Point defect scattering in Si nanowires

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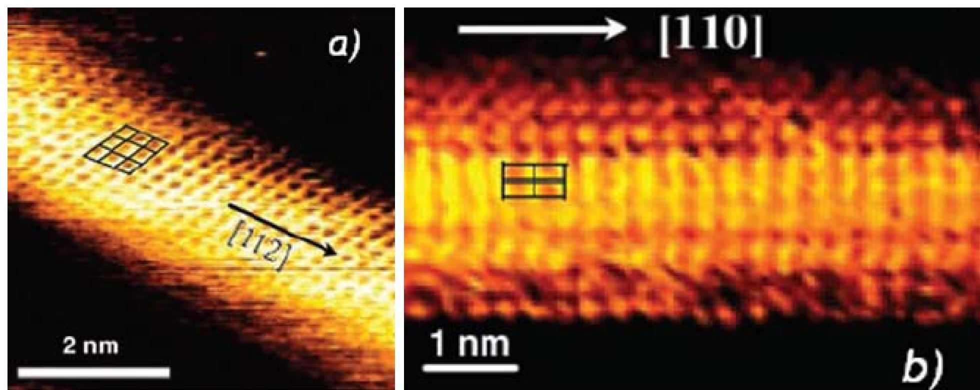
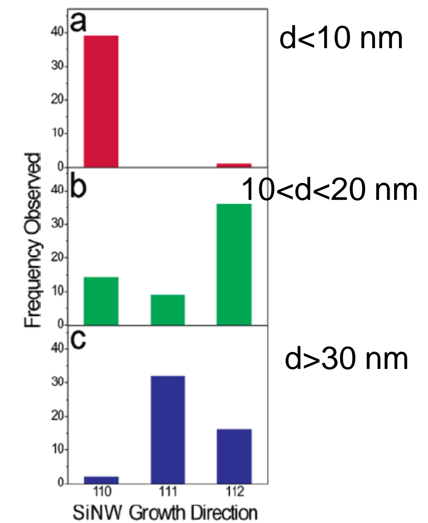
Outline

- Introduction
- DFTB and extensions to NEGF
- Results of charged defect scattering in SiNW

D. D. D. Ma. *et al.*, *Science*, vol. 299, pp. 1874-1877, 2003





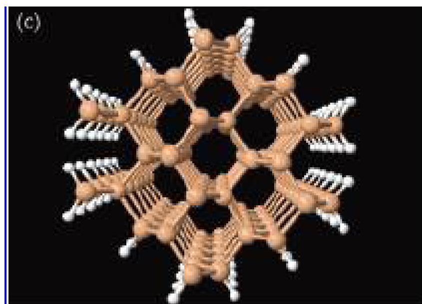
d<10 nm

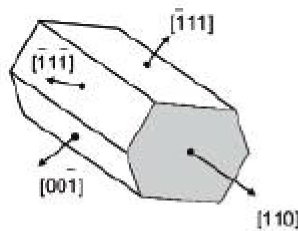
10<d<20 nm

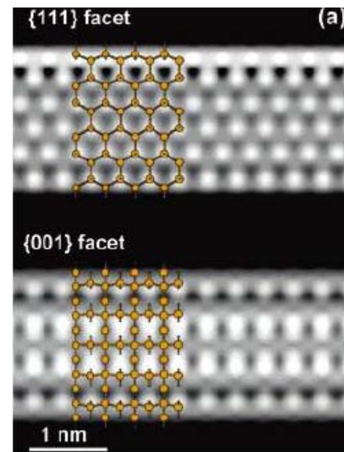
d>30 nm

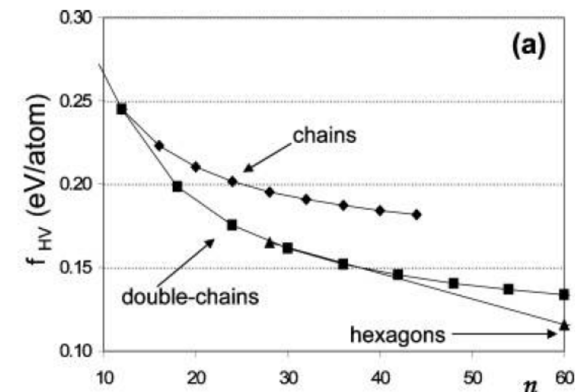
Low diameter (110) SiNW are energetically favoured

