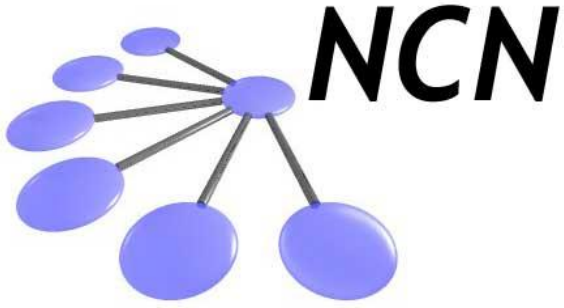
UC Berkeley, Univ.of Illinois, Norfolk State, Northwestern, Purdue, UTEP

1D Heterostructure Tool on nanoHUB.org



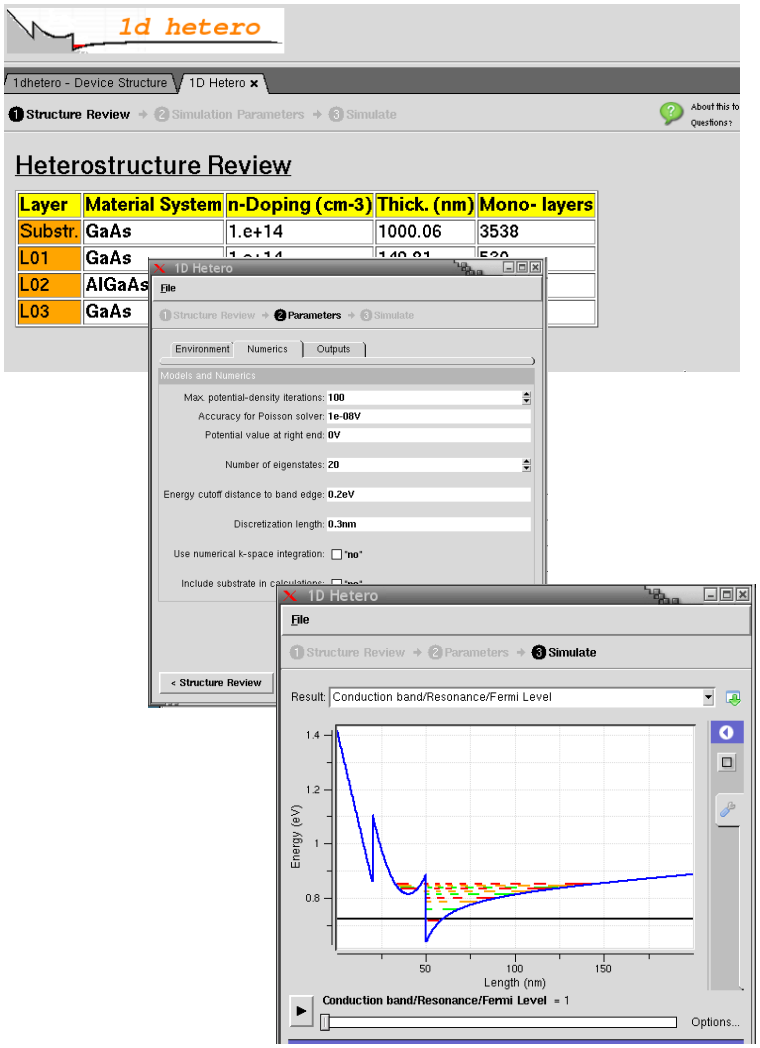
PURDUE UNIVERSITY

Sebastian Steiger
Arun Goud
Jean-Michel Sellier
Gerhard Klimeck

Electrical and Computer Engineering
