Physical models for nanowire device simulation

Dr. Vihar Georgiev, University of Glasgow, Glasgow, UK

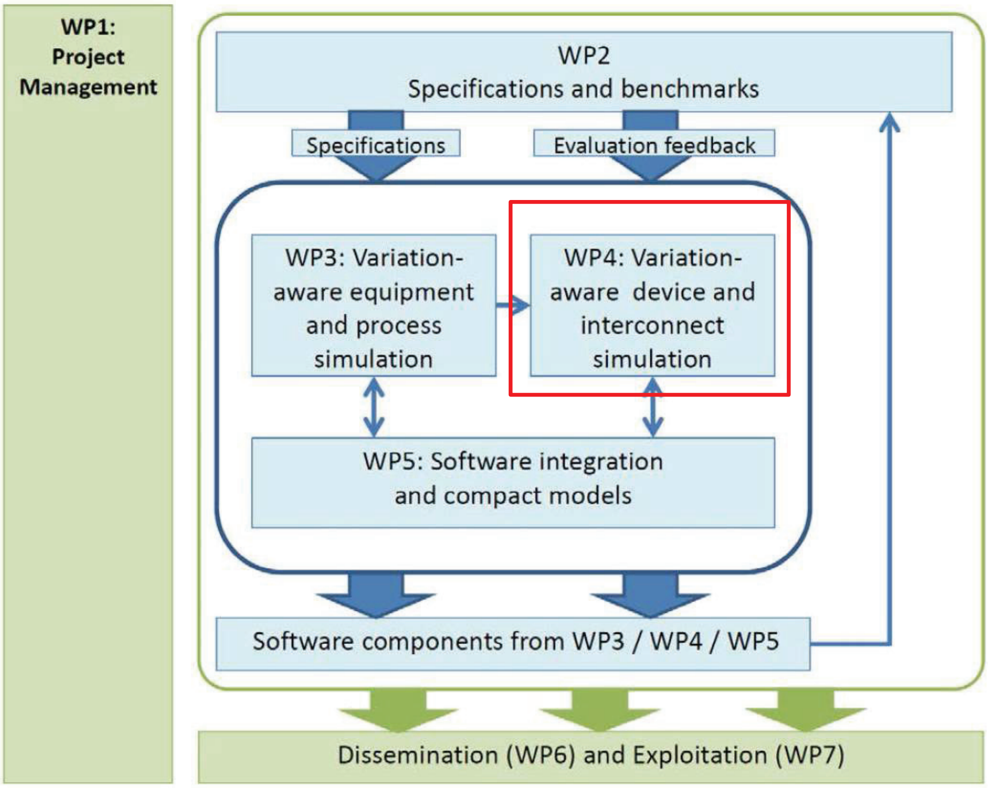
ESSDERC/ ESSCIRC Workshop "Process Variations from Equipment Effects to Circuit and Design Impacts"

September 3, 2018, Dresden, Germany

Outline

- Introduction
  - Project flow and link between the Work Packages
- Physical models and methods
  - Drift Diffusion Method (DD)
  - Kubo-Greenwood
  - Non-Equilibrium Green's Function (NEGF)
  - Wigner Monte Carlo
- Conclusions and outlook

Introduction - Project Context

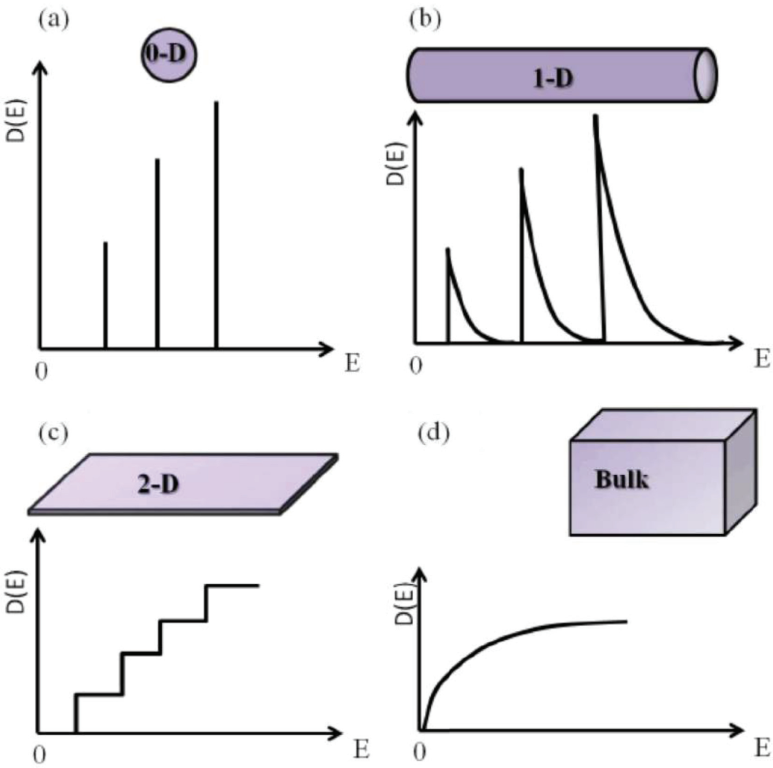


Introduction - Goals and Strategy of WP4

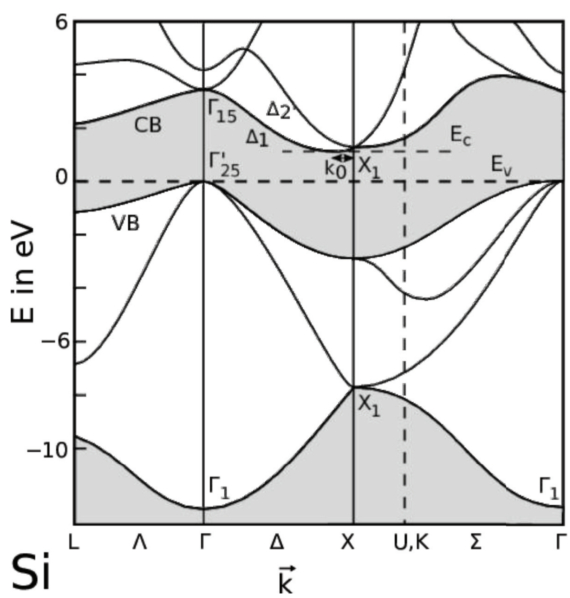
- The objective of this work package is to **enable device and advanced interconnect simulation tools** to deal with **realistic geometries including variability and process-induced variation**.

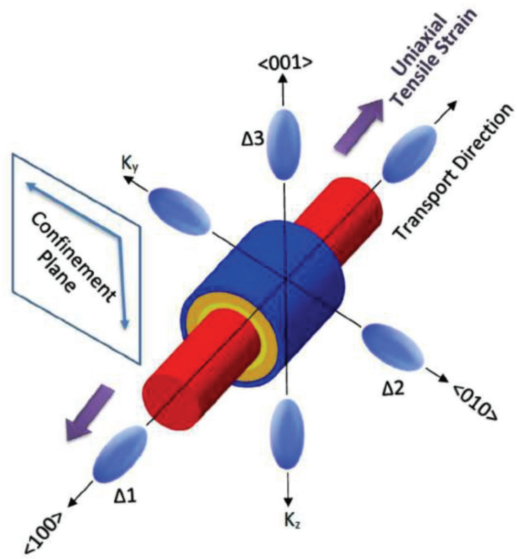
- **To develop and to implement refined physical models** which are needed for the **simulation of advanced More Moore devices like FinFETS and Nanowire Transistors**, especially when effects of ***confinement, quantum behaviour and charge granularity*** come into play. Interconnect models will be developed, which properly account for grain boundary and surface roughness effects on electron transport.

Introduction - Basic Physics



Introduction - Basic Physics





Conduction band consists of six energy ellipsoids (Δ) along the confinement plane and uniaxial tinsel strain.

