Nextnano: a predictive tool for mesoscopic semiconductor structures

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www.nextnano.de

nextnano overview

Goal: Provide quick global insight into basic physical properties of mesoscopic semiconductor structures

Simulation software for 3D semiconductor nanostructures

- Si/Ge and III-V materials, Nitrides, alloys, zb and wz
- Flexible structures and geometries
- Quantum mechanical electronic structure
- Equilibrium properties and carrier transport
- Typically 5-10 downloads/day worldwide

Calculation of electronic structure

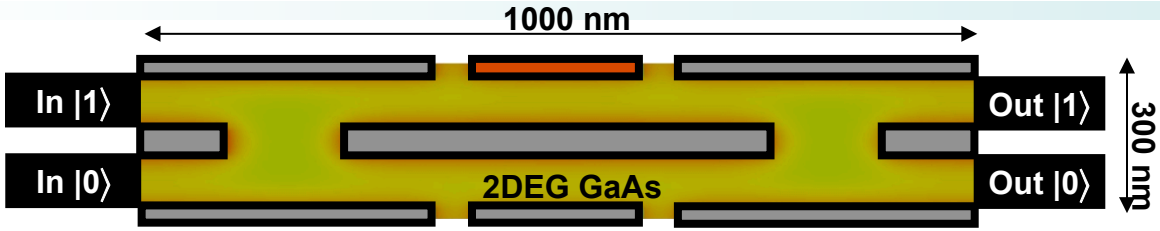
- 8-band k.p-Schrödinger (+LDA) and Poisson equation
- Global strain minimization
- Piezoelectric, pyroelectric charges, deformation potentials
- Exciton energies and optical matrix elements
- Magnetic field and spin effects
- ISFET: Surface reactions @ semicond./electrolyte interfaces

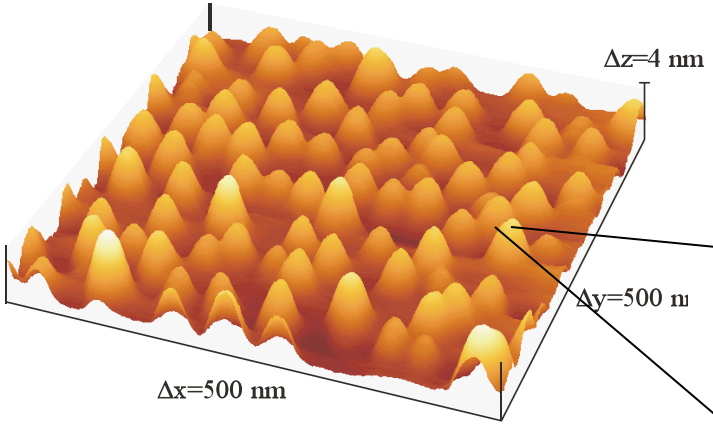
Calculation of charge current

- Quantum-drift-diffusion method : DD eq's + quantum densities
- Ballistic current through open systems: Contact Block Reduction
- Full quantum transport with scattering: NEGF for quasi-1D

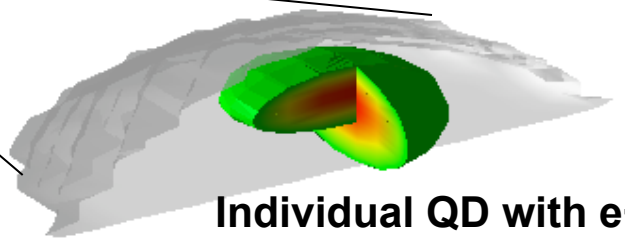
Examples of nanostructures

Mach-Zehnder-interferometer

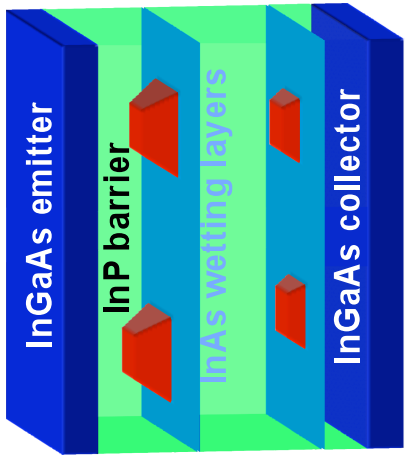




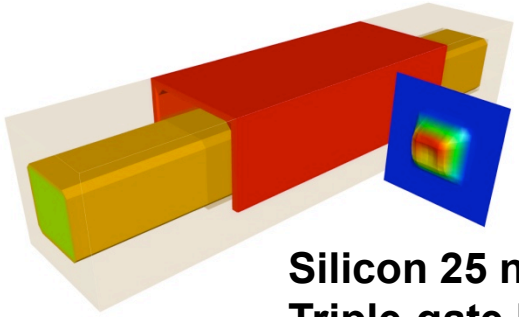
Self-assembled quantum dot array



Individual QD with e+h wave functions



Quantum dot-resonant tunneling diode



Silicon 25 nm Triple-gate FET

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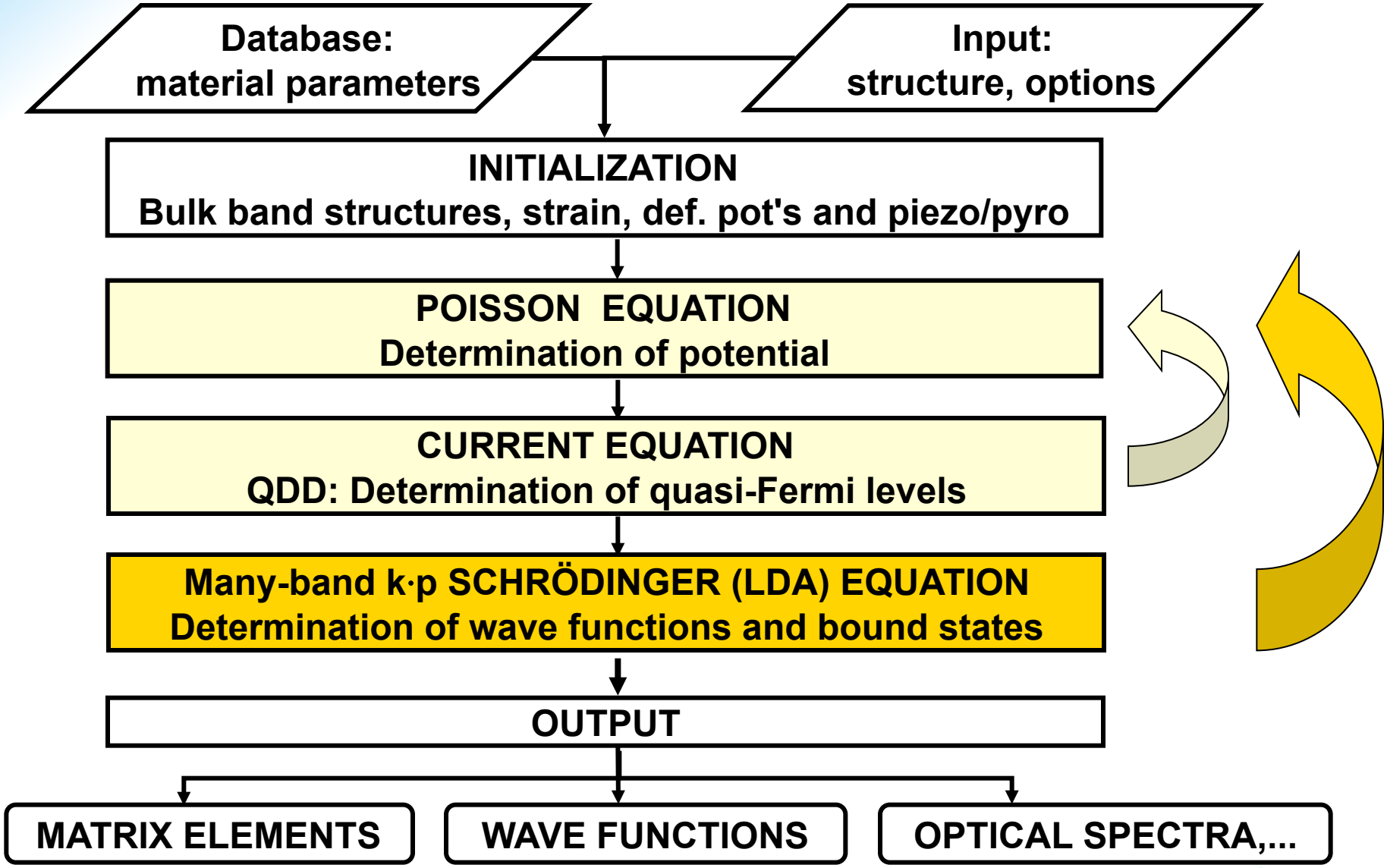
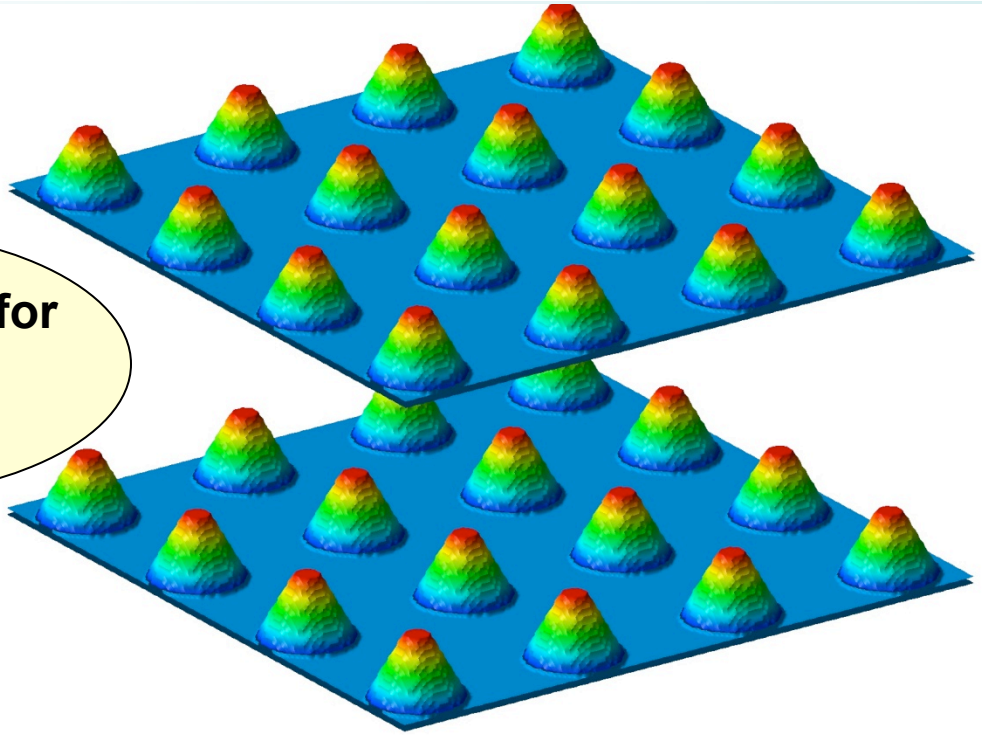
nextnano Program flow