Show less sensitivity to disorder and size variations



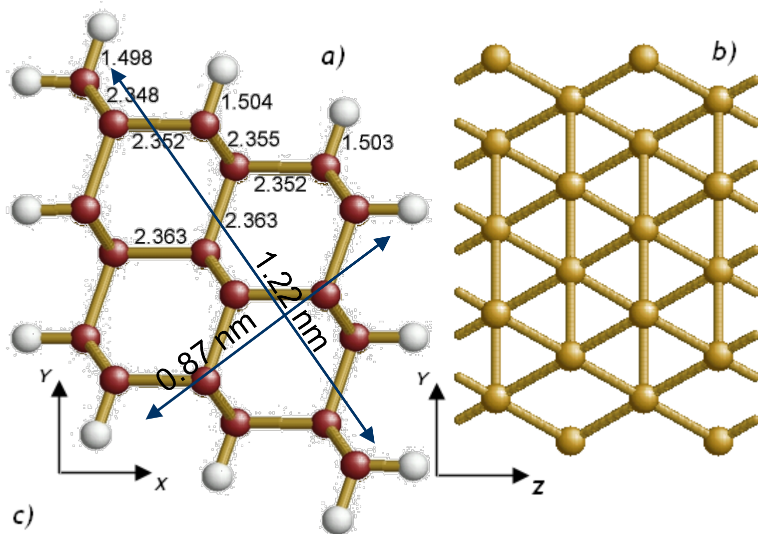






Tzu-Liang Chan, Nano Lett., Vol. 6, No. 2, 2006

Structures



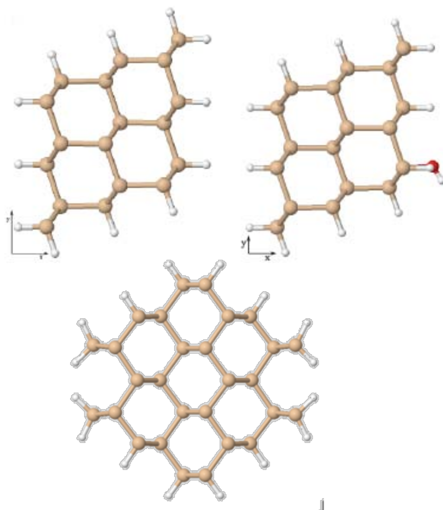
We considered [110] oriented SiNW

Total energy minimization has been performed with semi-empirical DFTB

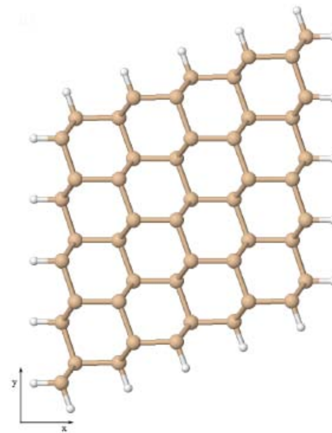
The structures are H-passivated

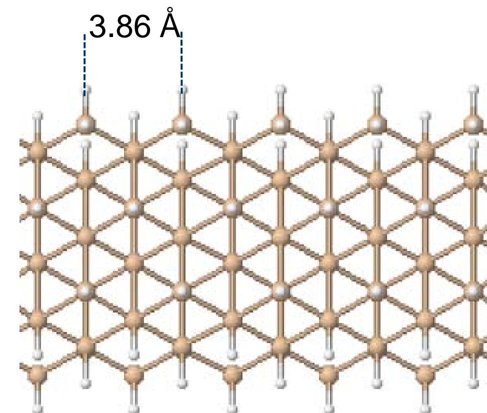
Calculations on SiNW of 1.2-2.0 nm

1.2 nm



2.0 nm





DFTB = DFT based Tight-Binding method

Kohn-Sham equation:

$$\sum_{\nu}\left[H^{0}_{\mu\nu} + H^{Scc}_{\mu\nu}[\delta n] - E_k S_{\mu\nu}\right]c^k_{\nu} = 0$$

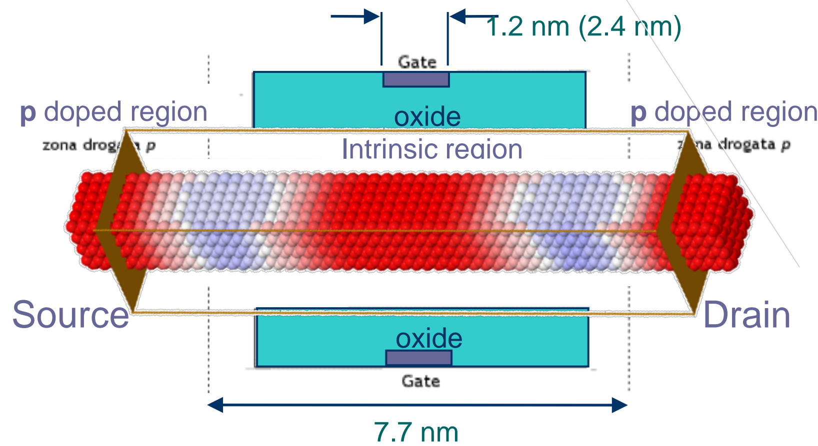
$$H_{\mu\nu} = \begin{cases} \varepsilon_{\mu} & \text{onsite atomic energy levels} \\ \langle \mu | V[n^0_{\mu} + n^0_{\nu}] | \nu \rangle & \text{two-centre density superposition} \end{cases}$$