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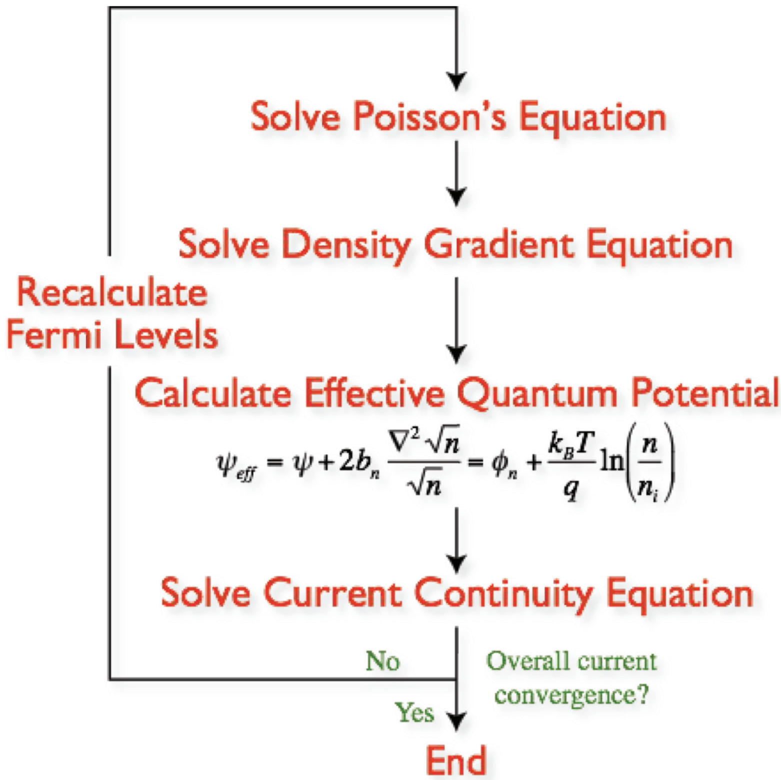
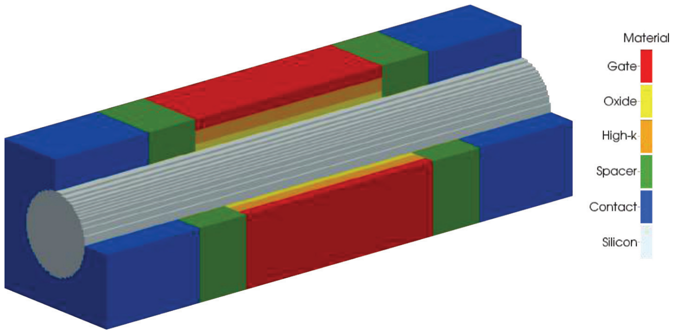
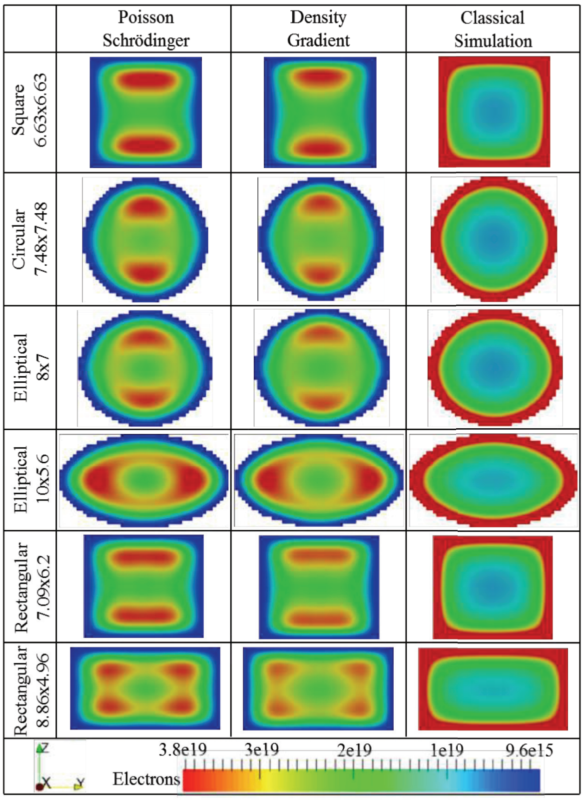
Physical Model - Drift Diffusion



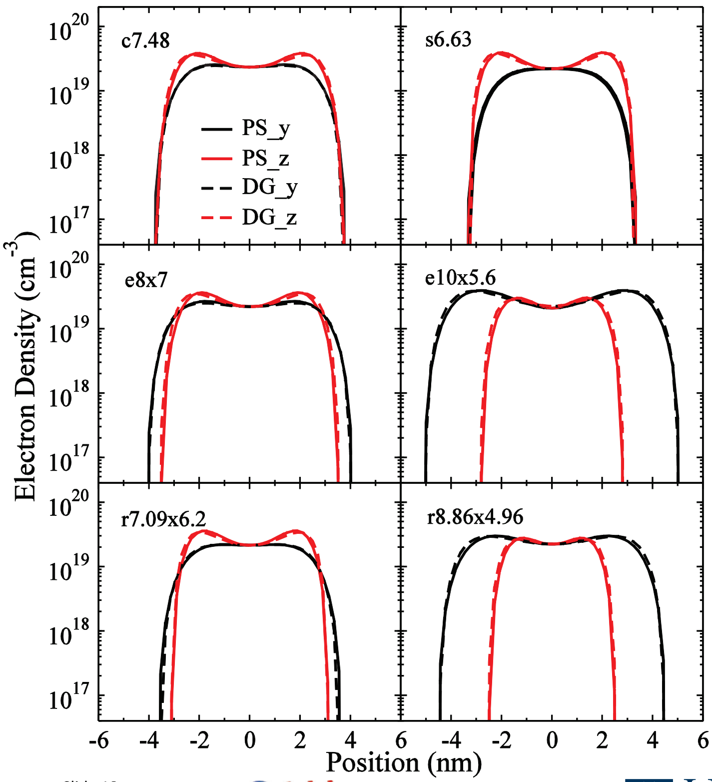
Physical Model - Drift Diffusion

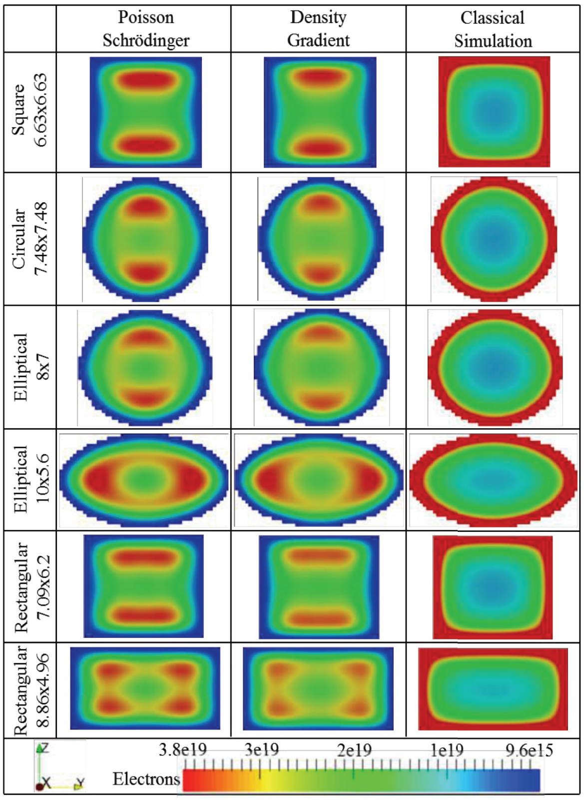
Parameters	Value
Gate length (nm)	18
Spacer thickness (nm)	5.0
S/D peak doping (cm^{-3})	2×10^{20}
Channel doping (cm^{-3})	10^{14}
Substrate orientation	(001)
Nanowire orientation	<110>, <100>
T_{oxide} (nm)	0.8