Compact geometry definition in input

User-Input: ASCII file defines geometry and materials

20 lines suffice for such a complex structure



- **Input file can be split up into template + very small steering file**
- **Parsed input is piped through validator (analogously to XML)**
- **Parser checks for syntax, validator checks content**

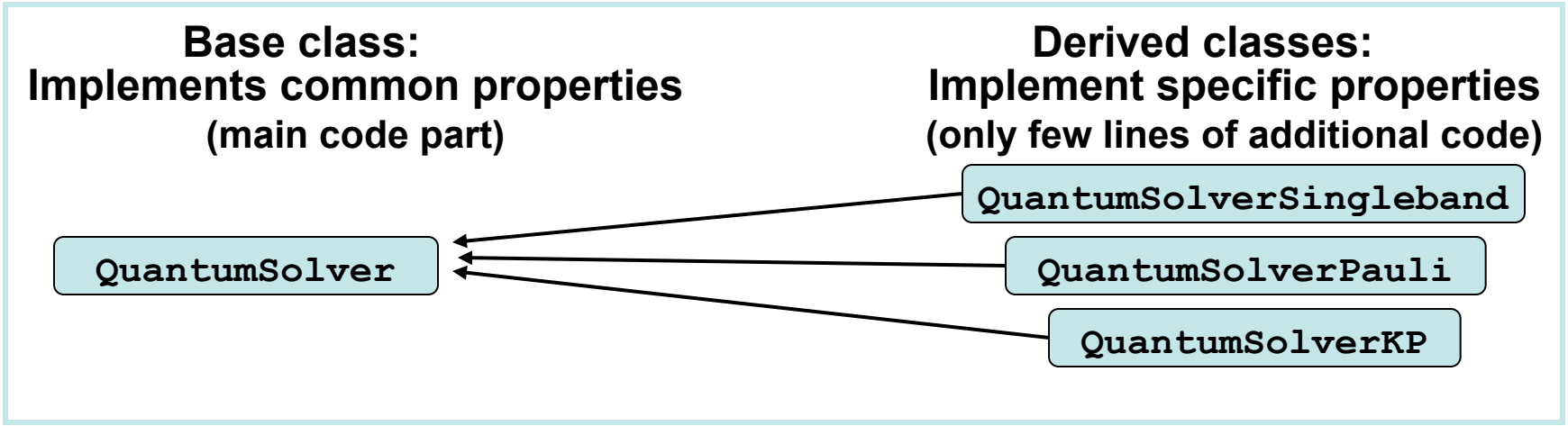
nextnano++ code structure

Old version is nextnano³: 250 K lines of F90 code, 400 files

New version: nextnano++ (written in C++)

- **Fully object-oriented design:**
  easy to maintain & to extend, reusable code
- **Use of generic programming:**
  single implementation for many types of data
- **Only 30K lines (without libraries)**
- **Typically 10 times faster**

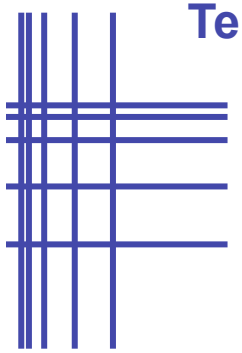
Example of object oriented schemes:



Numerical principles and techniques

Use state-of-the-art sparse linear systems solvers, CG methods , subspace projection methods for eigenvalue problems, but many still need significant improvements in efficiency for $N > 10^6$

Discretization:

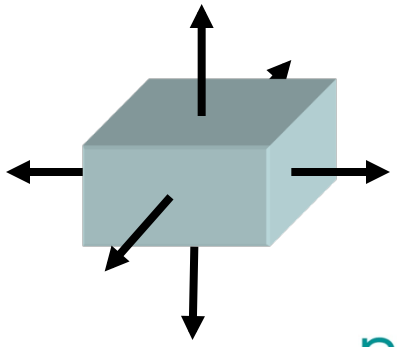


Tensor Grid

- **Robust, easy to control**
- **Nanostructures are edgy on nm-scale**
- **Schr. eq, Poisson eq., Elast. eq., smoothens interfaces**

Box integration technique:

- **div F(x) = k(x)** ⇒ $\int\int \mathbf{F} \cdot d\mathbf{A} = \langle k \rangle V$
- **Typically 100^d boxes = "nodes"**



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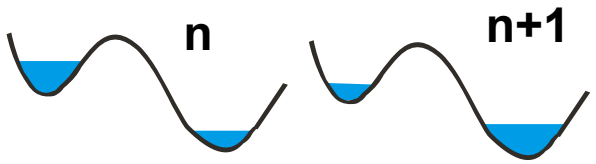
Numerical principles and techniques

Iterative Schrödinger-Poisson solution

$H[\phi]\,\psi_i = E_i\,\psi_i$ Schrödinger eqn.

$\Delta\phi = \rho[\phi, \psi]$ Nonlinear Poisson eqn.

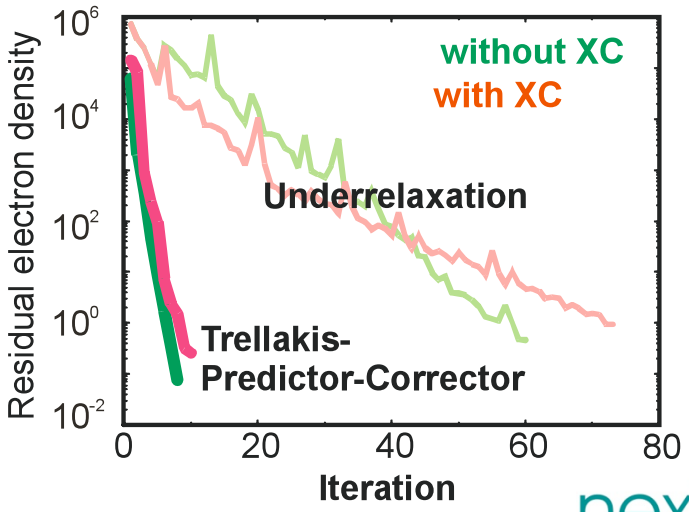


Problem: Slowly convergent with underrelaxation (charge sloshing)

Solution: Predictor-corrector procedure* + subspace iteration

1) Use perturbation theory to predict approx. $\tilde{\rho}[\phi]$ from ψ_i
2) Solve Poisson equation using $\tilde{\rho}$
3) Calculate correct $\rho[\phi]$ by solving Schrödinger equation
4) Each nth cycle (n~2), diagonalize H in subspace of previous iteration

- **Adaptive underrelaxation: slow, worse with V_{xc}**
- **Predictor-corrector: fast, no penalty for V_{xc}**



*Trellakis, JAP 81, 7880 (97)

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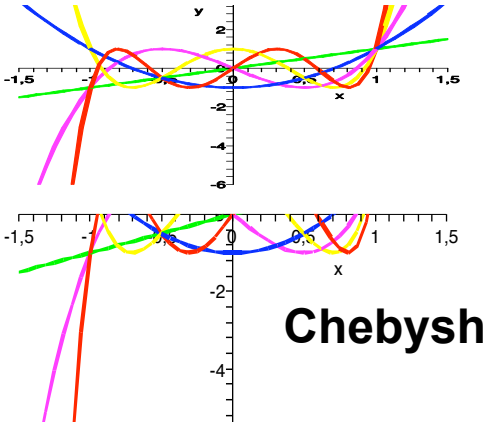
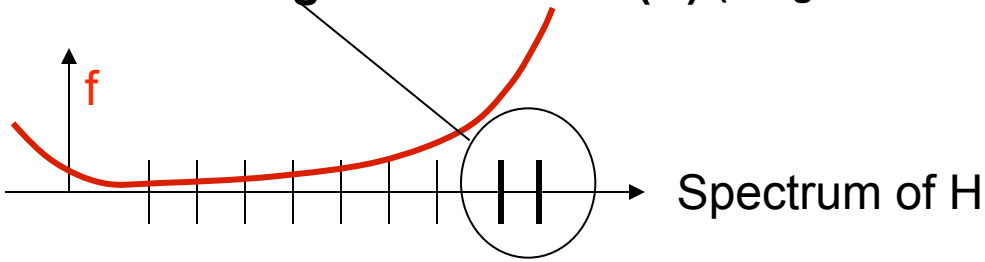
Numerical principles and techniques

Spectral transform for extremal eigenvalues:

- **Find H → f(H) that isolates large eigenvalues and their eigenvectors**
- **Calculate eigenvalues of H from eigenvectors of f(H) (= eigenvectors of H)**





Chebyshev polynomials $T_n(x)$

Excellent choice for f(H) for extremal eigenvalues:

- **Chebyshev spectral transformation (Kerkhoven et al 1993)**
- **Accelerates solution by at least factor of 10 for 2D problem**
- **$N=10^6$, 10 (30) E_n, 3Ghz P4, SC: 100 s (250 s)**

Best method for interior evals still not clear, currently use ARPACK: very robust, degenerate evals, but fairly slow.