Purdue University, West Lafayette IN, USA

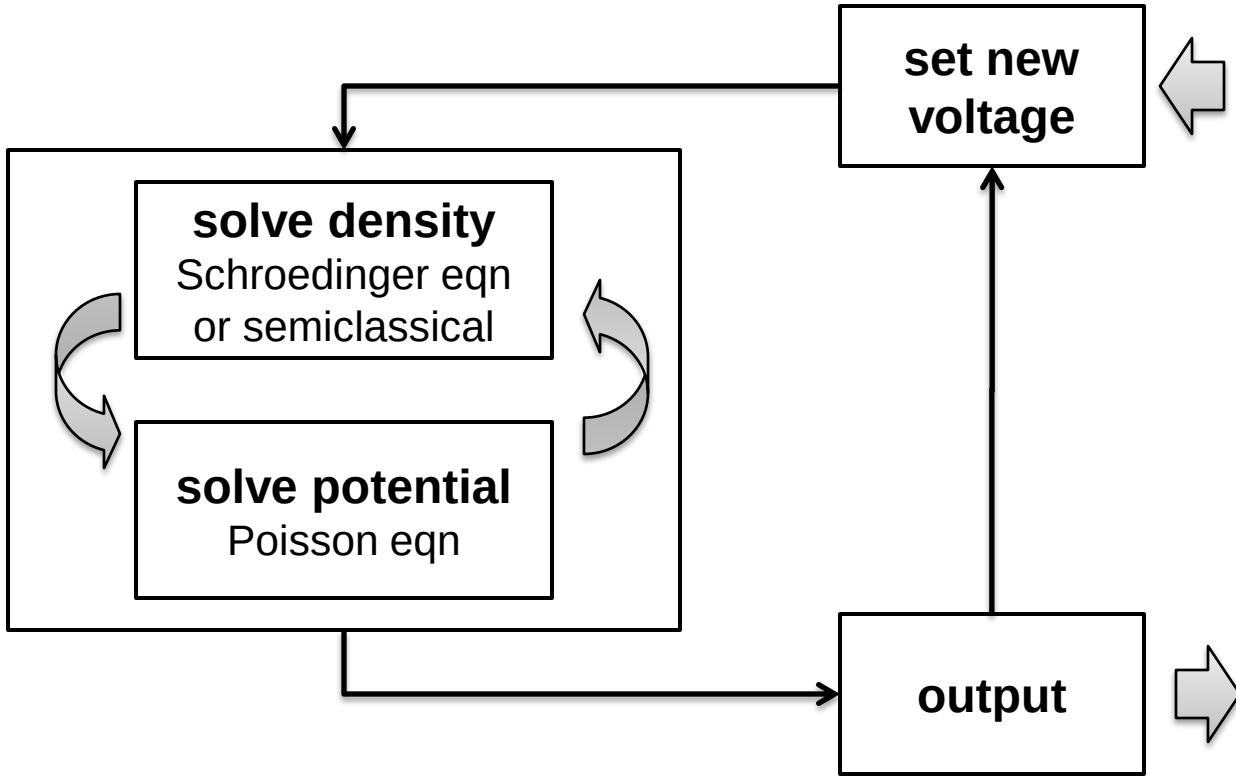
Outline

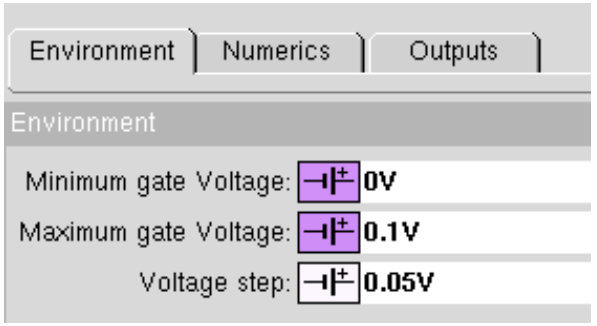
- **Tool overview**
- User **input**
- List of generated **output**
- List of available **materials** and their parameters
- Simulation **examples**
- Facts and parameters
- Validation
- Outlook
- History