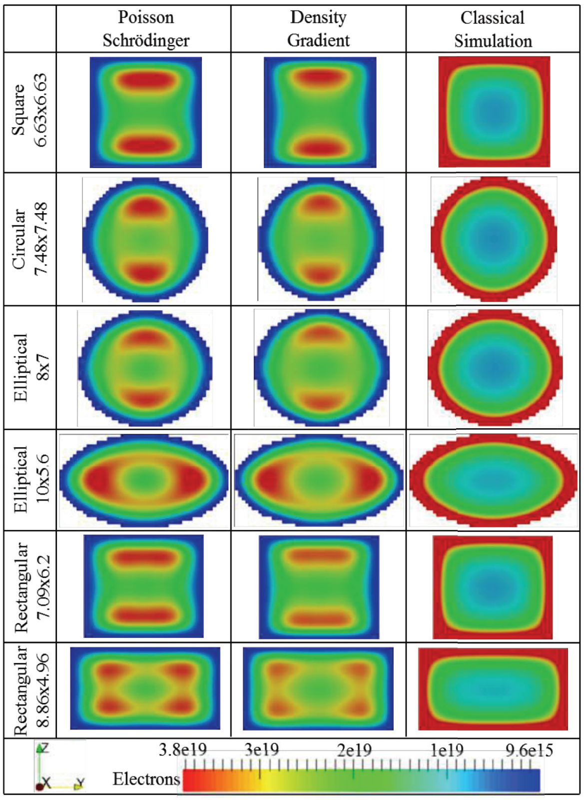
Physical Model - Drift Diffusion





Physical Model - Drift Diffusion

Device	Q_M (10^6/cm)	C_G (10^{-12}F/cm)	Q_M/C_G (10^{18}/F)
s6.63x6.63	7.208	5.915	1.219
c7.48x7.48	7.670	5.922	1.295
e8x7	8.229	6.171	1.334
e10x5.6	9.638	7.081	1.361
r7.09x6.2	7.971	6.130	1.300
r8.86x4.96	9.104	6.746	1.350
e5.6x10	6.771	6.312	1.073



The change in **shape** can have > 20% impact on performance

The change in **orientation** can have > 30% impact on performance

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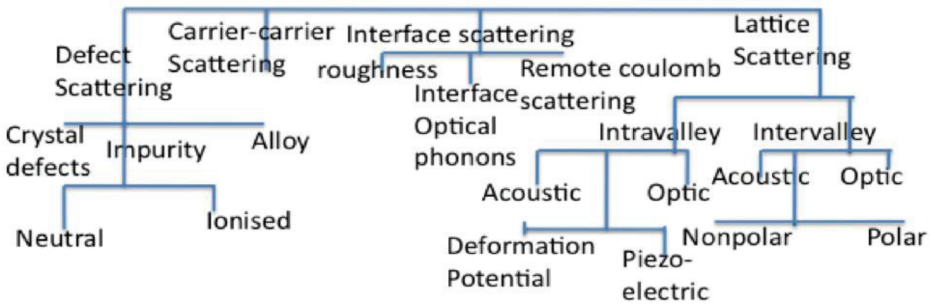
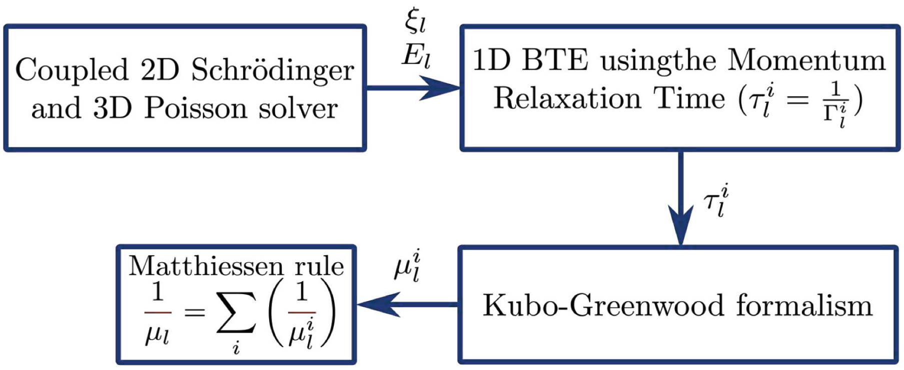
Physical Model - Kubo-Greenwood

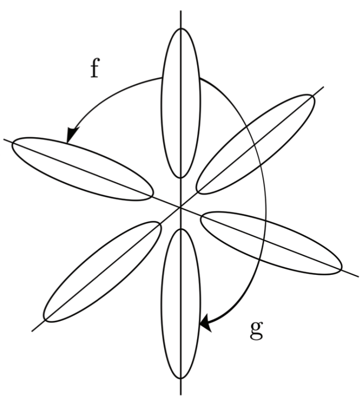
Scattering mechanism



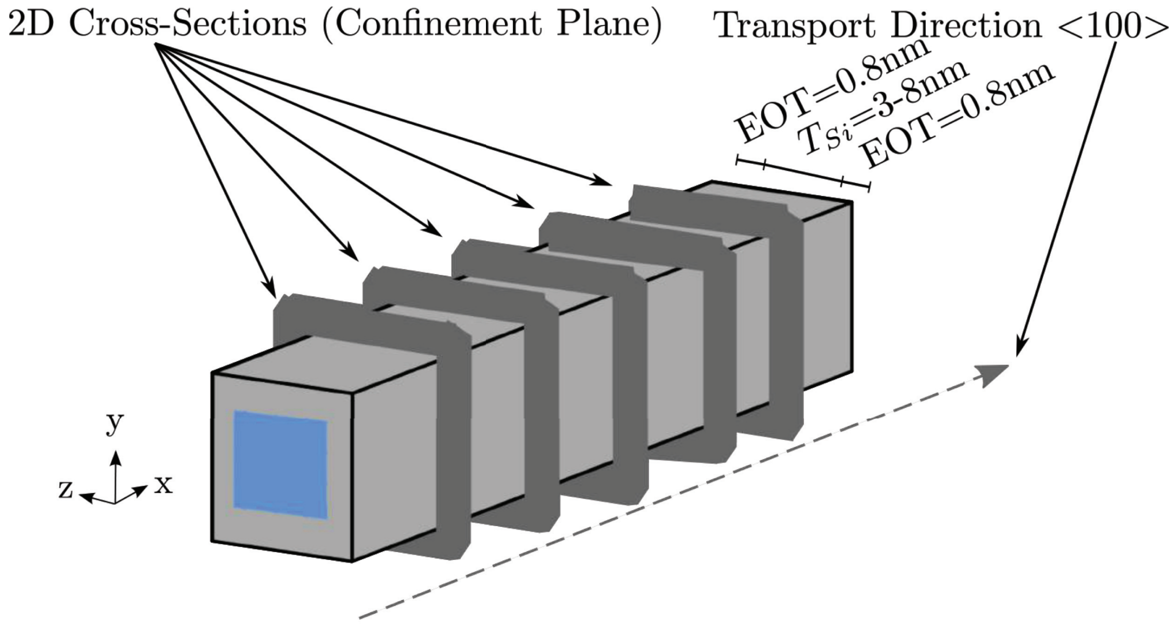


Physical Model - Kubo-Greenwood

- **Acoustic Phonon Scattering Mechanism**
  - Elastic and intra-valley transitions are only allowed
- **Optical Phonon Scattering Mechanism**
  - Inelastic mechanisms
  - The two different transitions among the six equivalent X minima of Si must be considered: g-type (intra-valley) and f-type (inter-valley) processes
- **Ionized Impurity Scattering Mechanism**
  - Elastic and intra-valley transitions are only allowed
  - Fixed uniform ionized impurity concentration:
    $n_0 = [10^{17} - 10^{19}]\ cm^{-3}$

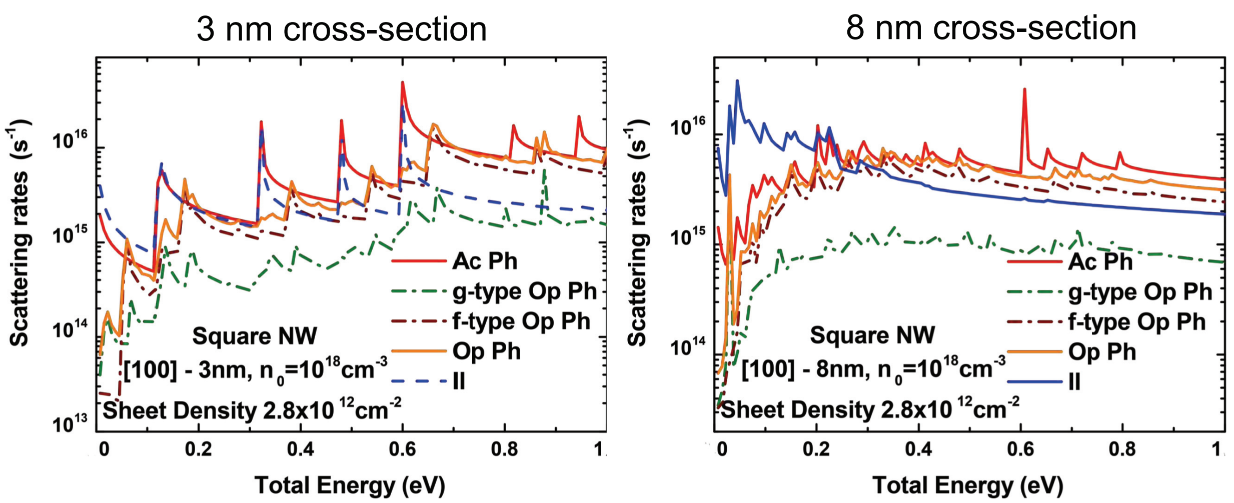


Physical Model - Kubo-Greenwood



Silicon gate-all-around (GAA) nanowire transistor (NWT) in [100] orientation. Thickness (T) and width (W) range from T=W=3nm to T=W=8nm for square and circular cross-sectional shapes including 20 sub-bands.

