers**

Our customers are the research labs of the leading semiconductor companies. So far we had successful projects with **Lucent Technologies** (Bell Labs) and **Infineon Technologies** on quantum cascade lasers, quantum wells and quantum dots.

**Customers' benefits**

- better understanding of device physics
- systematically improve and optimize devices
- less redesign cycles (optimum prototype)



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**Postal address**

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