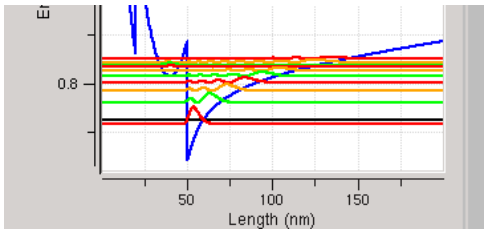


Tool Overview

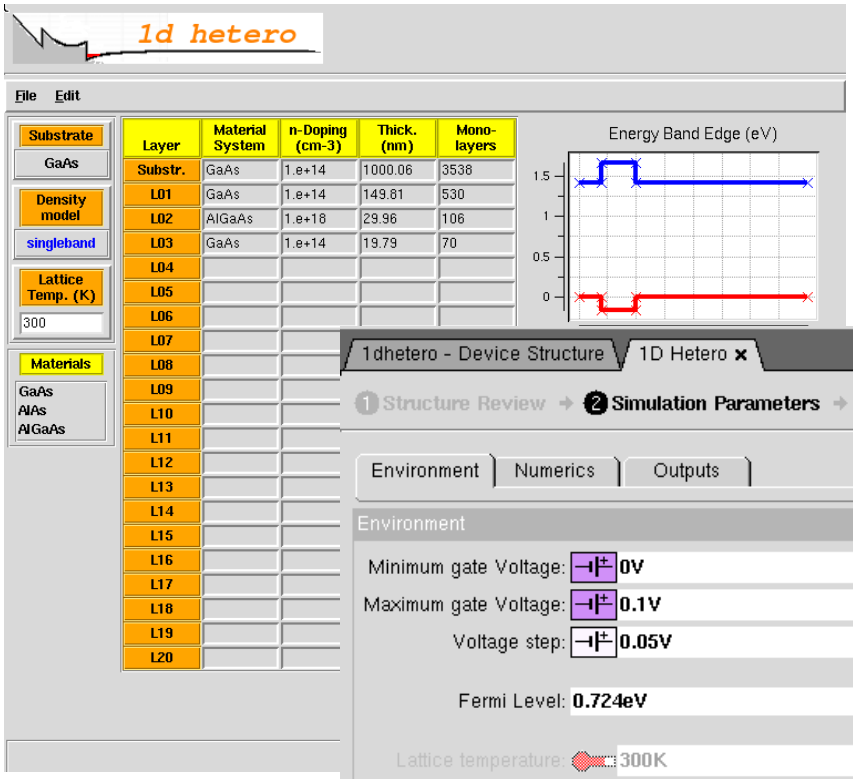
Find ***carrier densities***, ***electrostatic potential, eigenstates*** and other quantities in 1D-layered semiconductor heterostructures:





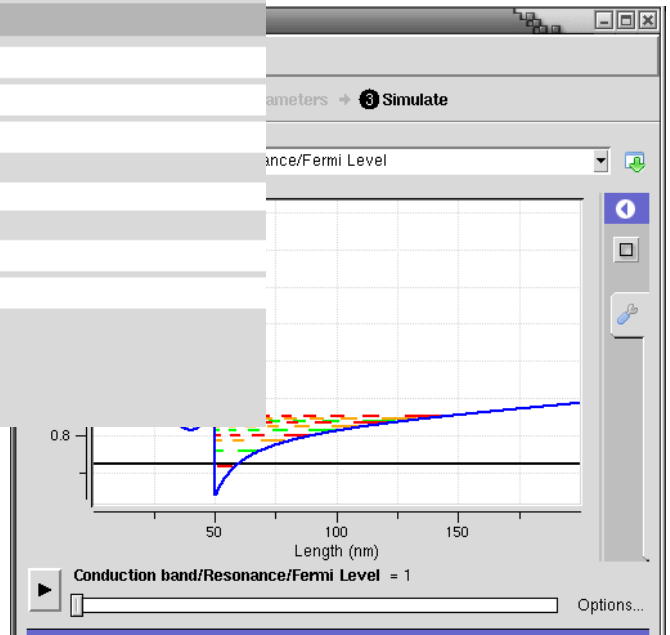


Tool Overview



- Structure definition
- Density model
- Temperature

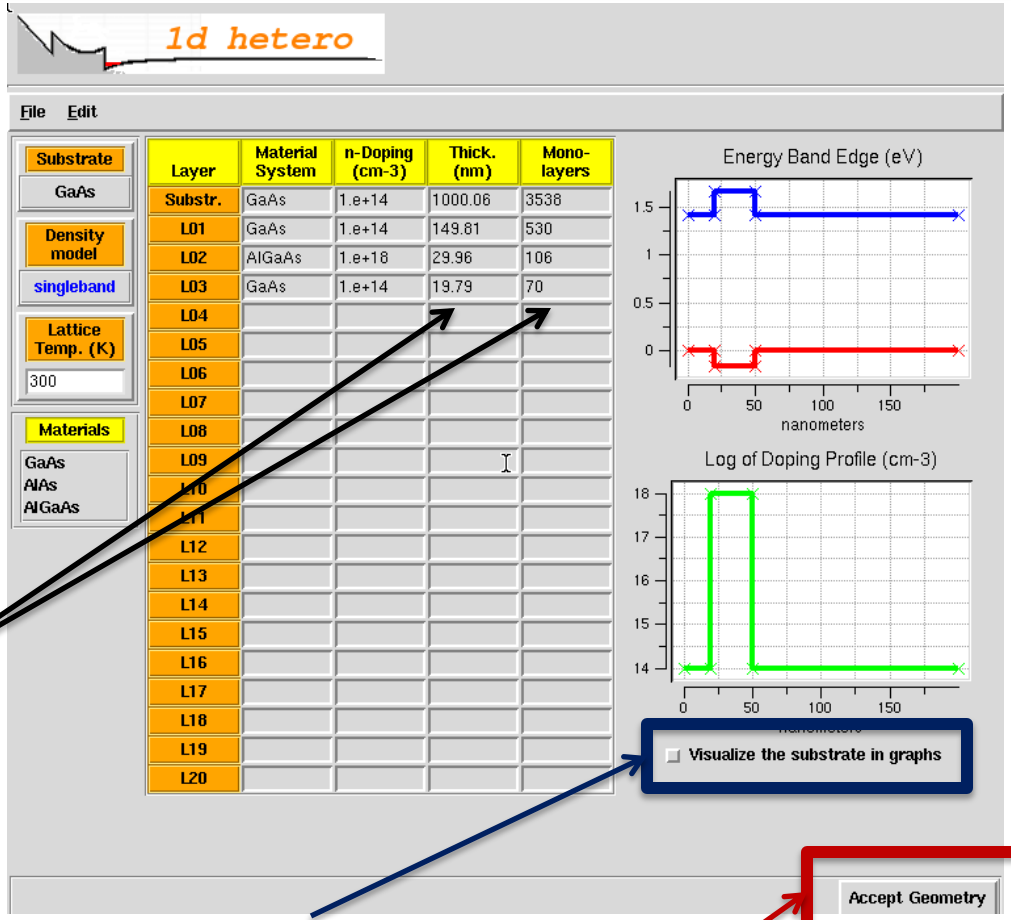
- Applied gate voltage
- Further parameters