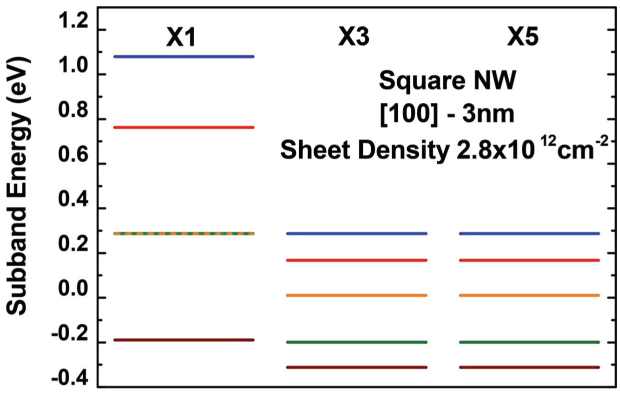
Physical Model - Kubo-Greenwood



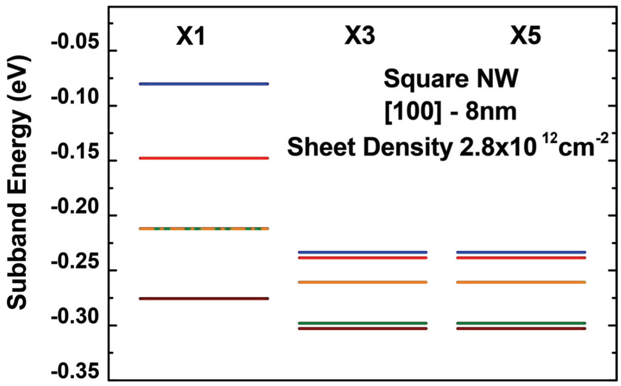
- The multisub-band effects in the scattering rates are generally more pronounced for smaller W.

Physical Model - Kubo-Greenwood

3 nm cross-section



8 nm cross-section



- The multisub-band effects in the scattering rates are generally more pronounced for smaller W.
- Higher energy difference between sub-bands minimizes the electron transitions.

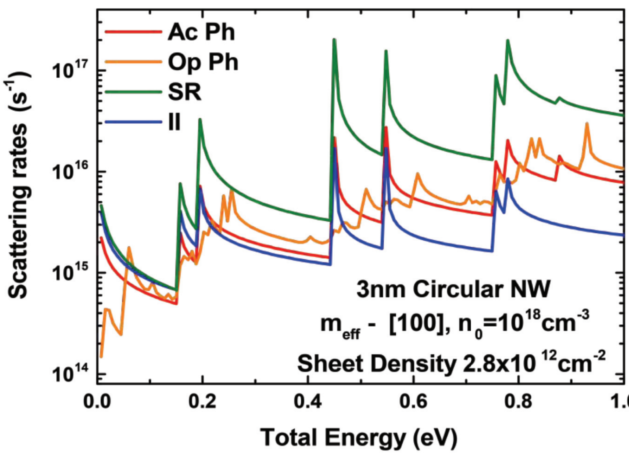
Physical Model - Kubo-Greenwood

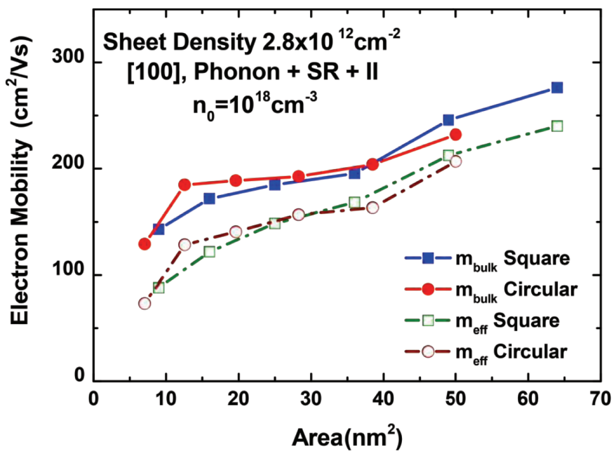
Scattering mechanisms:

- Elastic intra-valley acoustic phonon
- g- and f-type optical phonon
- Ionized impurity
- *Surface Roughness*

Si Nanowire transistors [100]:

- Effective mass calculation for each device
- Different width/height: 3nm – 8nm
- Different shape: square and circular





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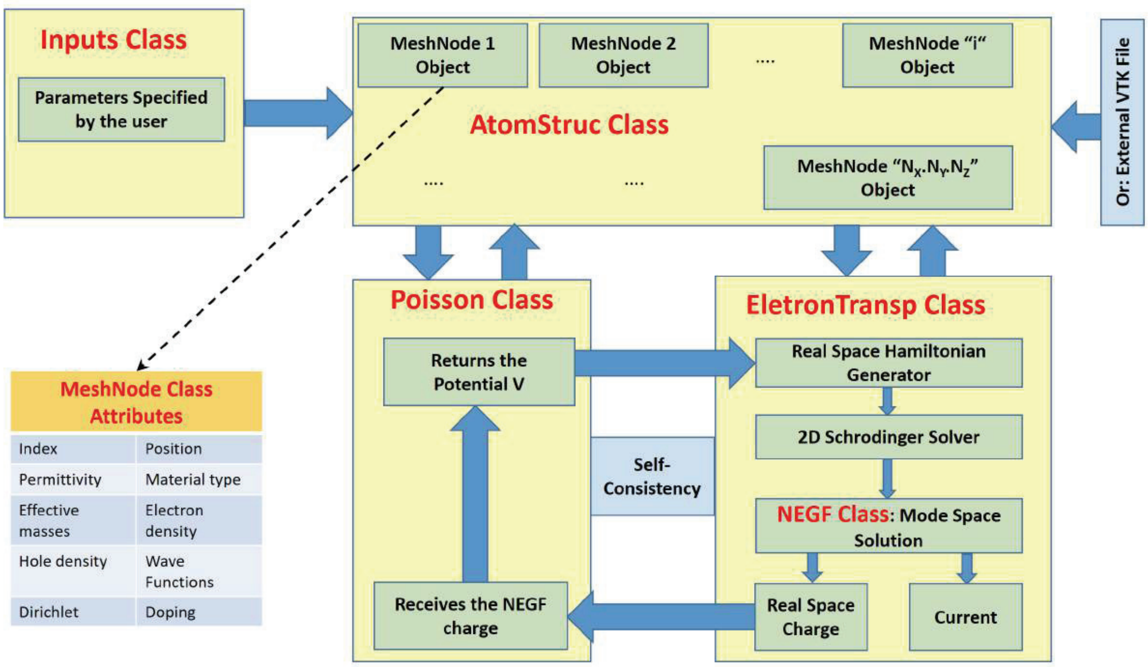
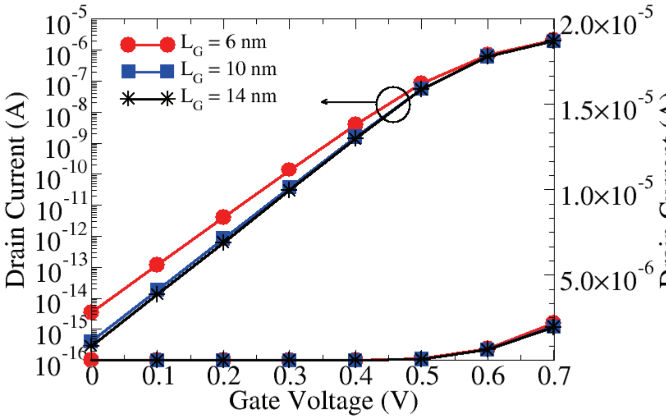
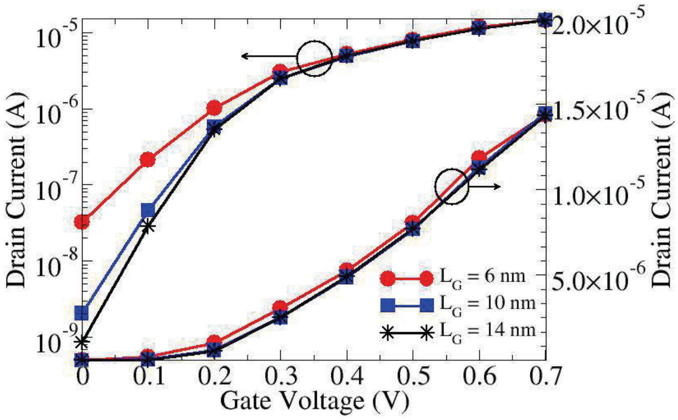
Physical Model - NEGF