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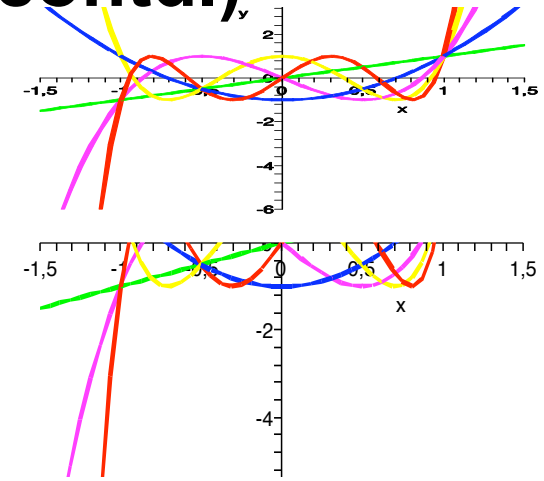
3.4. Solving the Schrödinger equations (contd.)



$$|T_n(x)| \le 1 \qquad ,|x| \le 1$$

$$|T_n(x)| > 1 \qquad ,|x| > 1$$

$$|T_n(x)| \propto x^n \qquad ,|x| \gg 1$$

Kerkhoven et al 1993

Chebyshev spectral transformation:

$$T_n\left(2\frac{\hat{H}-E_{cut}}{E_{\max}-E_{cut}}-1\right)\psi_m = \tilde{E}_m\psi_m$$

- **Suppression of unwanted eigenvals $E>E_{cut}$**
- **Enhancement of low-end eigenvals $E<E_{cut}$**

$$E_{\max} = \max_i\left(H_{ii}+\sum_{j\neq i}|H_{ij}|\right)$$

Gerschgorin upper eigenvalue bound

$$E_{cut} \approx E_F + 10k_BT$$

energy cutoff

$$E_m = \frac{\langle\psi_m|\hat{H}|\psi_m\rangle}{\langle\psi_m|\psi_m\rangle}$$

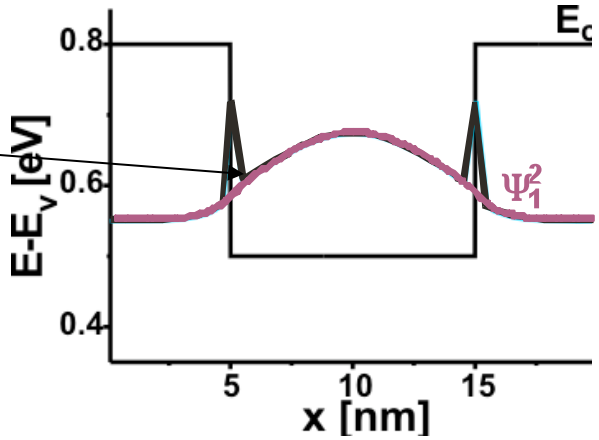
- **Use ARPACK on transformed problem to get ψ_n.**
- **Evaluate matrix polynomials using recursion.**
- **After running ARPACK determine eigenvals E_n.**

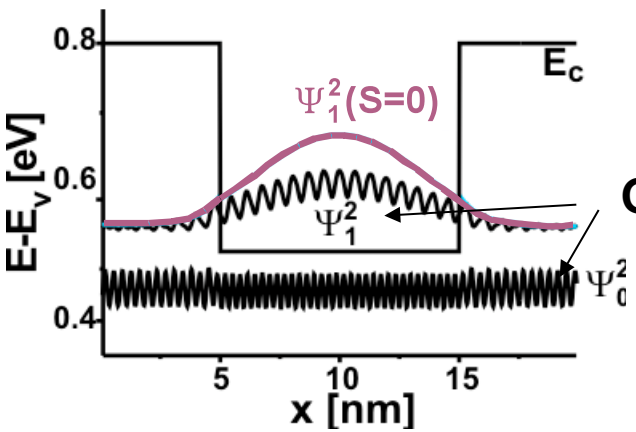
Electronic structure principles and techniques

Multiband k.p envelope function approach

- Based on "patching up" bulk Hamiltonians to build Hamiltonian for mesoscopic structures, is efficient and sufficiently accurate
- Method has built-in ambiguities that can lead to ghost states, spikes in density,...
- Spatial discretization can lead to instabilities and wrong oscillatory solutions

Spikes





Have eliminated artifacts in k.p+envelope function theory by

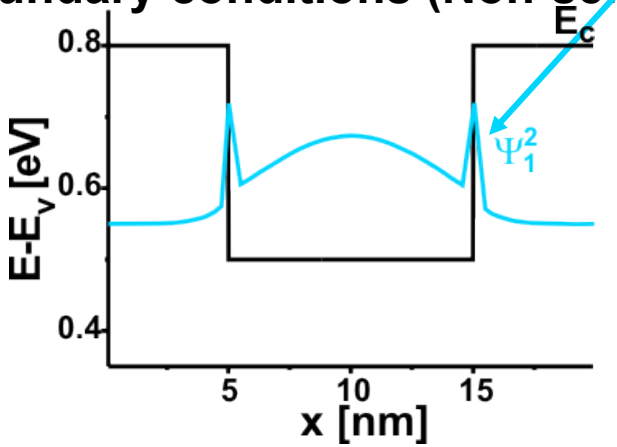
- careful treatment of far-band contributions
- using operator orderings that are manifestly self-adjoint
- employing upwinding scheme for discretizing derivatives

Multivalued operator ordering

$$H_{Vol}^{k\cdot p}(k) = \begin{vmatrix} E_c & i\,P\,k \\ -i\,P\,k & E_v + Lk^2 \end{vmatrix} \rightarrow H_{Vol}(\nabla):$$

$P(x)\,\partial/\partial x$ or
$\partial/\partial x\,P(x)$ or
$(P(x)\,\partial/\partial x + \partial/\partial x\,P(x))$

- Ordering unclear because of position dependent parameter P
- Different orderings yield Hermitian Ham., but cause contradictory boundary conditions (Non-self-adjointness)



Solution of Problem: Self-adjoint H

$$H_{Vol}(x) = \begin{vmatrix} E_c & P\,\partial/\partial x \\ -\partial/\partial x\,P & E_v - \partial/\partial x\,L\,\partial/\partial x \end{vmatrix}$$

Ref: B. A. Foreman, Phys. Rev. B 56, R12748 (1997)

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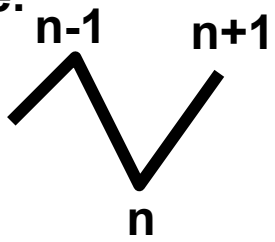
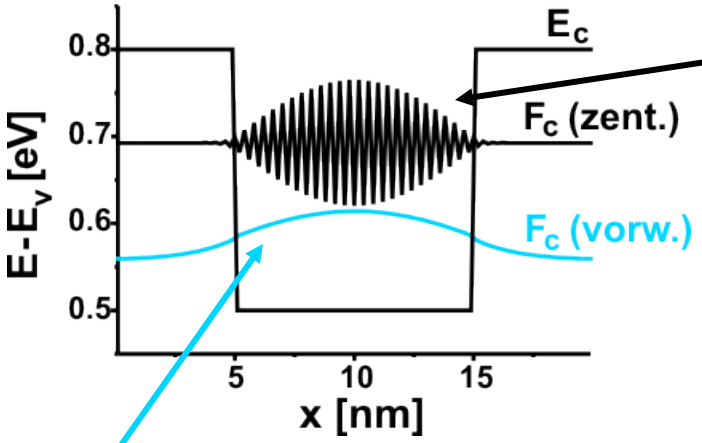
Electronic structure principles and techniques

Example: Eliminating oscillatory solutions

$H_{bulk}(k) \rightarrow H(\nabla)$: **Discretization of 1. derivates is not unique.**

$\nabla F(n) = F(n+1) - F(n-1)$ is compatible with





Solution:

$\nabla F(n) = \pm[F(n) - F(n \pm 1)]$ **excludes unphysical oscillatory solutions**

H = **Forward-Differencing** / **Backward-Differencing**

equivalent to upwinding scheme

Ref: Andlauer et al, to be publ.

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Electronic structure principles and techniques

Problem: How to solve Schrodinger equation for nanodevice in B-field?
Vector potential A(x) diverges with x ⇒ Discretized version of H violates gauge invariance ⇒ arbitrary results

$$H = \frac{(-i\partial + A(x))^2}{2m} + V(x)$$

Invariance under gauge transformation is violated if $\frac{\partial f}{\partial x} = \lim_{\varepsilon \to 0} \frac{f(x+\varepsilon) - f(x)}{\varepsilon}$

Solution:*

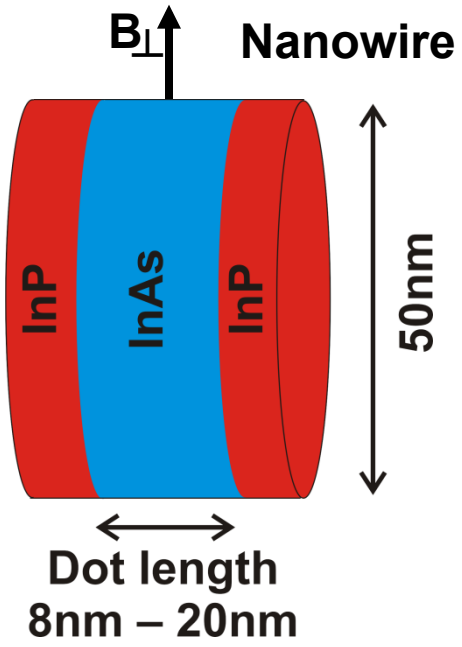
- Define $U(x,y) = \exp\left(-i \int_x^y A(z)\, dz \right)$
- Define $D = \frac{1}{\varepsilon}[f(x+\varepsilon) - U(x+\varepsilon,x)\, f(x)]$
- Use Hamiltonian $H = \frac{D^2}{2m} + V(x)$

guarantees local gauge invariance

- This Hamiltonian is gauge invariant and suitable for discretizing the Schrodinger equation in magnetic fields
- Works for any multi-band, relativistic k.p Hamilonian for nanostructures