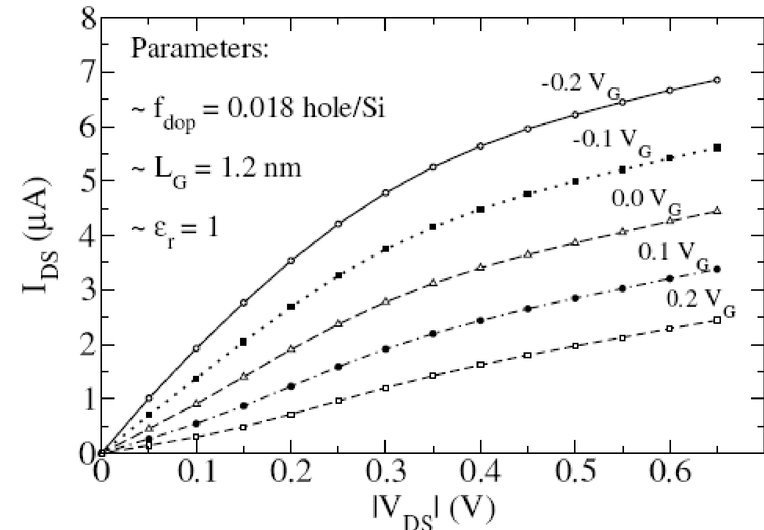
$$S_{\mu\nu} = \langle \mu | \nu \rangle$$

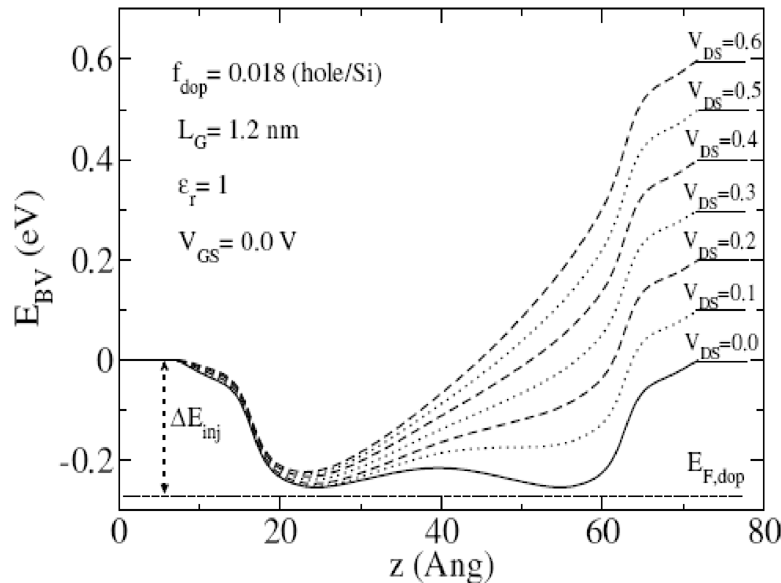
$$H^{Scc}_{\mu\nu} = \frac{1}{2} S_{\mu\nu} \sum_{\sigma} \left(\gamma_{\mu\sigma} + \gamma_{\nu\sigma}\right) \Delta q_{\sigma}$$

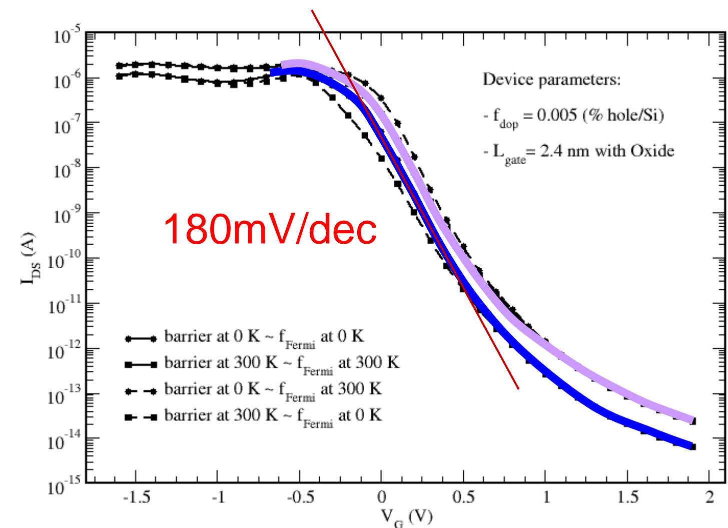
[Elstner, et al. Phys. Rev. B 58 (1998) 7260]