- Output graphs

Structure Definition

- Currently only lattice-matched structures are possible (no strain)
- Availability of materials depends on the selected density model
- Enter thickness *or* #MLs other quantity gets adjusted



has no influence on simulation

click when done

→ afterwards structure cannot be changed anymore

Physical Models for the Density

Density model

singleband

$$\rho = e(p - n + N_D)$$

- **Semiclassical density** (no Schroedinger equation needs to be solved):

$$n(x) = N_c \, F_{0.5}\left(\frac{E_c(x) - e\varphi(x) - E_F}{k_B T}\right), \quad p(x) = N_v \, F_{0.5}\left(\frac{E_F - E_v(x) + e\varphi(x)}{k_B T}\right)$$

- **Quantum density:**

$$n(x) = \sum_n \sum_k f_{FD}\left(\frac{E_{nk} - E_F}{k_B T}\right)\left|\psi_{nk}(x)\right|^2, \quad p(x) = 0$$

  - » Single-band effective mass Schroedinger equation:

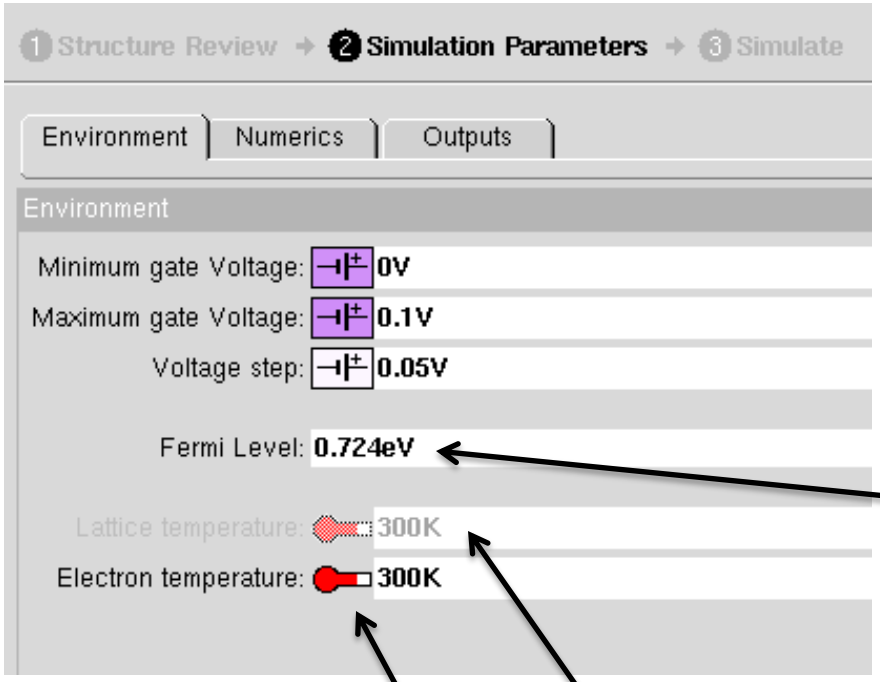
$$\left(-\frac{d}{dx}\frac{\hbar^2}{2m^*(x)}\frac{d}{dx} + E_c(x) - e\varphi(x)\right)\psi_{nk}(x) = E_{nk}\psi_{nk}(x)$$