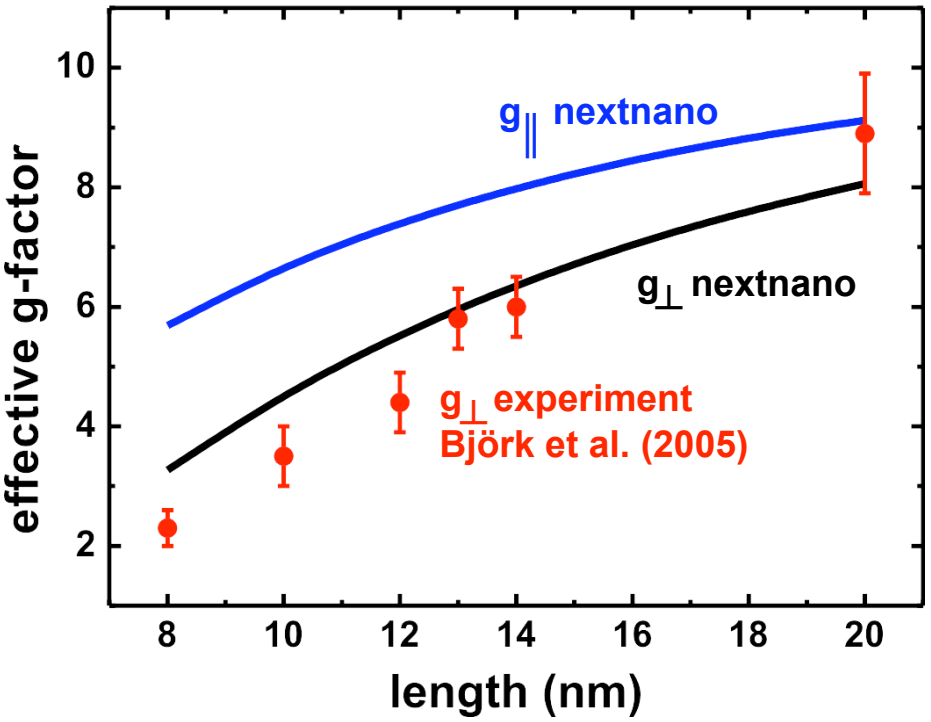
*) Morschl et al, to be publ.

Prediction of g-tensors in nanowire dots



Nonperturbative inclusion of B-Field into 8-band k.p method

Electron ground state g-factors



Excellent agreement between calculated g-factors and experiment without any fitting parameters

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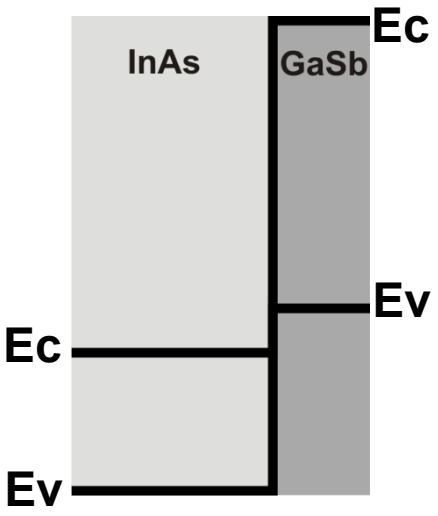
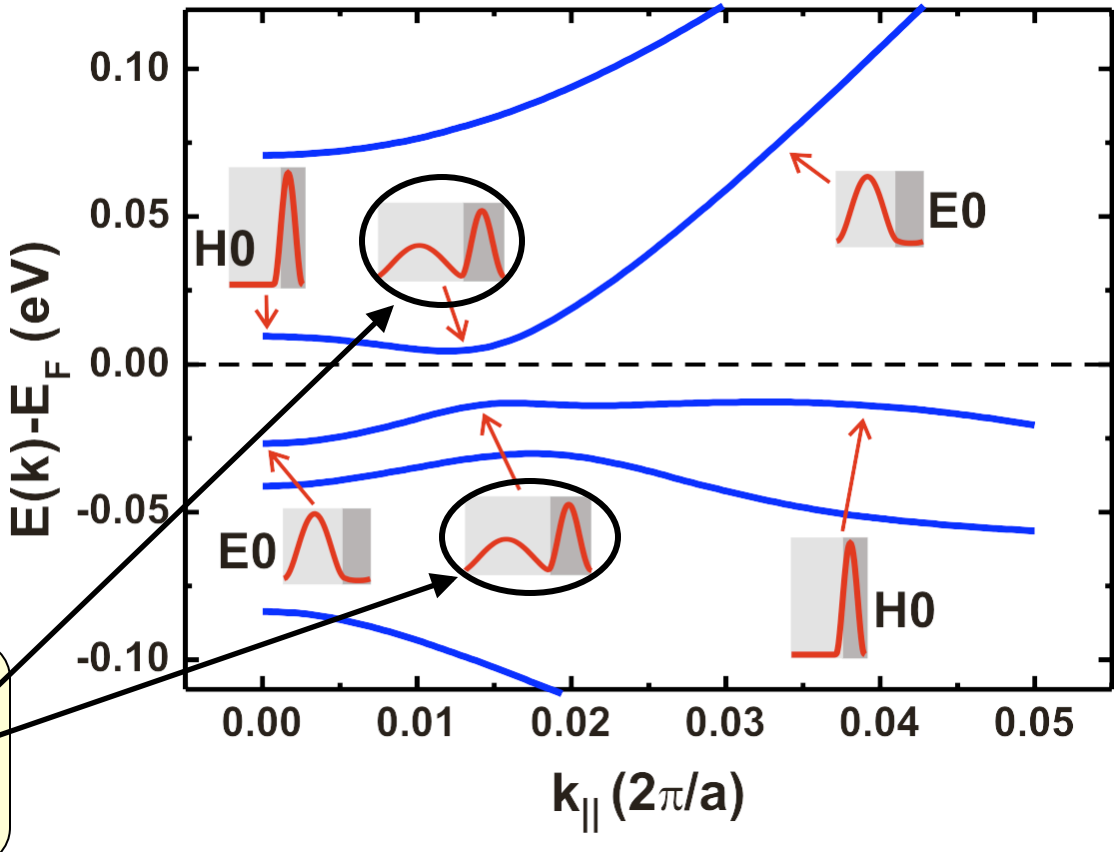
Electronic structure principles and techniques: Broken gap superlattices

Band lineup



Subband dispersion



Hybridized states can not be assigned to be either electron or hole

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Novel method for charge density calculation

Problem:

Charge contributions can not be split into electrons and holes

$$\rho(x) = \int_{\Omega_{BZ}} d^2k_{||} \{-\sum |\Psi_{n,k}(x)|^2 f(E_{n,k}) + \sum |\Psi_{n,k}(x)|^2 [1 - f(E_{n,k})]\}$$

electrons? holes?

Solution:

Occupy all states as electrons and subtract background charge

$$\rho(x) = - \int_{\Omega_{BZ}} d^2k_{||} \sum |\Psi_{n,k}(x)|^2 f(E_{n,k}) + \rho_{bg}(x)$$

all states

- Increased computational effort:
  Calculate $N_{Bands} \cdot N_{Grid}$ states instead of only a few close to Fermi level

- For charge neutrality: $\rho_{bg}(x) = N_{VB} N_{Grid} \Omega_{BZ} / L_{SL}$

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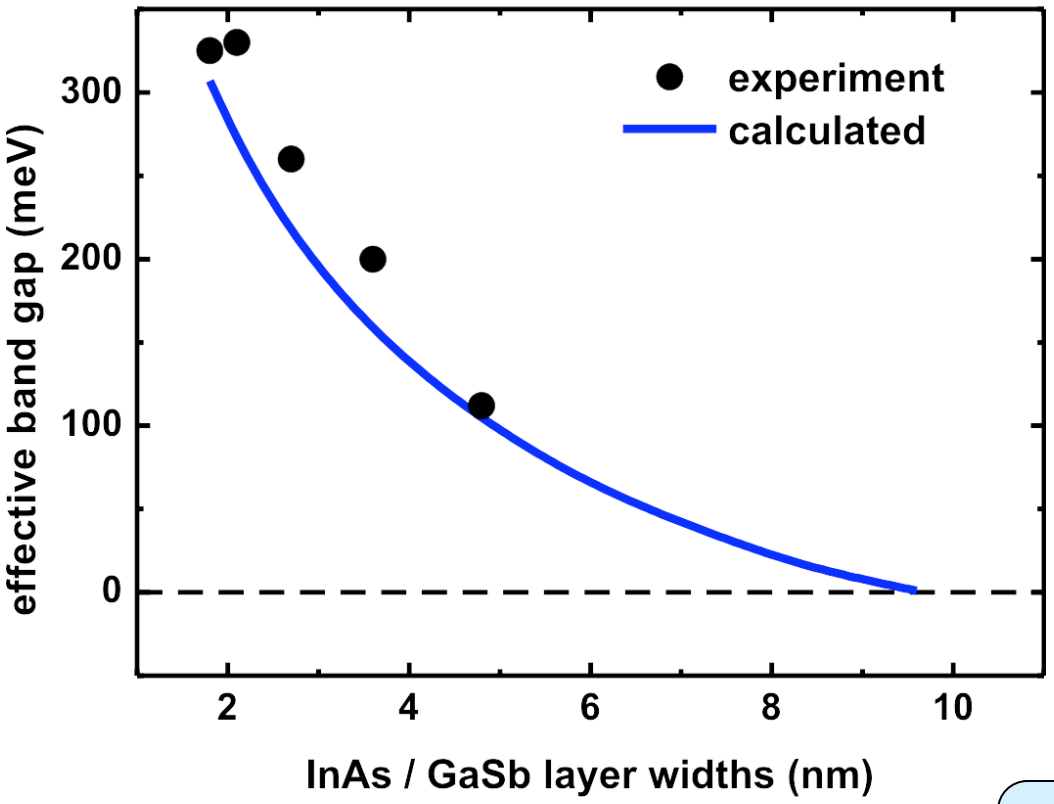
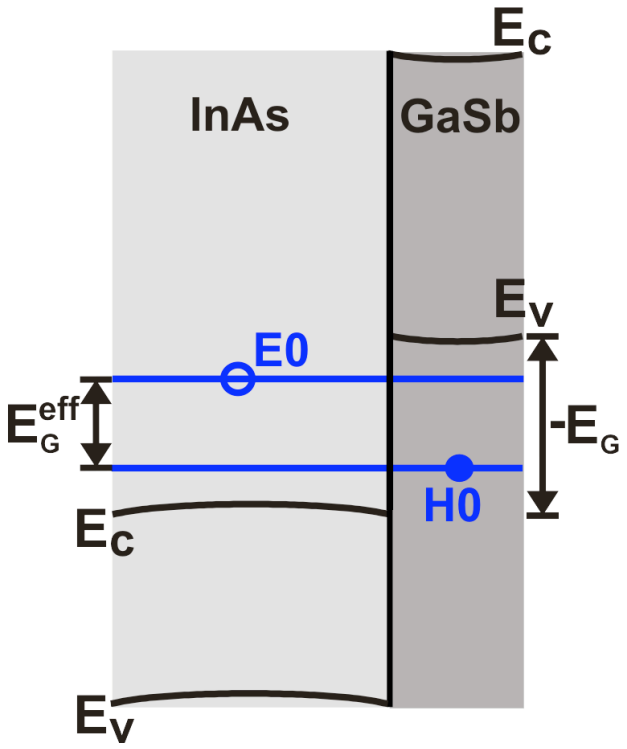
Effective band gap of InAs/GaSb SL