SiNW MOSFETs



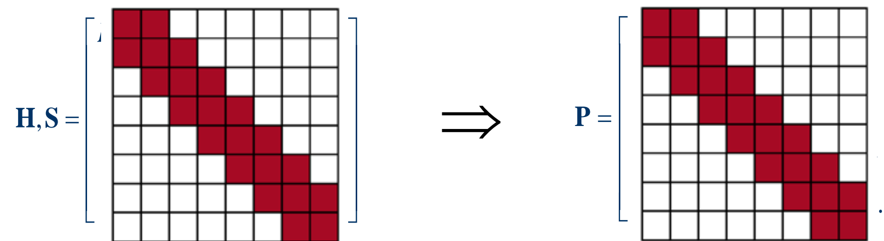




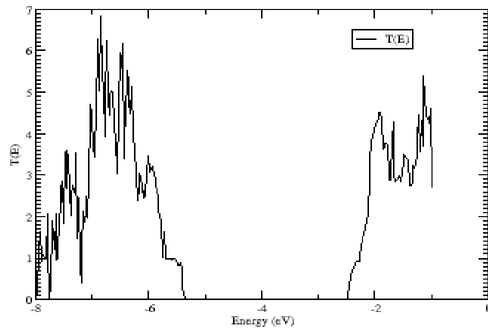


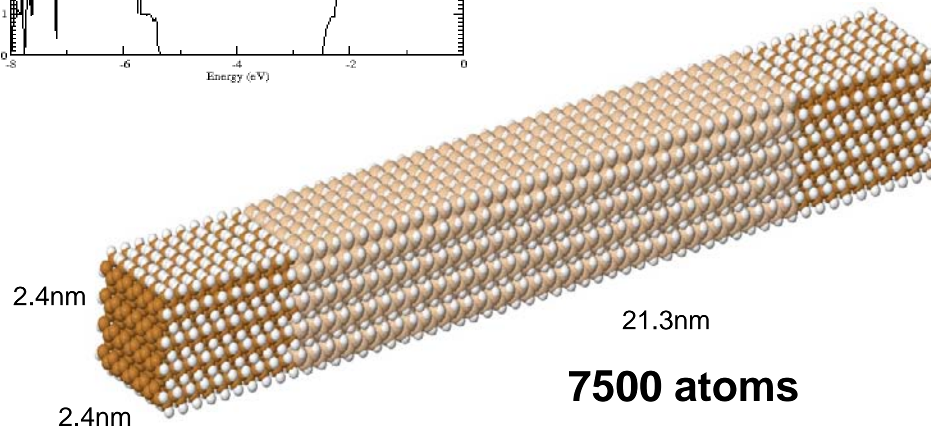
[Pecchia et al., IEEE trans. nanotechnol. (2007)]

Iterative scheme



$$q_\mu = \sum_\nu \mathbf{P}_{\mu\nu} \mathbf{S}_{\nu\mu}$$



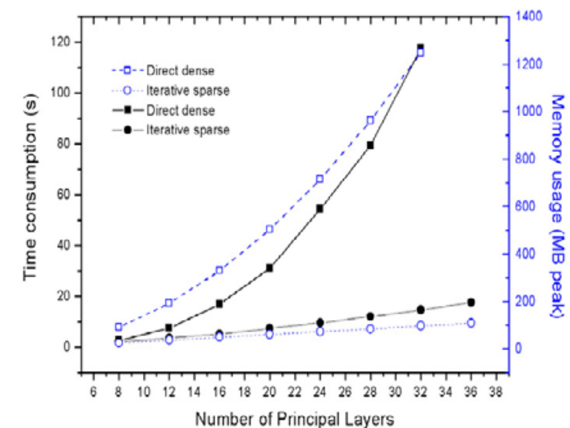


7500 atoms

PROFILING

Charge density and potential:	20 h
Density of States (350 points):	6 h
Peak memory:	876 MB

Calculations on single PC Linux core
Intel(R) Core(TM)2 CPU 6600 @ 2.40GHz

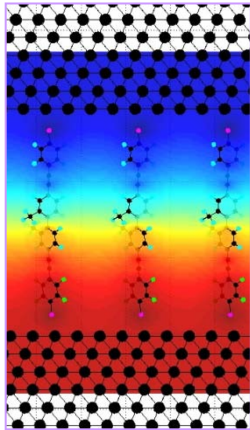


O(N m^3)

[Penazzi, et al. New J. Phys. 10 (2008)]

Poisson solver

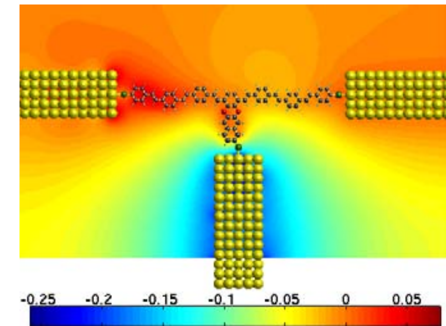
2-terminals



Discretize in real space

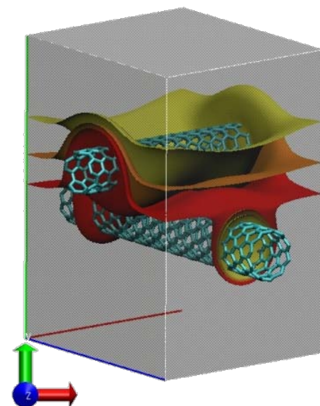
$$\Delta\rho(r) = \sum_{\mu} \Delta q_{\mu} n_{\mu}(r)$$

gated (3-term.)