  - » Multi-band empirical tight-binding (LCAO) Schroedinger equation:

$$H\psi_{nk}(x) = E_{nk}\psi_{nk}(x), \quad H_{ij} = \left\langle \phi_i \middle| H \middle| \phi_j \right\rangle$$

ϕ = atomic orbitals

Gate Voltage

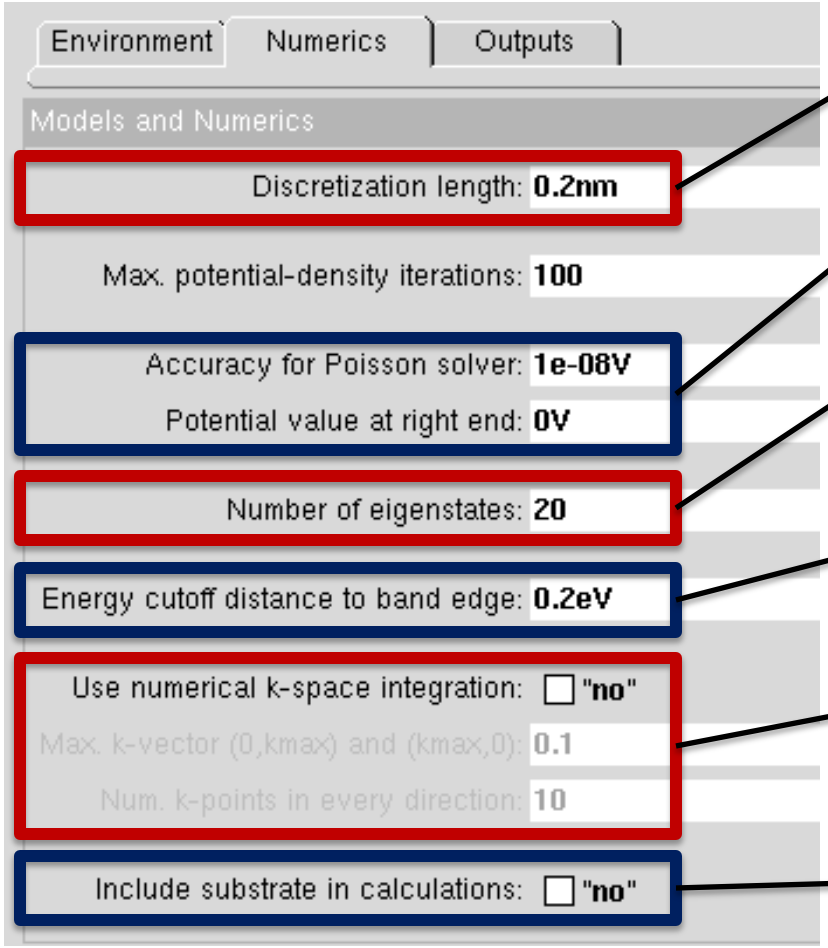


Electrostatic potential at the left end will be ramped given by these steps

Globally constant Fermilevel

- Lattice temperature was given in previous screen → influences lattice constant
- Electron temperature influences Fermi-Dirac population of eigenstates

Numerical Parameters



Real-space discretization for semiclassical and effective-mass simulations

Poisson solver numerical parameters

Number of computed eigenstates for quantum density simulations

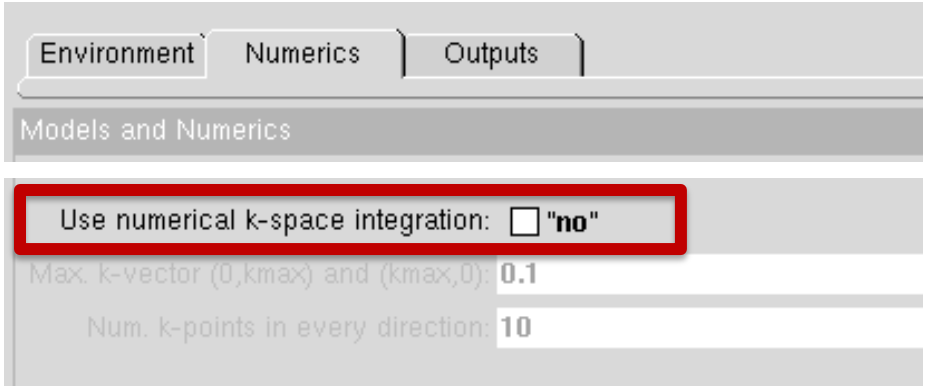
Numerical parameter for discrimination between electrons and holes

Options for the treatment of 2D k-space (see next slide)

Allow substrate layer to have density (makes simulation slower)