Narrow superlattices have positive effective band gap although $E_G < 0$





E_G^{eff} decreases due to reduction of confinement

Ref: G. C. Dente et al, J. Appl. Phys. 86, 1420 (1999)

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Carrier transport in nextnano

- **Quantum drift-diffusion (QDD) equations:**

$$\vec{\nabla} \cdot \vec{j}(\mathbf{x}) = \vec{\nabla} \cdot \left[\mu n(\mathbf{x}) \vec{\nabla} E_F(\mathbf{x}) \right] = 0$$

$$n(\mathbf{x}) = \sum_i \left| \psi_i(\mathbf{x}) \right|^2 f\left(\frac{E_F(\mathbf{x}) - E_i}{k_B T} \right)$$

  - **WKB-type approach, suitable for diffusive transport near equilibrium**
  - **Good for barrier-limited transport**
  - **Misses quantum resonances and interference effects**

- **Contact block reduction-method (CBR):** **Mamaluy, Sabathil, V., PRB 05**
  - **Efficient method to calculate strictly ballistic transport through open device with arbitrary number of leads**
  - **Scales with N^2 rather than N^3**
  - **Suitable for very short quantum devices close to resonance**

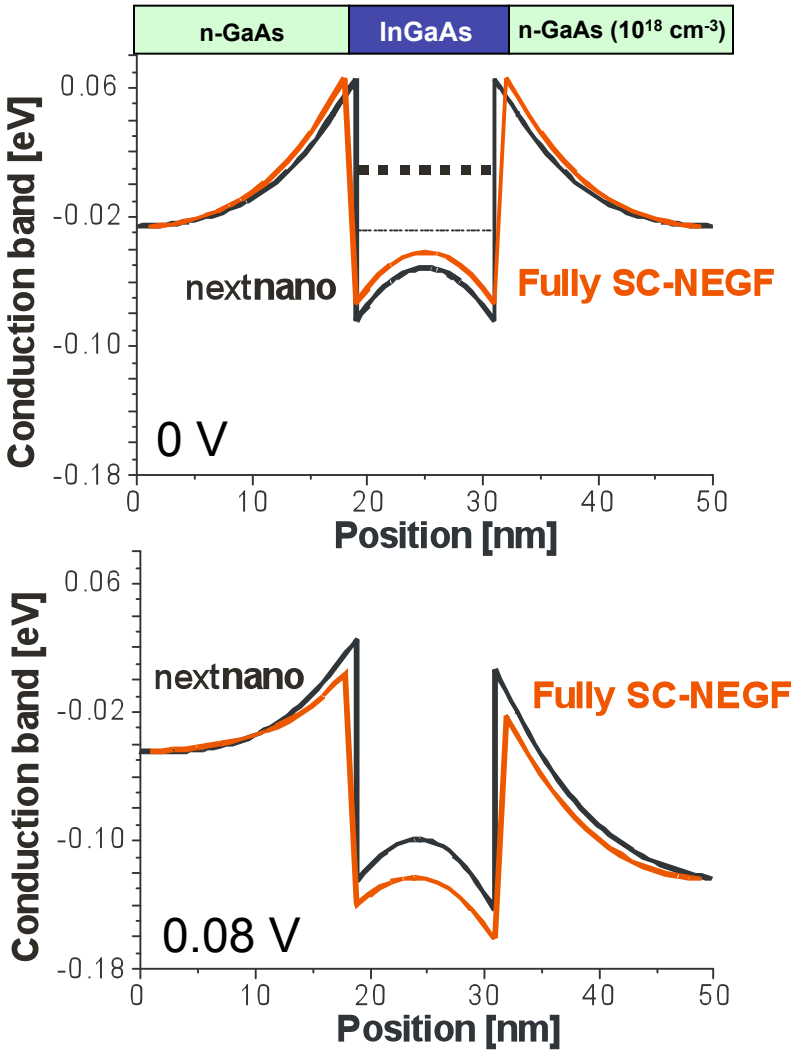
- **Non-equilibrium Green's function method (NEGF):** **Kubis, V., subm.**
  - **Full quantum transport with all relevant scattering mechanisms**
  - **Only for vertical transport (quasi-1D)**

Assessment of QDD

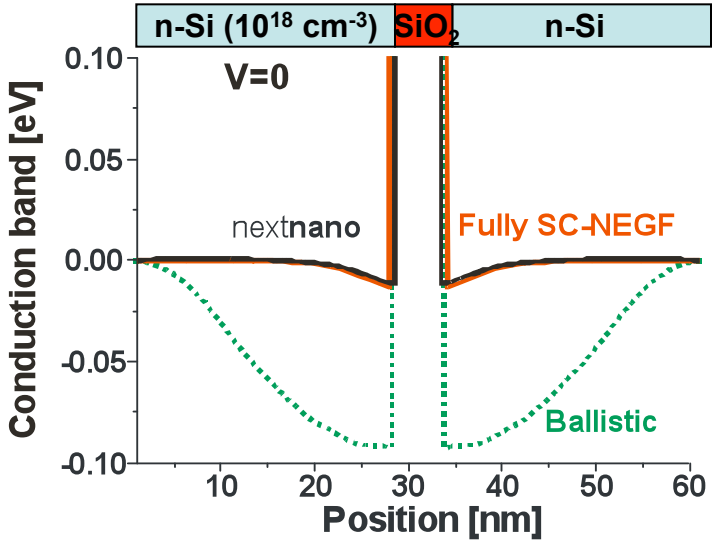
Comparison of QDD with fully self-consistent NEGF*) shows good agreement...

- **close to equilibrium**
- **in situations where interference effects are weak**

Carrier capture by quantum well



Tunneling through thin barrier



*) Kubis et al, Poster #96

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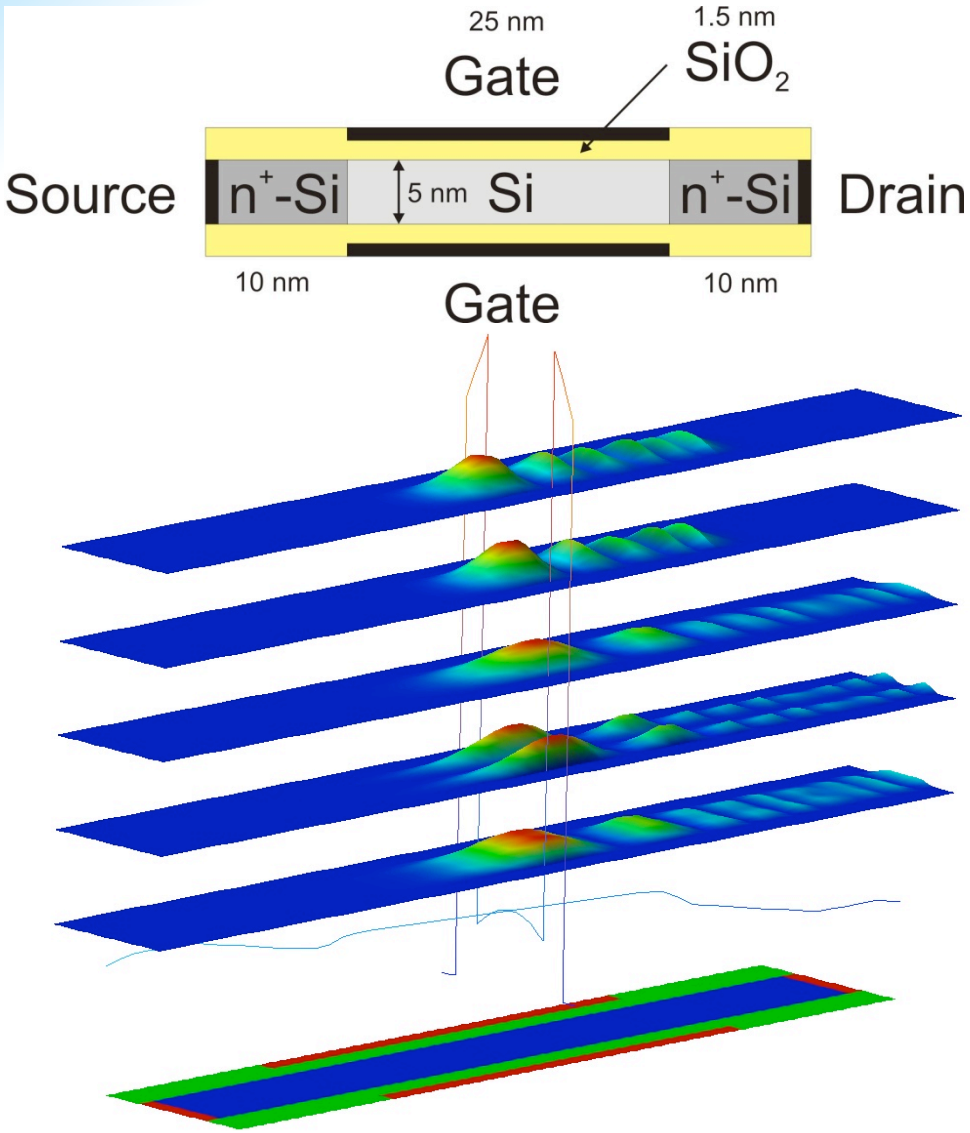
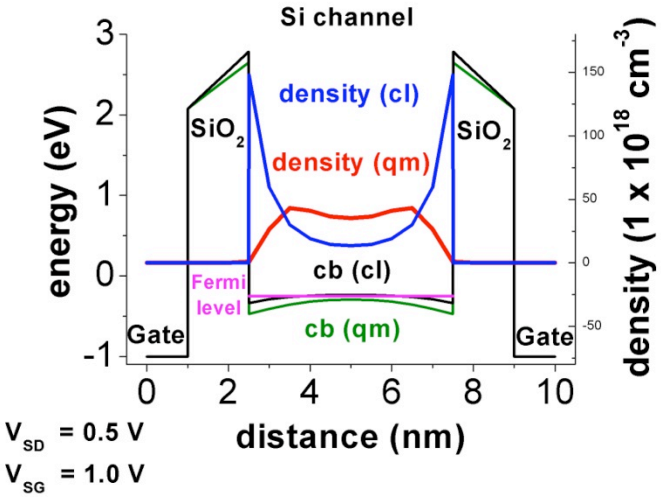
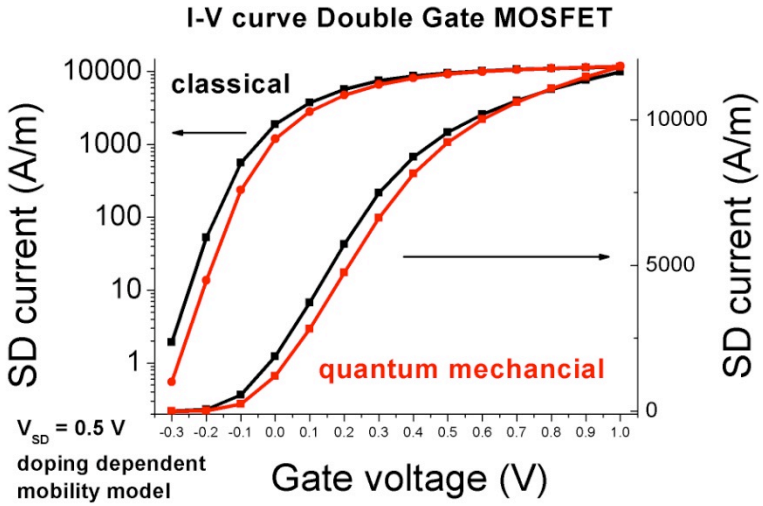
2D Results: Equilibrium + QDD for Si DG-FET