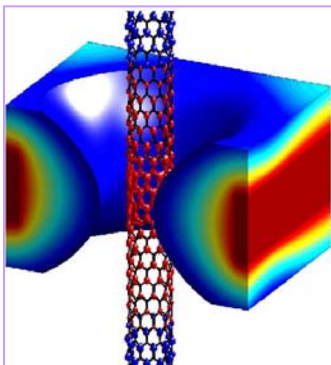


The Poisson equation is solved with a multi-grid algorithm (MUDPACK).

4-terminals



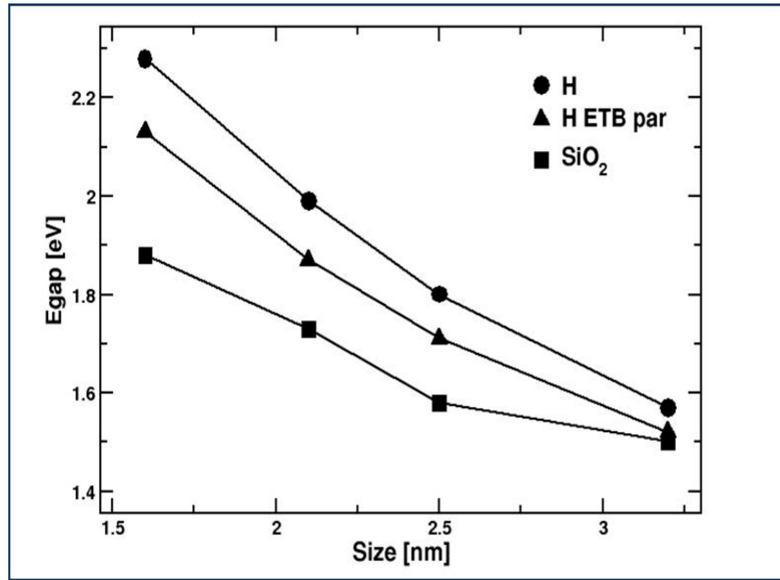
coaxially-gated

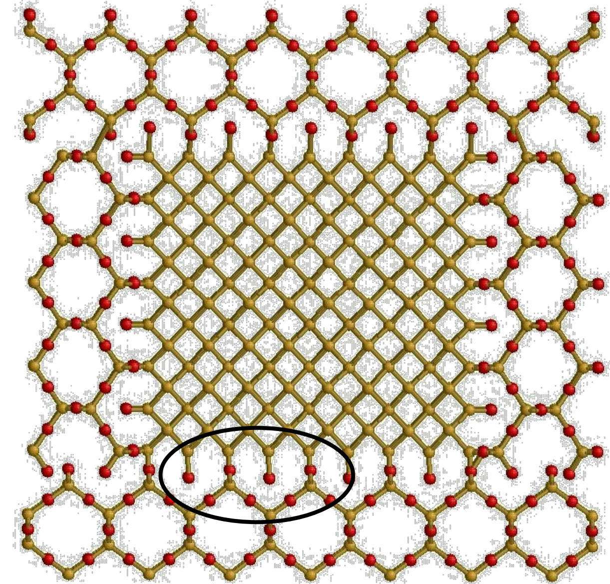


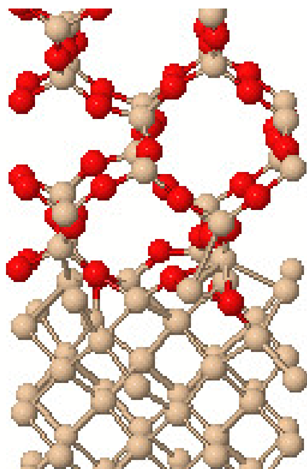
This allows to solve complex boundary conditions (bias, gate)

$$\nabla^2 V = -4\pi\Delta\rho$$

Bandgap vs passivation







DFTB can be used to relax medium-sized structures/intrerfaces

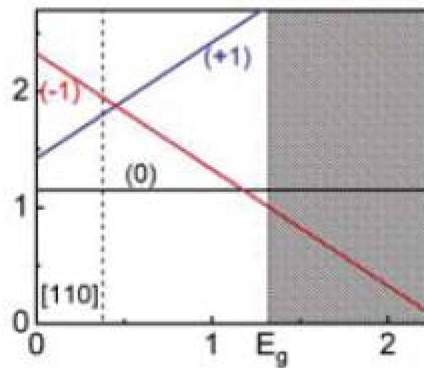
Challenge: realistic oxide around a NW (defect).