Default settings are good enough for most users

k-space Treatment



For Schroedinger simulations two alternatives exist:

1. **Solve only *k*=0** and use

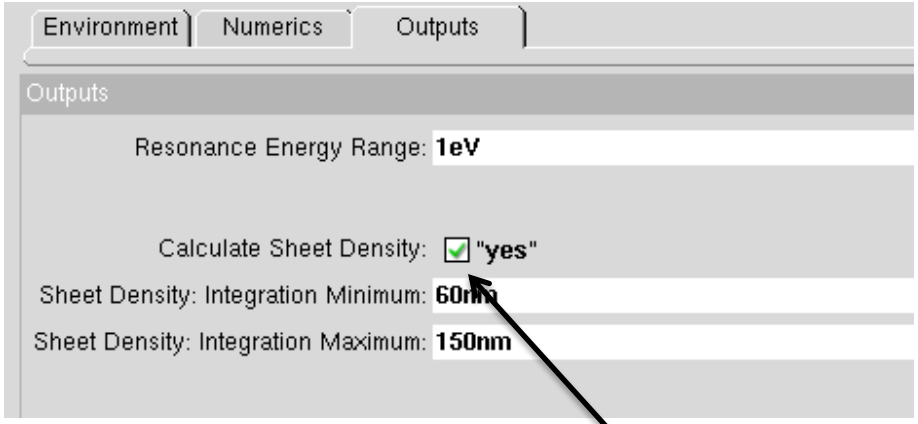
$$\sum_k f_{FD}\left(\frac{E_{nk}-E_F}{k_BT}\right)\left|\psi_{nk}(x)\right|^2 \approx \sum_k f_{FD}\left(\left(E_{n0}+\frac{\hbar^2k^2}{2m^*_{avg}}-E_F\right)/k_BT\right)\left|\psi_{n0}(x)\right|^2 = \frac{m^*_{avg}k_BT}{2\pi\hbar^2}\log\left(1+\frac{E_F-E_{n0}}{k_BT}\right)\left|\psi_{n0}(x)\right|^2$$

For effective mass simulations with constant effective mass this method is exact.

2. Do **numerical integration** using solutions of several *k*-points.

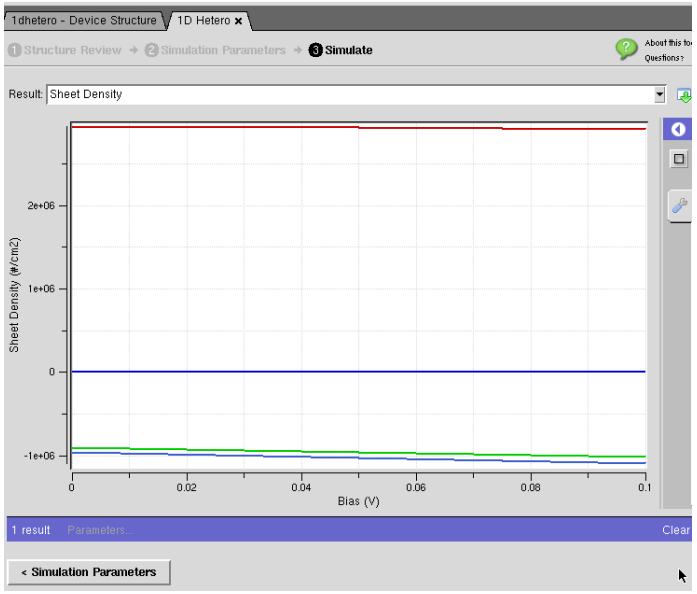
This option submits the job onto a Purdue supercomputer.
It is computationally much more expensive and takes longer.

Output Parameters



For quantum density simulations, states in the range $E_F \pm \Delta$ will be displayed.

If checked, the 3D density will be integrated between the specified boundaries to obtain a 2D density



List of Output Graphs

Graph	Available when?
CB / Resonances / EF	quantum density simulations
CB / EF	semiclassical density simulations
CB / VB / Resonances / EF	quantum density simulations
CB / wave functions	quantum density simulations
Electrostatic potential	always
Doping density	always
Electron density	always
CB / VB w/o electrostatics	always
Sheet density vs. gate voltage	when option is checked
Eigenenergies vs. gate voltage	quantum density simulations

CB = conduction band (including electrostatic potential)

VB = valence band (including electrostatic potential)