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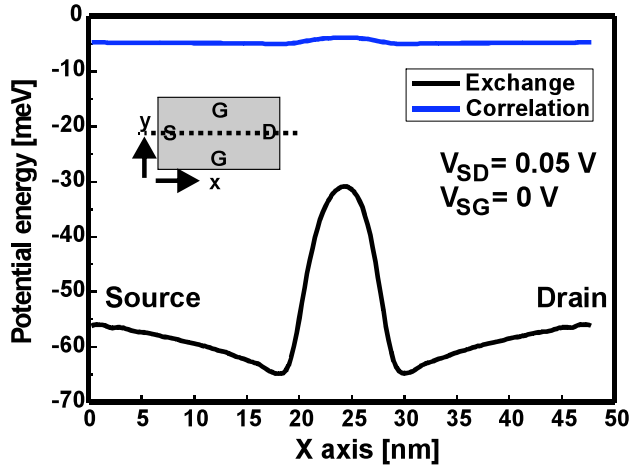
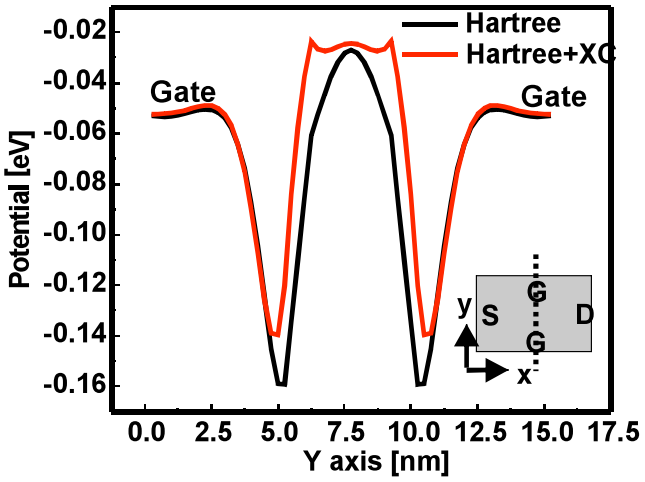
Effect of el-el interaction: exchange-correlation potential

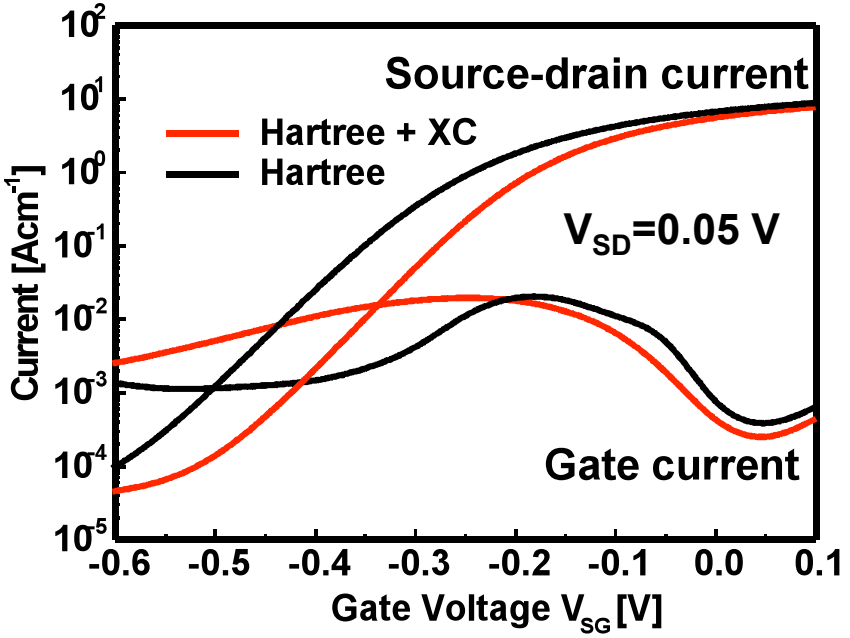
Local density functional theory adds $V_{XC}=V_X+V_C$ to $V_{Hartree}$





$V_X >> V_C$

$V_X = \alpha\, n^{1/3} = 50$ meV for $n=10^{20}$ cm^{-3}



V_{XC} has very large effect for small V_{SD}

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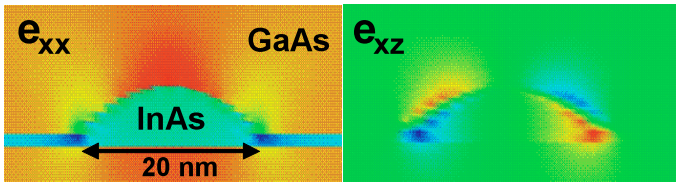
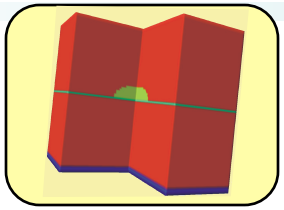
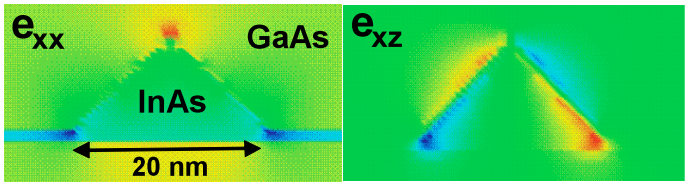
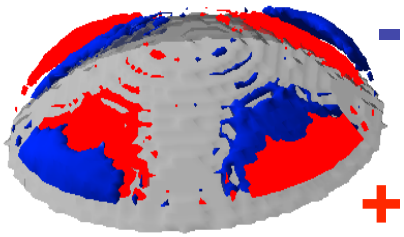
3D results: Self-assembled buried QD