Charged impurity DB

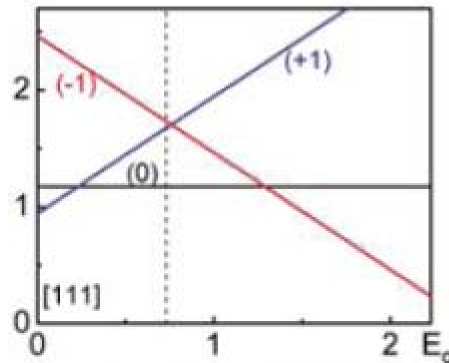
Ki-Ha Hong et al., *Nano Lett. 2010, 10, 1671-1676*

Phase stability diagrams of charged db defects

$$E_F^q = E_{SDB}^q - E_{SiNS}^0 + \mu_H + q(\varepsilon_{VBM} + \varepsilon_F)$$

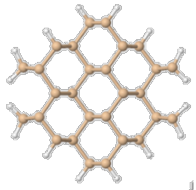


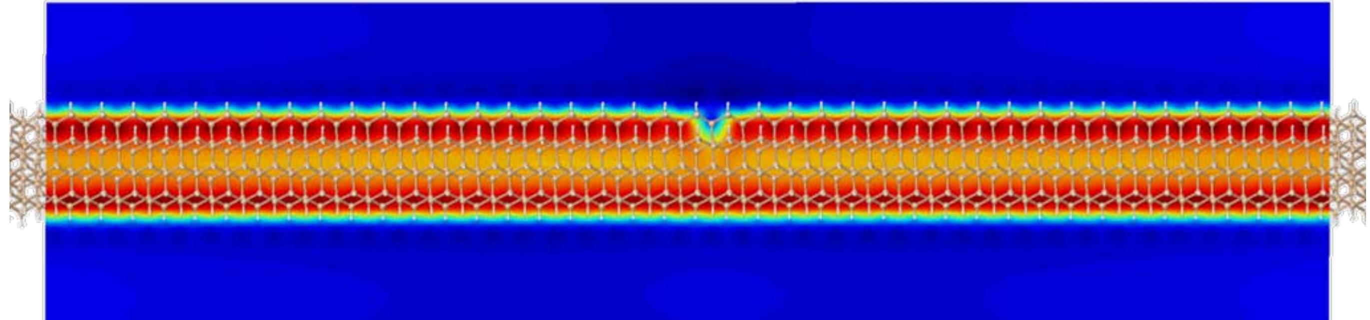
SiNW [110]
- can have negatively charged surface DB
- for Fermi Energy close to the CB.
- no positively charged DB.



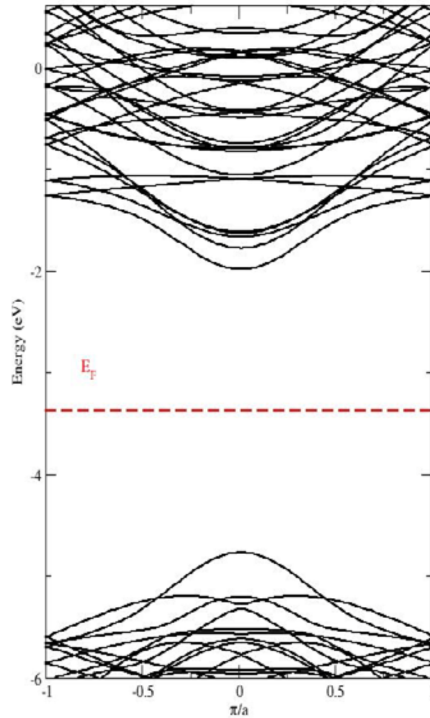
SiNW [111]
- can have negatively and positevely charged DB