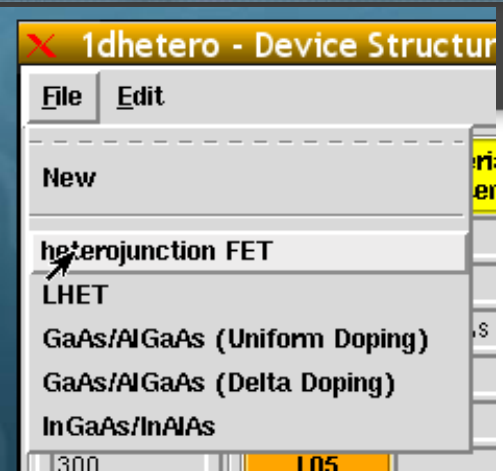
EF = Fermilevel (spatially constant)

Available Material Systems

substrate	material	Ec	Ev	me	sp3s*?	sp3d5s*?
GaAs	GaAs	1.422	0.000	0.067	✔	✔
	AlGaAs	1.672	-0.159	0.067		
	AlAs	1.634	-0.530	0.361	✔	✔
GaP	GaP	1.803	-0.470	0.504	✔	✔
	AlP	1.548	-0.940	0.401	✔	✔
GaSb	GaSb	1.497	0.770	0.039	✔	✔
	AlSb	2.006	0.390	0.274	✔	✔
InP	InP	1.213	-0.140	0.080	✔	
	In53GaAs	0.948	0.205	0.044	✔	
	In52AlAs	1.505	0.015	0.075	✔	
Si	Si	1.125	0.000	1.084	✔	✔
	Ge	1.448	0.545	0.869		✔
	SiO2	4.295	-4.705	0.3		✔

- Most effective mass parameters are taken from Vurgaftman 2001. Effective DOS masses are taken for indirect semiconductors.

Heterostructure Examples (1)



Heterojunction FET:

GaAs, 1e14, 20nm
AlGaAs, 1e18, 30nm
GaAs, 1e14, 150nm
GaAs, 1e14, 800nm

InGaAs/InAlAs:

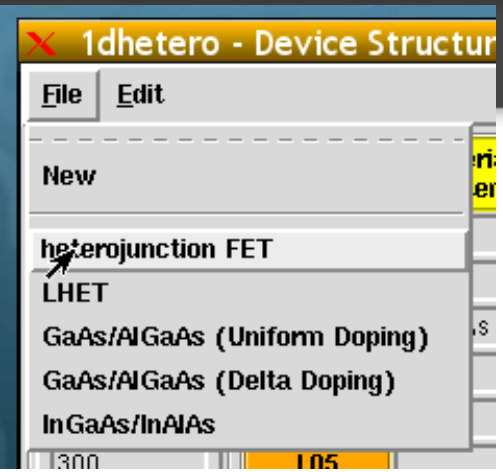
5 nm $In_{0.53}Ga_{0.47}As$ (2×10^{18} cm^{-3})	*Cap layer*
30 nm $In_{0.53}Al_{0.47}As$ (1×10^{18} cm^{-3})	*Buffer layer*
10 nm undoped $In_{0.53}Al_{0.47}As$	*Spacer*
25 nm undoped $In_{0.53}Ga_{0.47}As$	*Quantum well*
250 nm undoped $In_{0.53}Al_{0.47}As$	
SI InP (001) substrate	

example courtesy of Prof. D. Vasileska, ASU

LHET:

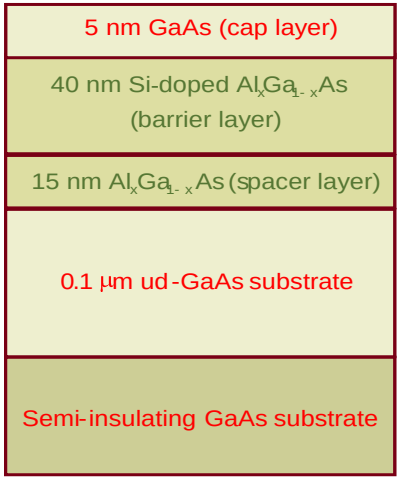
20nm AlGaAs	
5nm AlGaAs	δ-dop 5e11cm^{-2}
5nm AlGaAs	δ-dop 5e11cm^{-2}
5nm AlGaAs	δ-dop 5e11cm^{-2}
5nm AlGaAs	δ-dop 5e11cm^{-2}
25nm AlGaAs	δ-dop 5e11cm^{-2}
40nm AlGaAs	
50nm GaAs	
200nm GaAs (001)	

Heterostructure Examples (2)