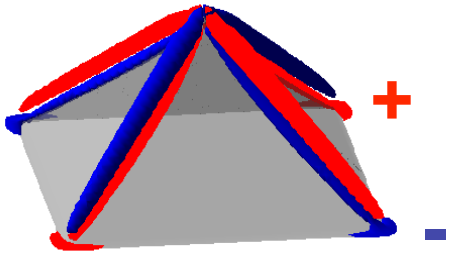


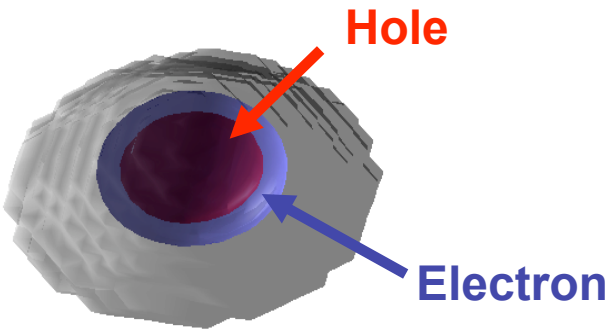
Material strain



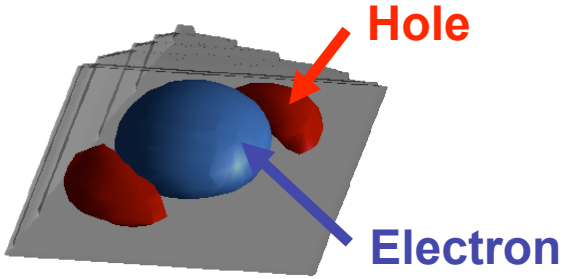


Piezoelectric polarization charge





Modified exciton states



Efficient light emission

No light emission

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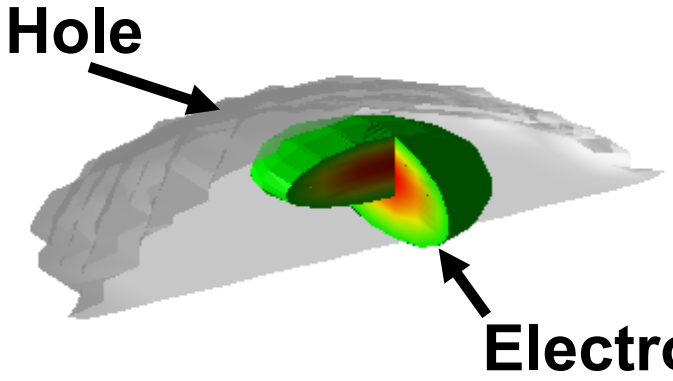
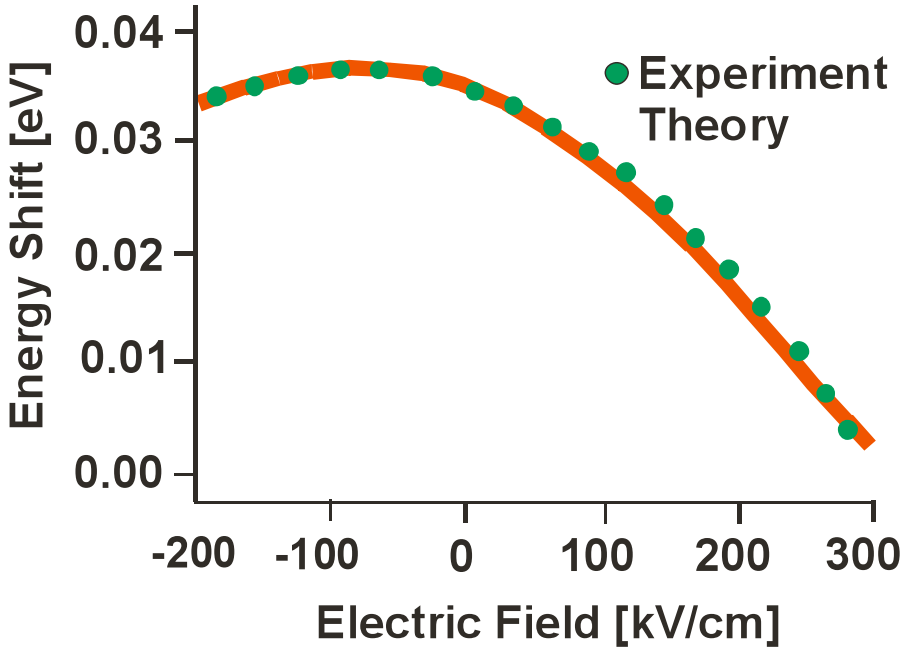
3D results: Stark shift of exciton line in QD

$In_{.5}Ga_{.5}As$ WL on GaAs



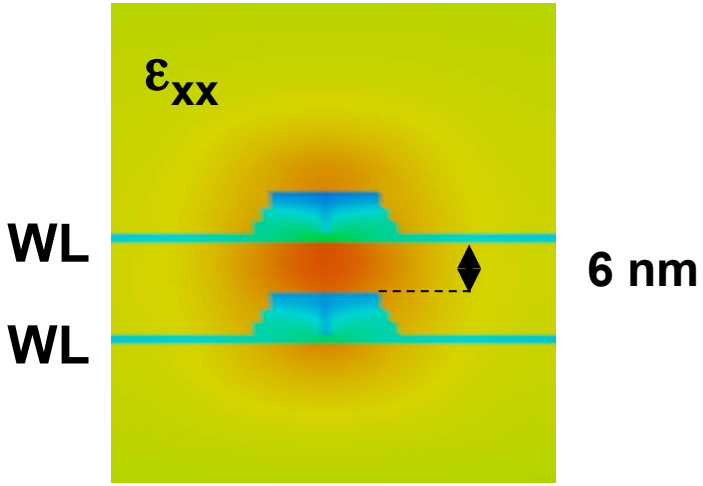


- Detailed comparison with exp allows precise characterization of shape and alloy composition
- Hole sits at tip, electron at bottom
- Depending on QD's width, height is 5-6 nm, In-concentration varies from 50% at base to 100% at tip

3D results: Quantum Dot Molecule

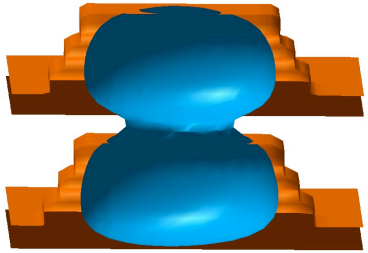
Vertically stacked InGaAs/GaAs QD

Strain field (next**nano**)

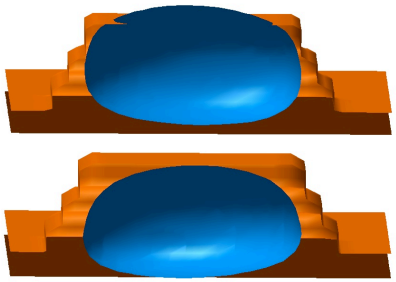


Electron & hole wave functions

bonding



antibonding



Calculate exciton energies

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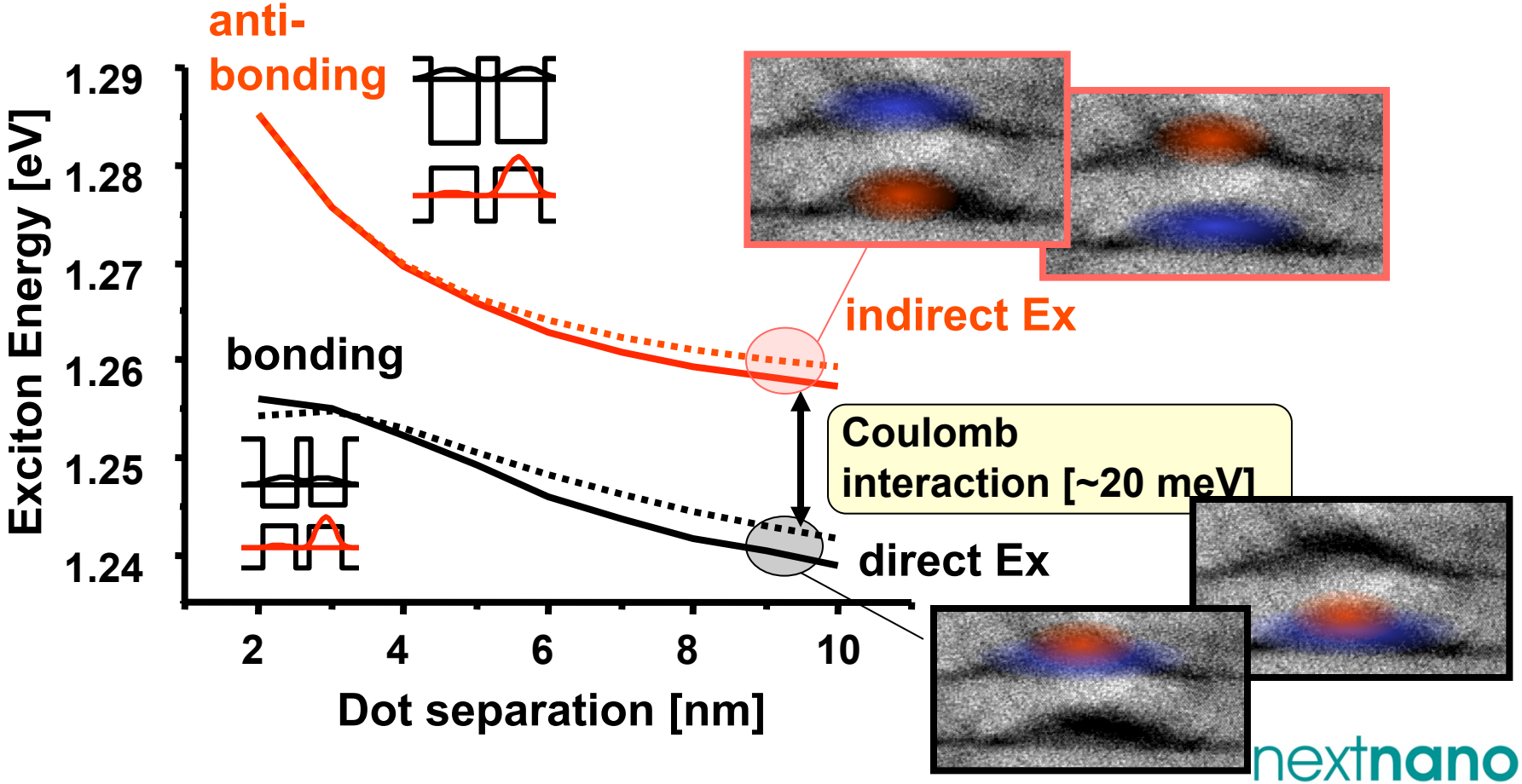
3D Results: Neutral excitons in QD-Molecule

Quantum coupling + strain + Coulomb interaction

- Large separation: direct and indirect excitons
- Small separation: el-dominated bonding and antibonding excitons