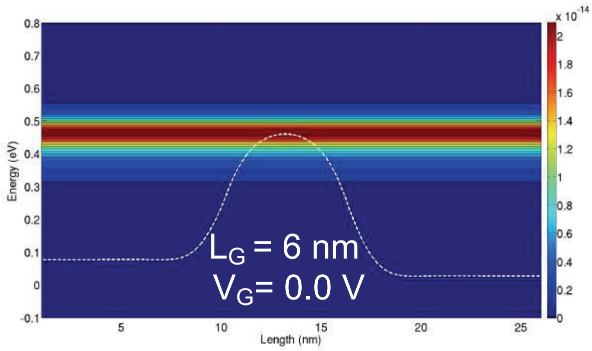
- Nano-Electronic Simulation Software (NESS) - University of Glasgow Device Simulator

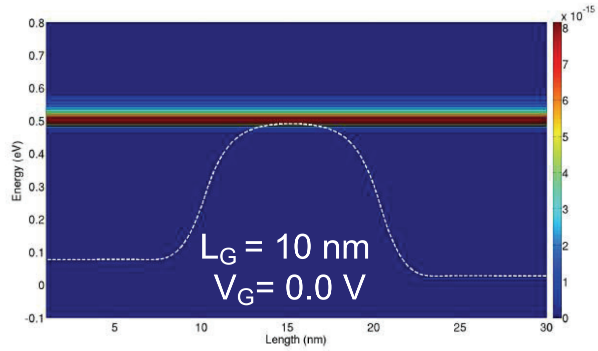
Physical Model - NEGF

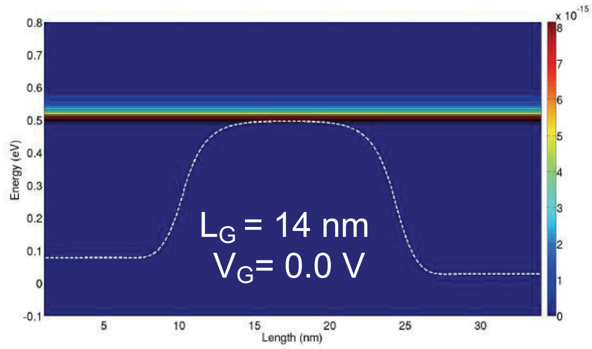




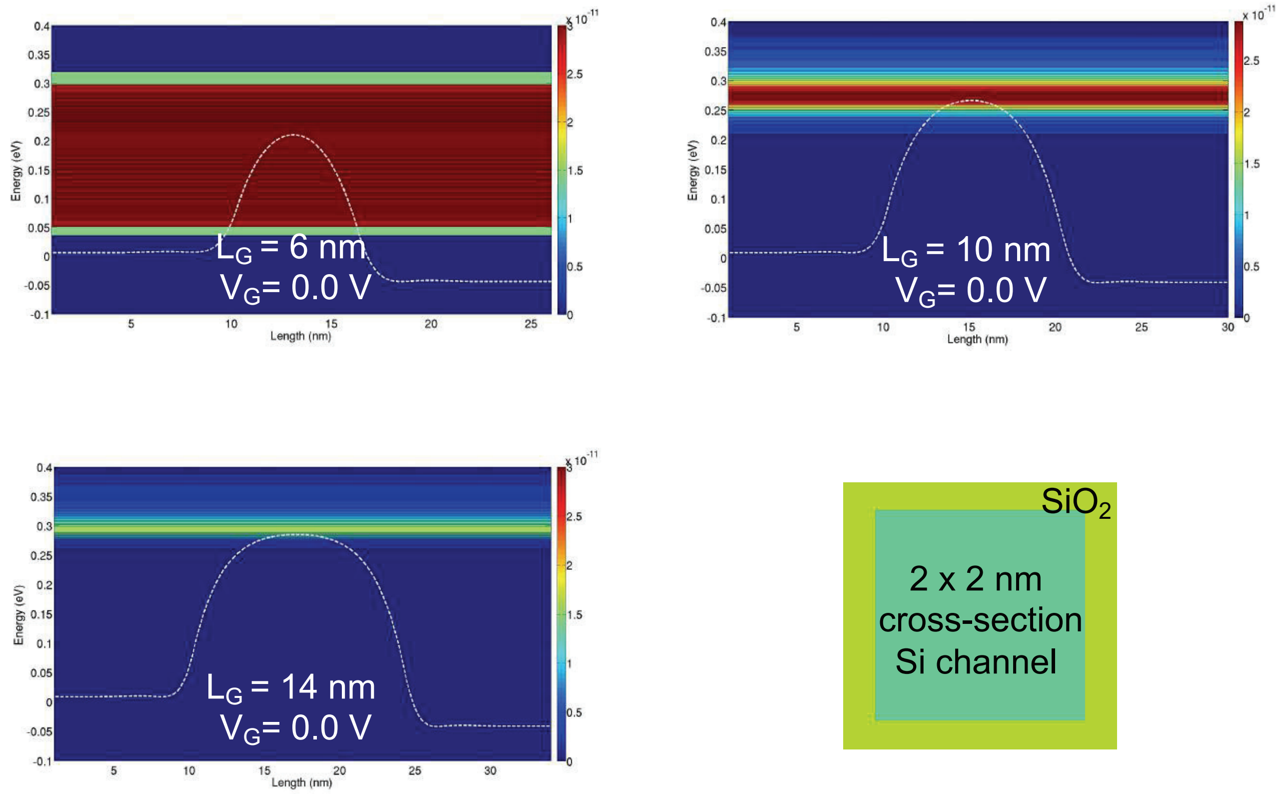
Physical Model - NEGF



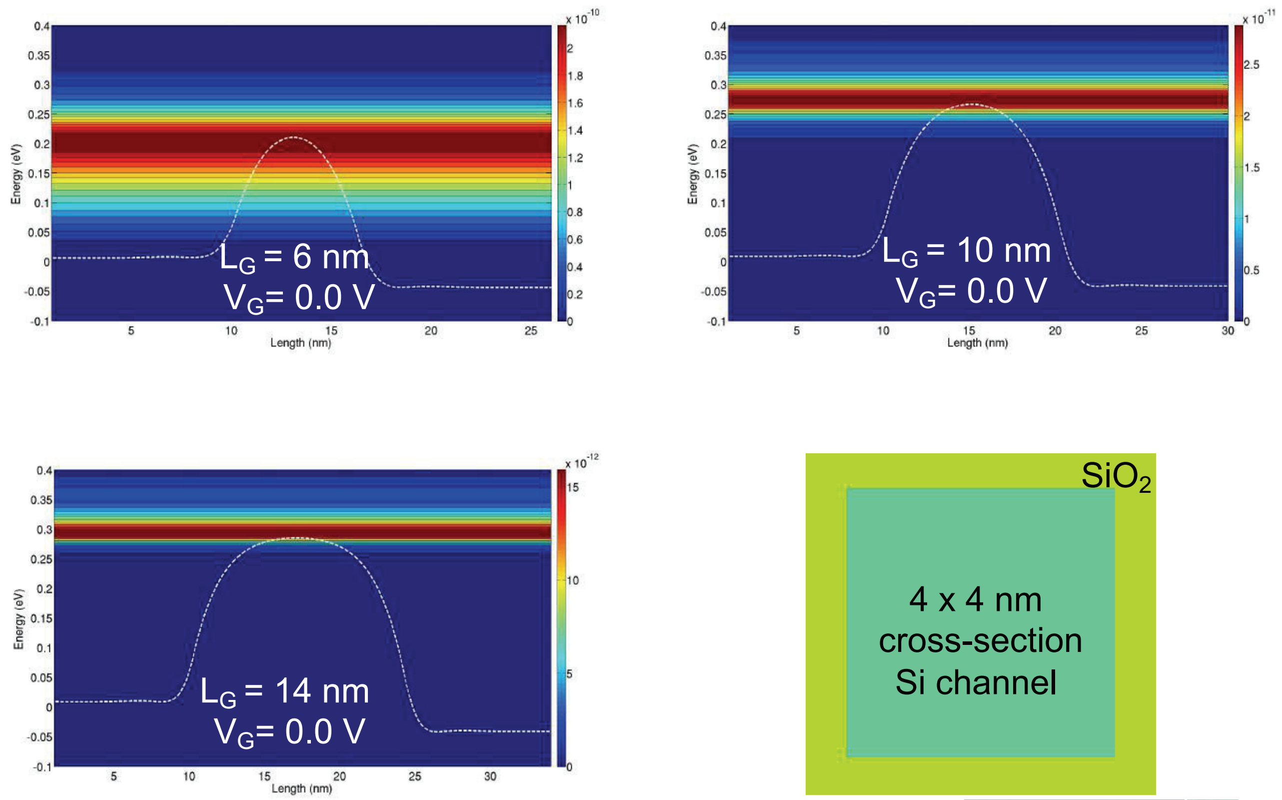




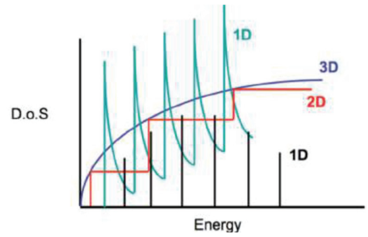
Physical Model - NEGF

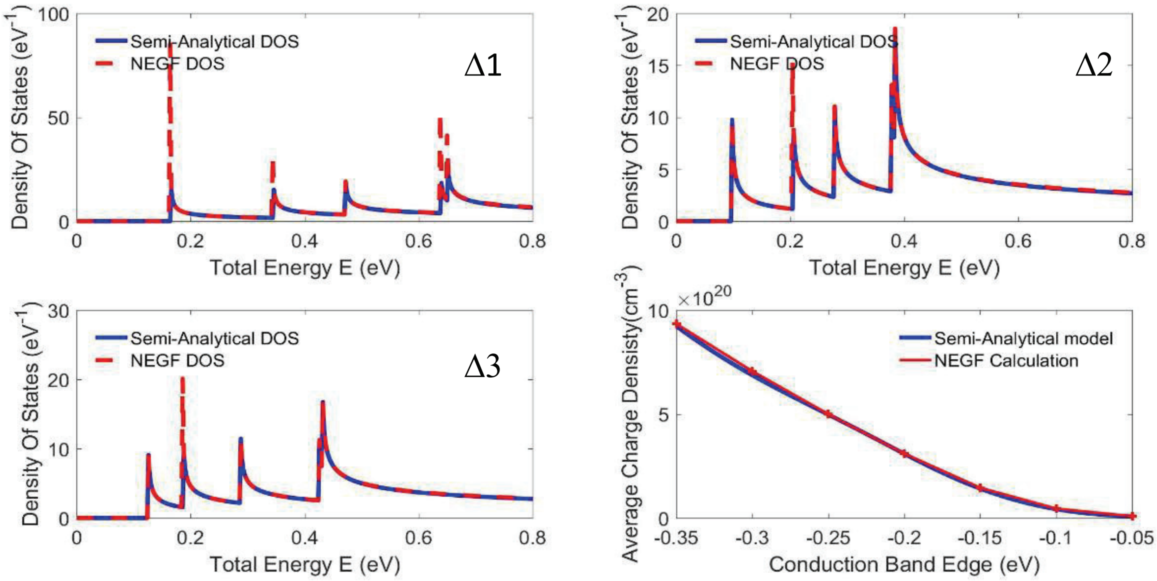


Physical Model - NEGF



Physical Model - NEGF





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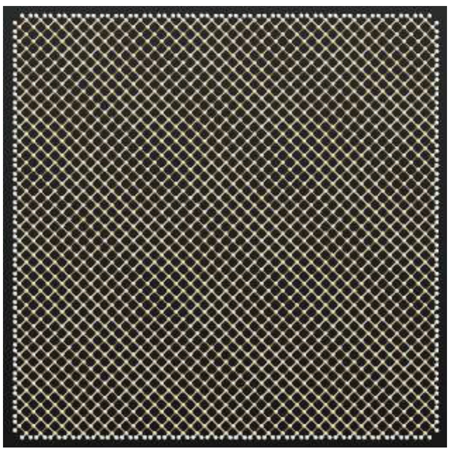
Physical Model - Band Structure

8nm Square Si NW

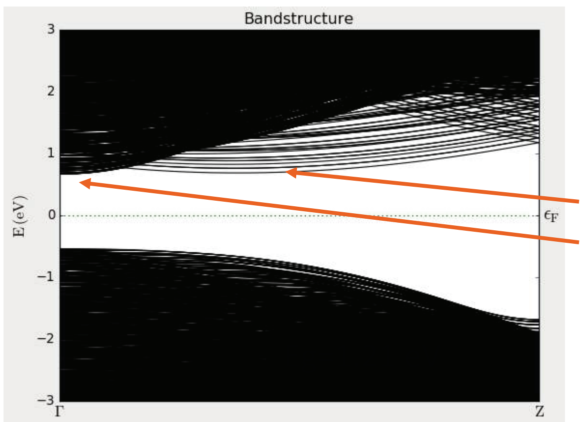