Bandstructures and DB states

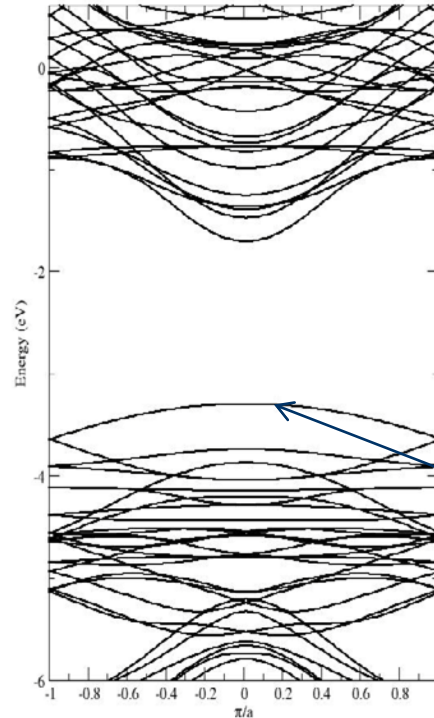




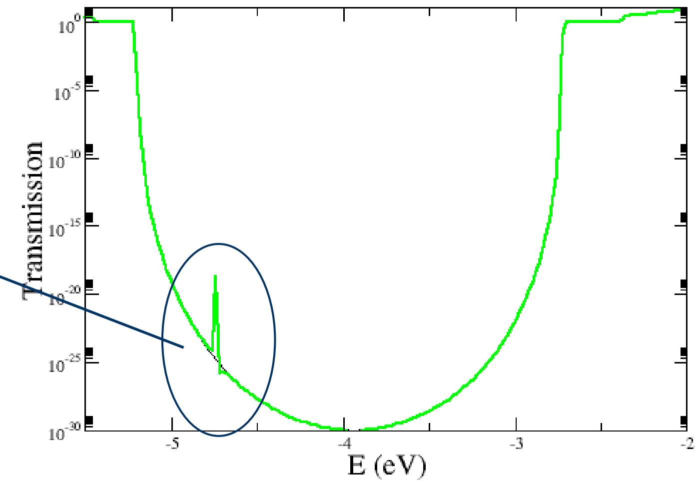
[110]SiNW H-passiv.



[110]SiNW

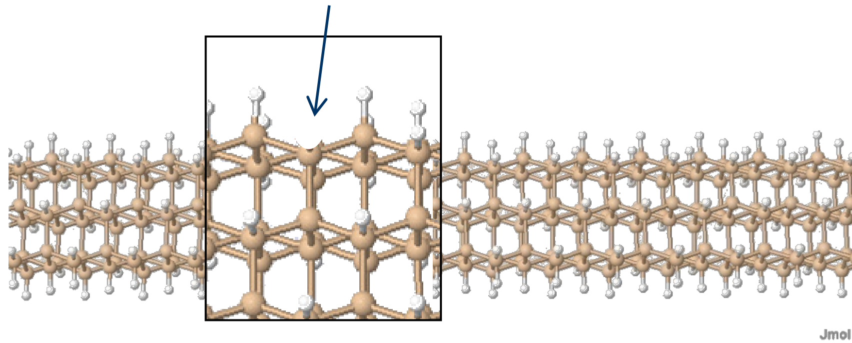


DB state

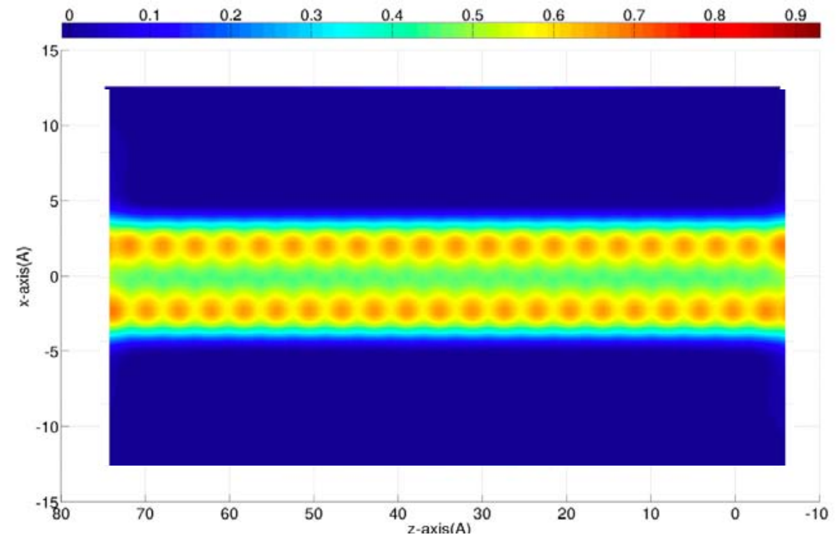


DB in p-doped SiNW

- Si dangling bond on **p-doped** SiNW (110)

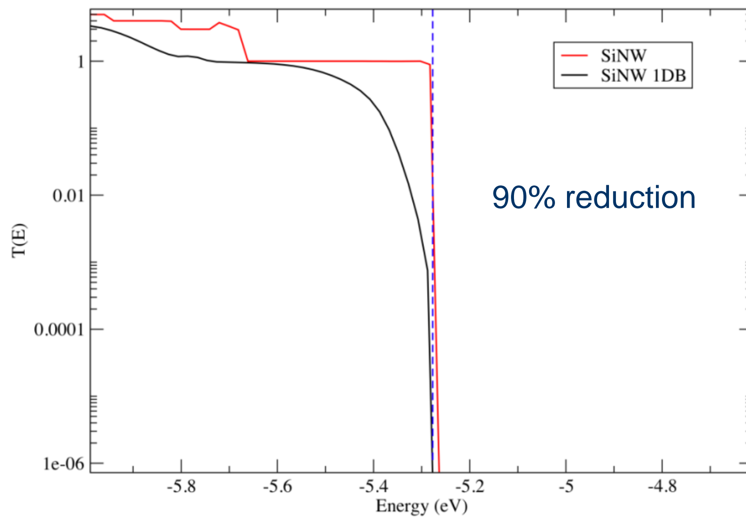


Potential (V)