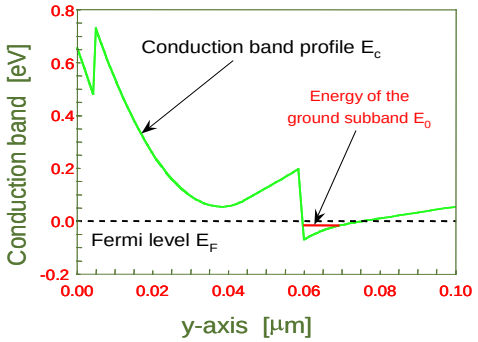


- GaAs/AlGaAs w/ uniform doping

MBE Grown Heterostructure with uniformly doped layer

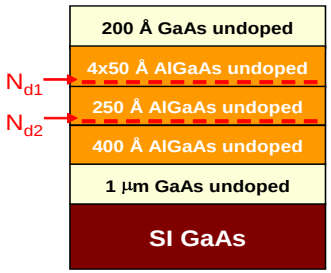


Conduction band profile along the growth direction



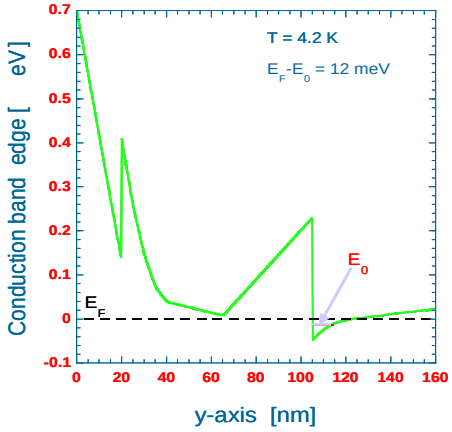
Calculated channel electron density for the ungated structure is N_s=4.26x10^{11} cm^{-2}. The experimental measurements revealed N_s=4.1x10^{11} cm^{-2}, in close agreement with our simulation results.

MBE Grown Heterostructure with δ-doped layers



N_{d1}=1x10^{12} cm^{-2} Si

N_{d2}=3x10^{12} cm^{-2} Si



- GaAs/AlGaAs w/ δ-doping

examples courtesy of Prof. D. Vasileska, ASU

Facts and Parameters

- For multi-band simulations the discretization is given by the atomic lattice.
- The Fermilevel is spatially constant and fixed during the simulation.
- Zero density in the “substrate” material is assumed except when the designated option is checked.
- In the case of varying effective masses and analytical k-space, the assumed effective mass for the lateral dispersion is

$$m^*_{avg} = \int m^*(x) \left|\psi(x)\right|^2 dx.$$

- For numerical k-space integration, by default a sample of 100 k-points is taken over the square [0,2pi/4a]x[0,2pi/4a] (and multiplied by 4).
- The multiband tight-binding parameter sets are *not* temperature-dependent so changing the temperature will have no effect on the simulation.
- For multiband simulations, a quantum state E_{nk} is assumed to be an electron according to the (spatially dependent) criterion

$$E_{nk} > E_c - e\varphi(x) - \Delta.$$

The parameter Δ is 0.2 eV by default and adjustable in the Numerics section of the GUI.

Validation

- Bulk E(k) band structure diagrams of most materials and models were validated against literature:

Model	Source
Ec, Ev, me	Vurgaftman et al., JAP 89, 5815 (2001)
sp3s*	Klimeck et al., Superlatt. 27, 519 (2000) Klimeck et al., Superlatt. 27, 77 (2000) NEMO-1D
sp3d5s*	Jancu et al., PRB 57, 6493 (1998) Boykin et al., PRB 69, 115201 (2004)

- The Poisson solver was validated against analytical results.
- The Schroedinger-Poisson iteration result was compared to previous versions of the tool that had an independent codebase.

Outlook

- Ternary materials with flexible mole fractions
- Holes
- Strain
- Varying crystal orientations (multiband only)
- Nitrides

History of the Tool

1d_hetero is an ongoing outreach effort by the Klimeck group @Purdue:

- First *Matlab* prototype by Samarth Agarwal (<1.0.3).
- *New-NEMO 3D* simulation engine by Sunhee Lee (1.0.3-2.x).
- *NEMO 5* simulation engine by Sebastian Steiger, Michael Povolotskyi, Tillmann Kubis and Hong-Hyun Park (>3.0). Material database by Ben Hailey (>3.0).
- Initial *Tcl/Tk* and *Rappture* GUIs by Jean-Michel Sellier (1.0.3-2.x) and Xufeng Wang (<1.0.3).
- Current (>3.0) GUI and maintenance by Arun Goud under supervision of S. Steiger.
- General supervision: Gerhard Klimeck. Counseling: Dragica Vasileska.

Last update of this document: Jan 2011