Simulation Method

- ***sp3d5s* tight binding*** with a Boykin parameter set
- No geometric optimization
- [100] transport direction

From reference [PRB 69 115201 (2004)]

- Effective mass of bulk Si: 0.891, 0.201 m_e (longitudinal, transverse)
- Bandgap: 1.131 eV



Effective mass (parabolic fit)

m_l: 0.900 m_e

m_t: 0.215 m_e

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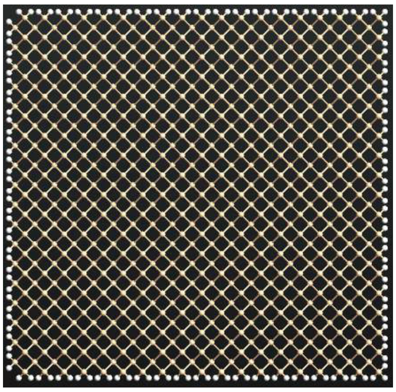
Physical Model - Band Structure

5nm Square Si NW



Simulation Method
- ***sp3d5s* tight binding*** with a Boykin parameter set
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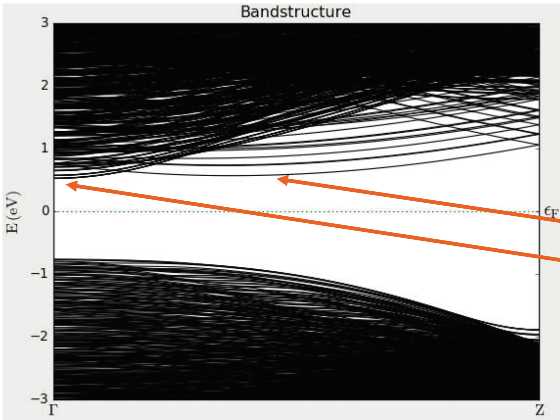
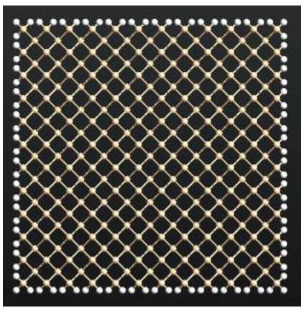