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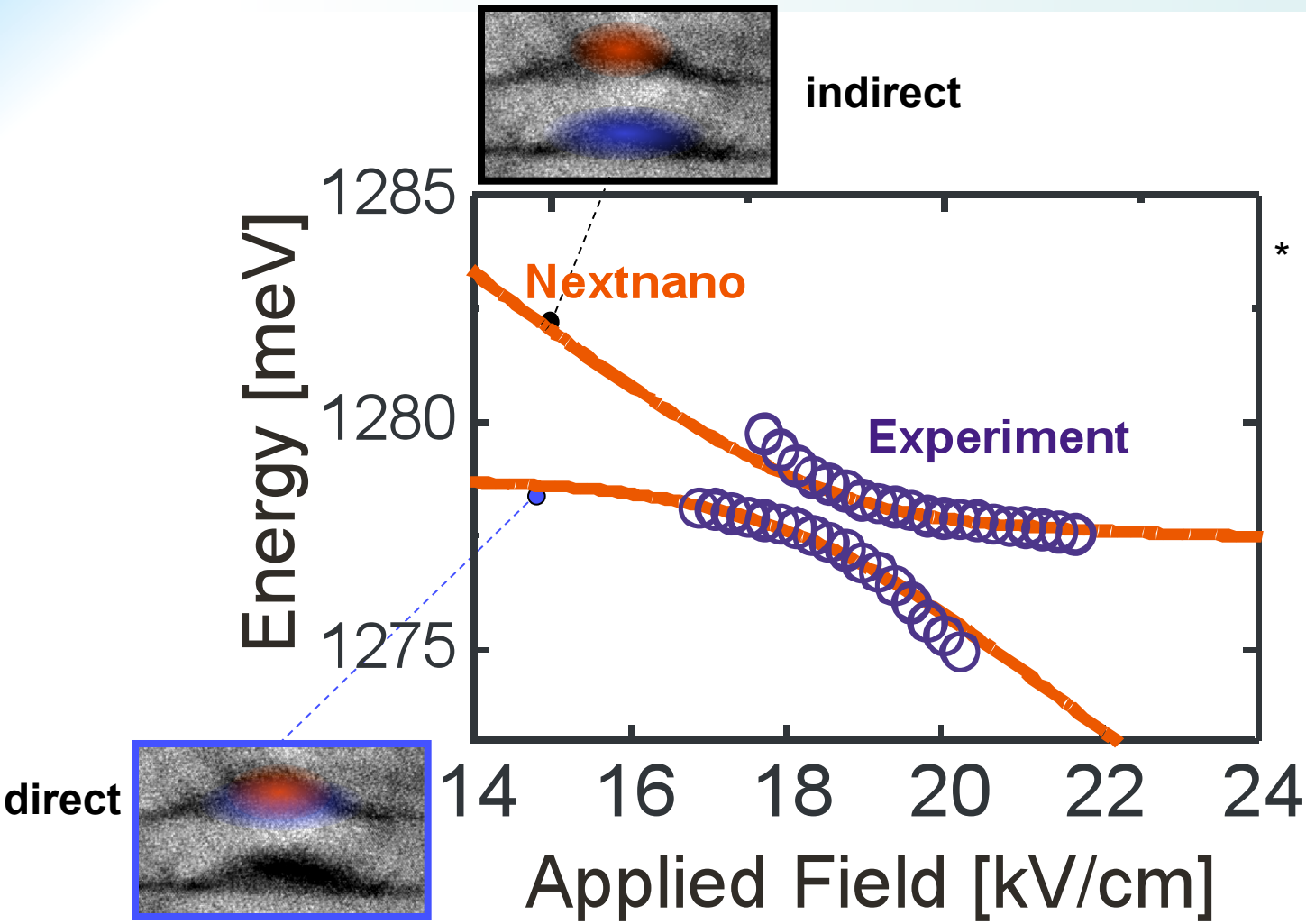
3D Results: Anticrossing of direct + indirect states



*) P.W. Fry et al, PRL 84, 733 (2000), G. Ortner *et al.*, PRL 94, 157401 (2005)
H. J. Krenner *et al.*, PRL 94, 057402 (2005), G. Bester *et al.*, cond-mat/0502184

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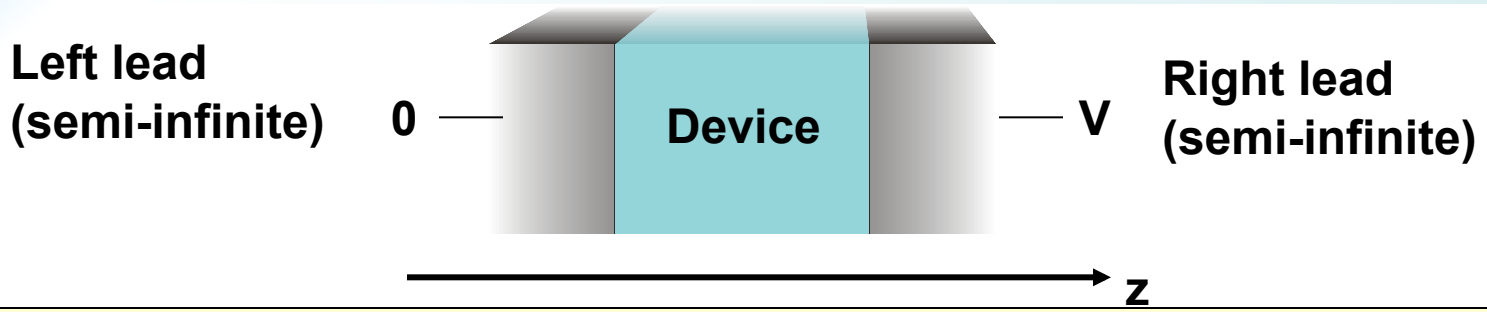
Nonequilibrium Green's function method

T. Kubis (PhD)



Full implementation of NEGF for laterally homogeneous devices

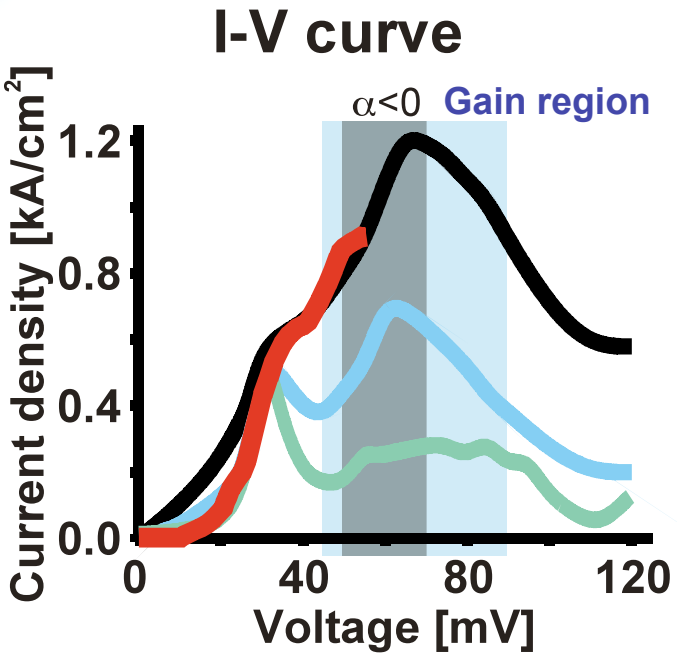
- Open device boundary conditions, take into account contacts
- Coupling of all Green's functions with one another is included
- Elastic and inelastic scattering within sc Born approximation
- Electron-electron scattering (Hartree)
- Momentum and energy dependent self-energies
- Spatially off-diagonal self-energies

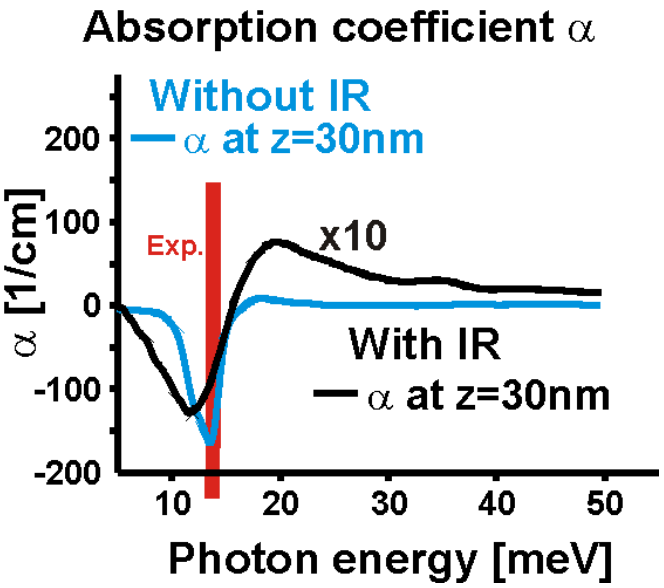
$$H_0 = -\frac{\hbar^2}{2}\nabla\frac{1}{m^*(z)}\nabla + E_c(z)$$ Electrons in heterostructure

$$V_{e-e} = -e\Phi_{Hartree}(z)$$ .. feel electrostatic potential

$$H = (H_0 + V_{e-e}) + \Sigma_{phonon} + \Sigma_{impurity} + \ldots$$ .. and scattering by phonons,...

QCL-Results: Current and Gain





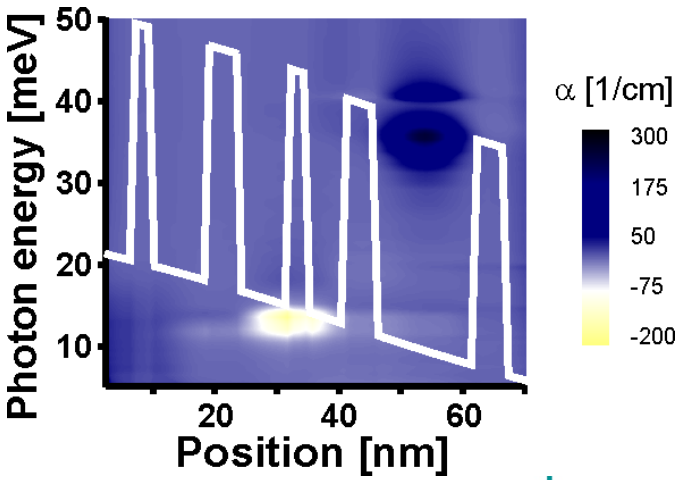
Theory (NEGF) with rough interfaces

Theory (NEGF) with perfect interfaces

Theory: purely ballistic ($k_{//}$ conservation)

Experiment

(Callebaut et al APL 83, 207 (03))



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How to get nextnano?

- **Software including source is free (nextnano³ Fortran)**
- **Online documentation is free**
- **Online registration is free**
- **Support, customized input files + on-site training available on request (by S. Birner)**
- **Some complex tutorial files (QCLs, MOSFETs) are not free**
- **nextnano++ (C++ executable) will be available soon**

www.wsi.tum.de/nextnano3
www.wsi.tum.de/nextnano
www.nextnano.de

Summary

- Nextnano provides base for physics of 1D, 2D, and 3D semiconductor nanostructures
- Handles equilibrium electronic structure, optics, magnetic fields
- Nonequilibrium: QDD approach, ballistic current, and NEGF
- Successful application to 2D+3D nano-MOS, QD molecules, excitons, magnetic field effects, QCL‘s,...