Effective mass (parabolic fit)
m_l: 0.917 m_e
m_t: 0.231 m_e

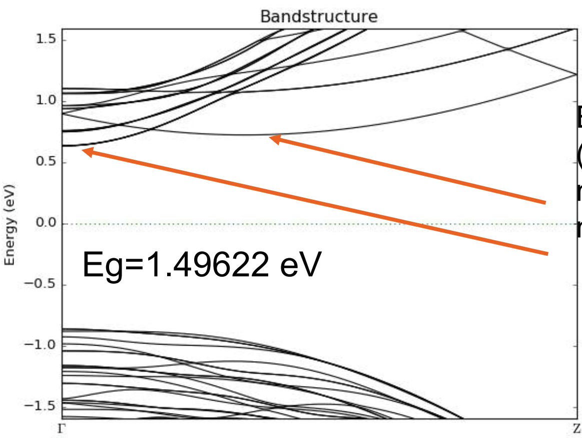
Physical Model - Band Structure

3nm Square Si NW



Simulation Method
- ***sp3d5s* tight binding*** with a Boykin parameter set
- No geometric optimization
- [100] transport direction

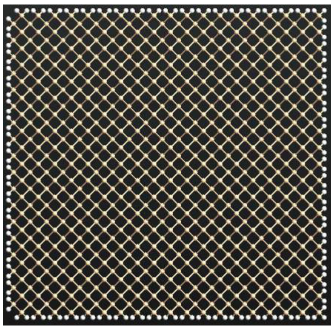
From reference [PRB 69 115201 (2004)]
- Effective mass of bulk Si: 0.891, 0.201 m_e (longitudinal, transverse)
- Bandgap: 1.131 eV

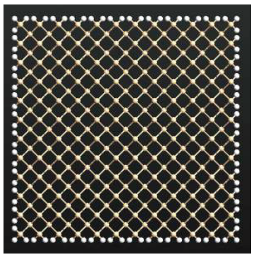


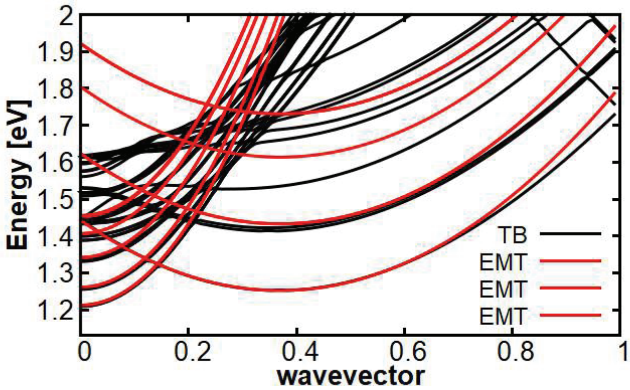
Effective mass (parabolic fit)
m_l: 0.951 m_e
m_t: 0.268 m_e

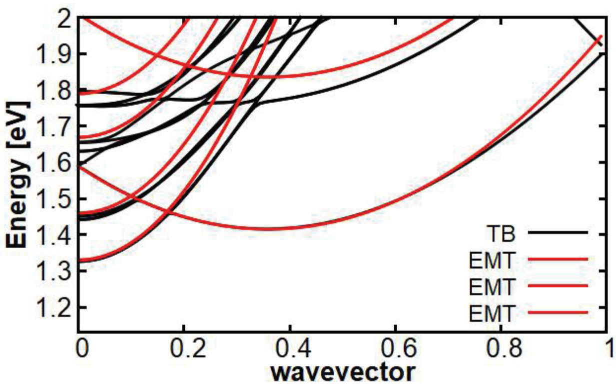
Physical Model - Band Structure

5nm Square Si NW | **3nm Square Si NW**

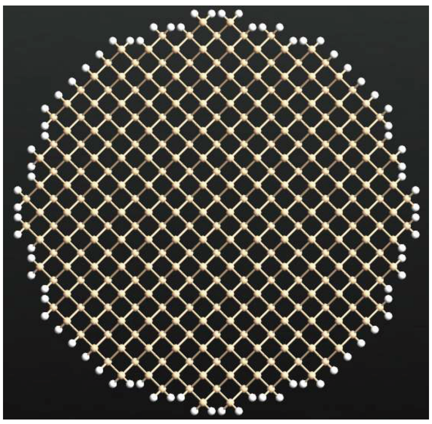


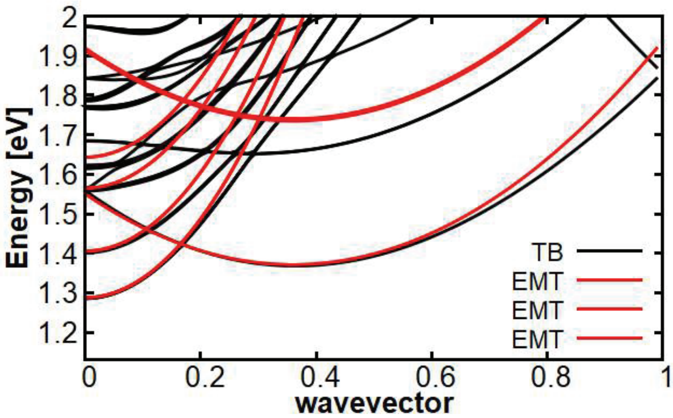






Physical Model - Band Structure (Task 4.1.4)





Atomic structure of Si NW (3.82 nm)

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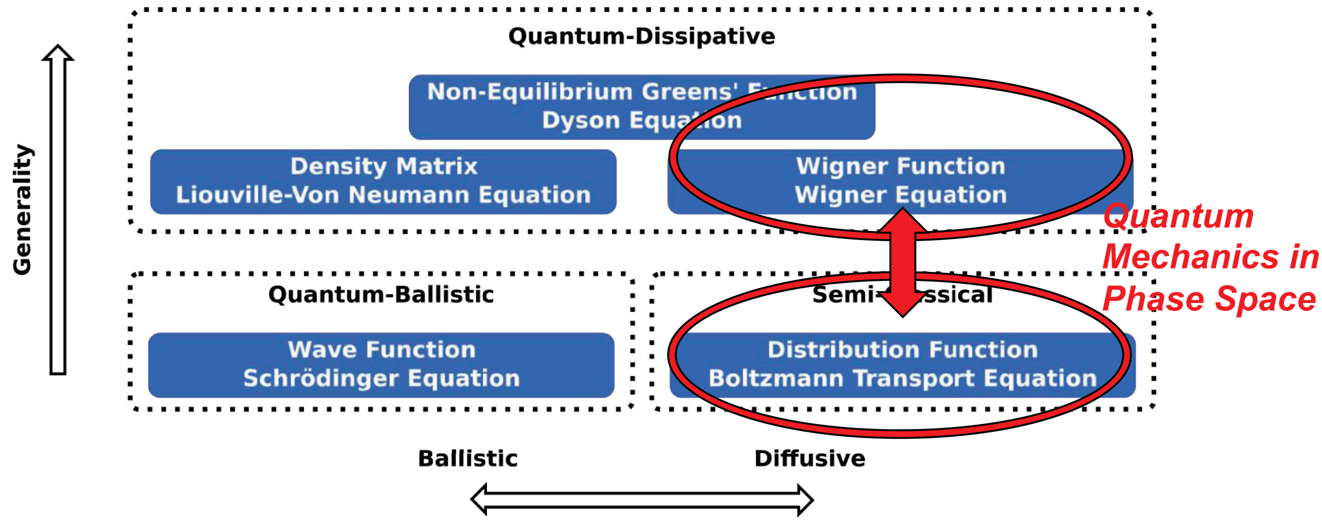
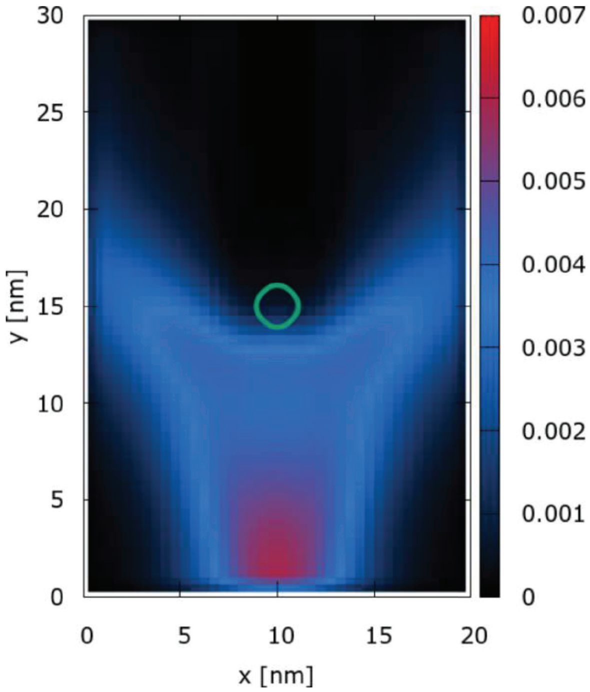
Physical Model - Wigner MC



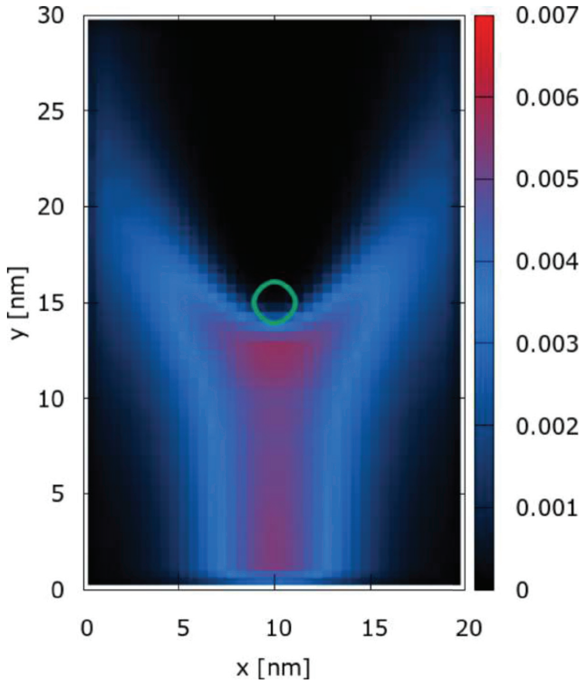
Signed particle **approach supports switching between**

- **Quantum particle evolution: Wigner transport**
- **Classical particle evolution: Boltzmann transport**

Physical Model - Wigner MC

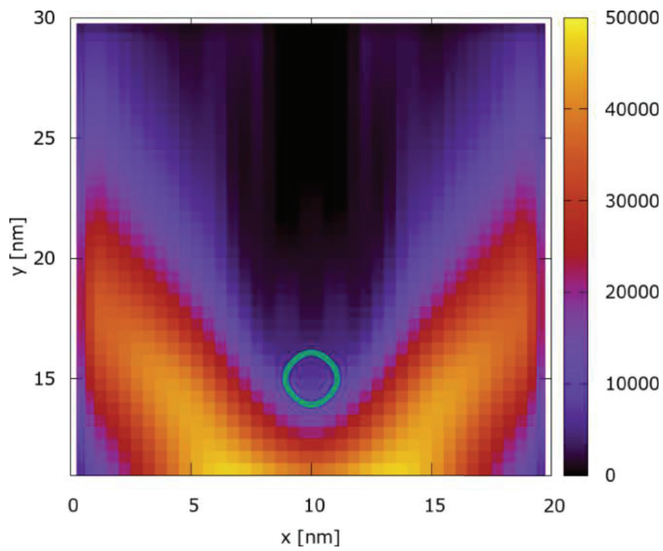


Quantum electron density [a.u.]

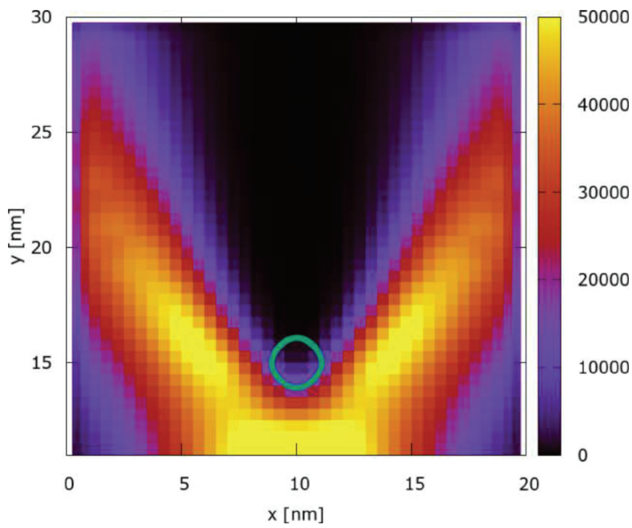


Classical electron density [a.u.]

Physical Model - Wigner MC

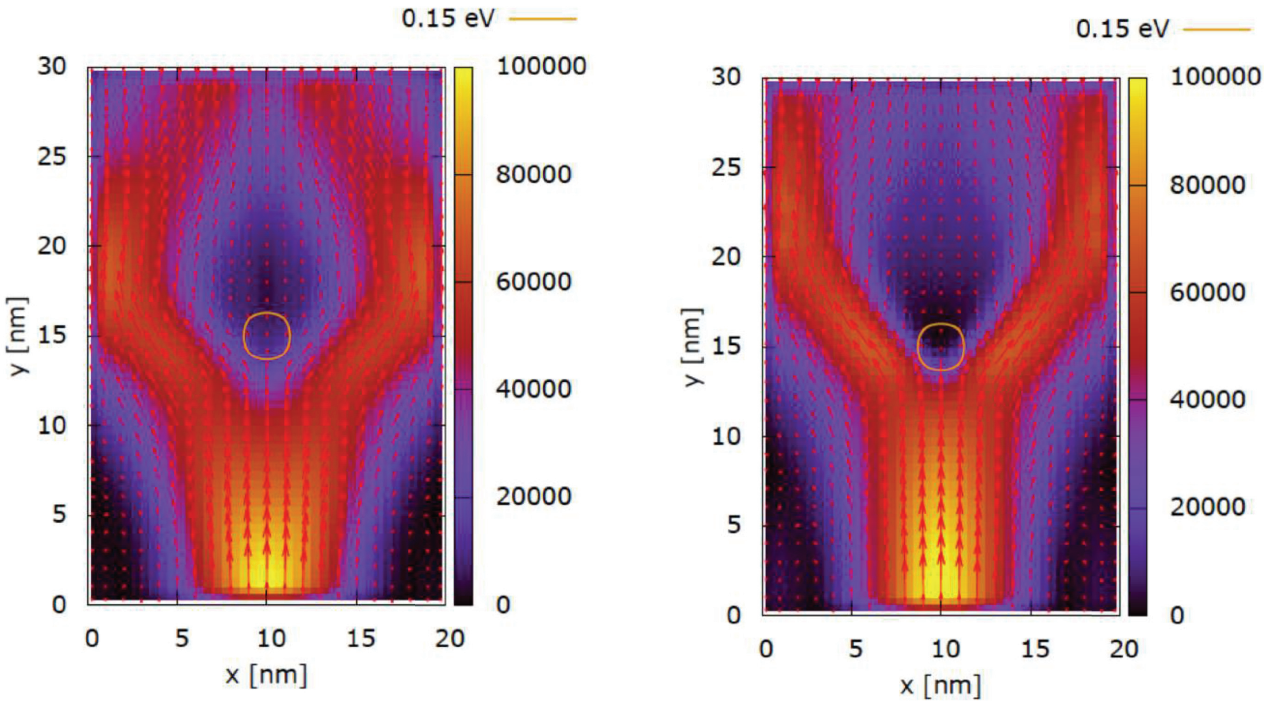


Quantum current density [a.u.]



Classical current density [a.u.]

Physical Model - Wigner MC



With lateral reflecting boundaries

Quantum current density [a.u.]   Classical current density [a.u.]

Conclusions and Outlook

- Physical models and methods
  - Drift Diffusion Method (DD)
    - Fast and well established method but needs quantum corrections
  - Kubo-Greenwood
    - Particle statistical method, needs the appropriate scattering models, good for evaluating mobility in the devices
  - Non-Equilibrium Green's Function (NEGF)
    - Wave representations of the carriers, able to capture quantum mechanical tunneling
  - Wigner Monte Carlo
    - Particle statistical method, quantum mechanics in phase space