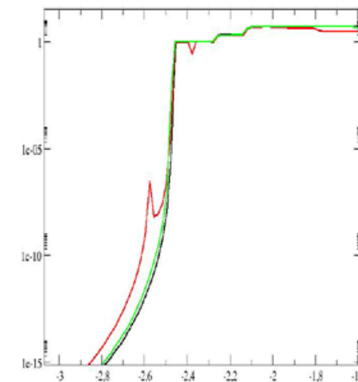


0.002 e/atom ⇔ $9.3\ 10^5\ cm^{-1}$
⇔ $10^{20}\ cm^{-3}$

Valence band



Conduction band

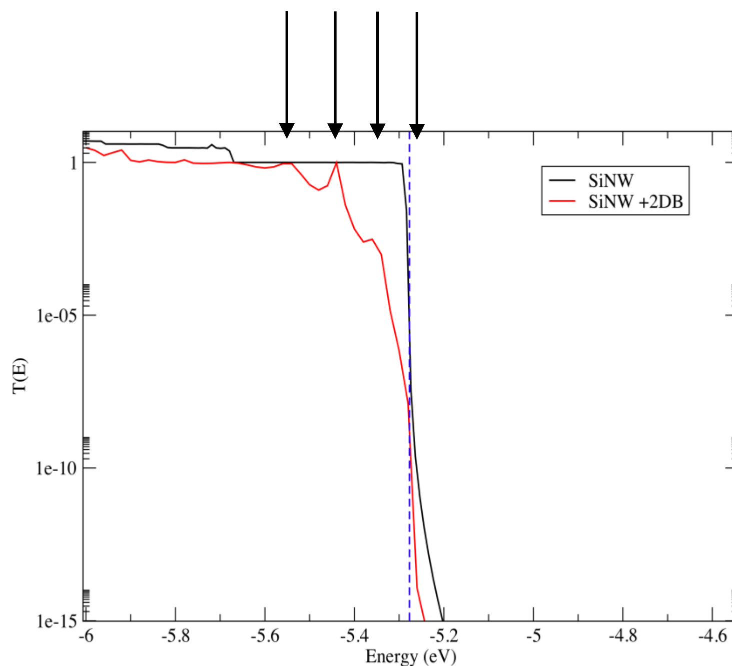


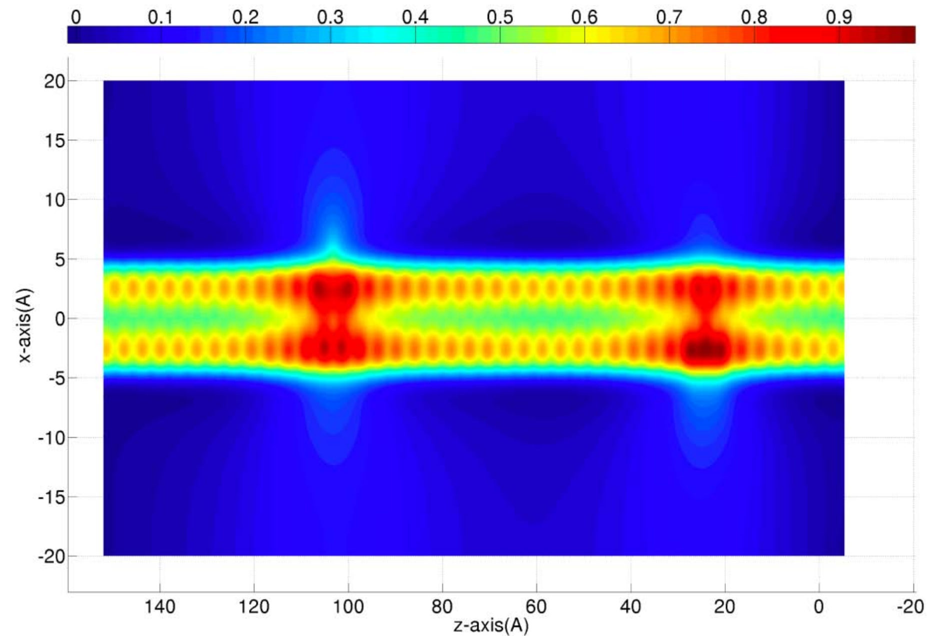
Effects of two defects

2 DG bonds produce a further reduction

DG bonds are on 2 random sides

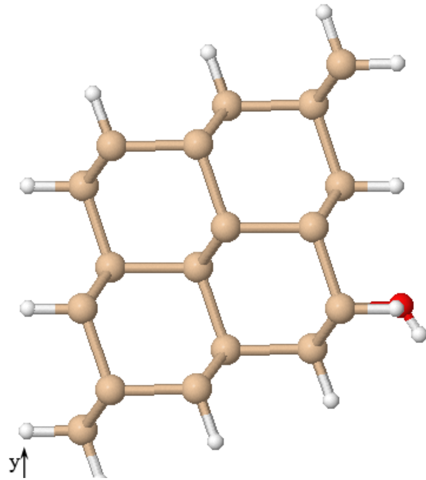
Interference peaks

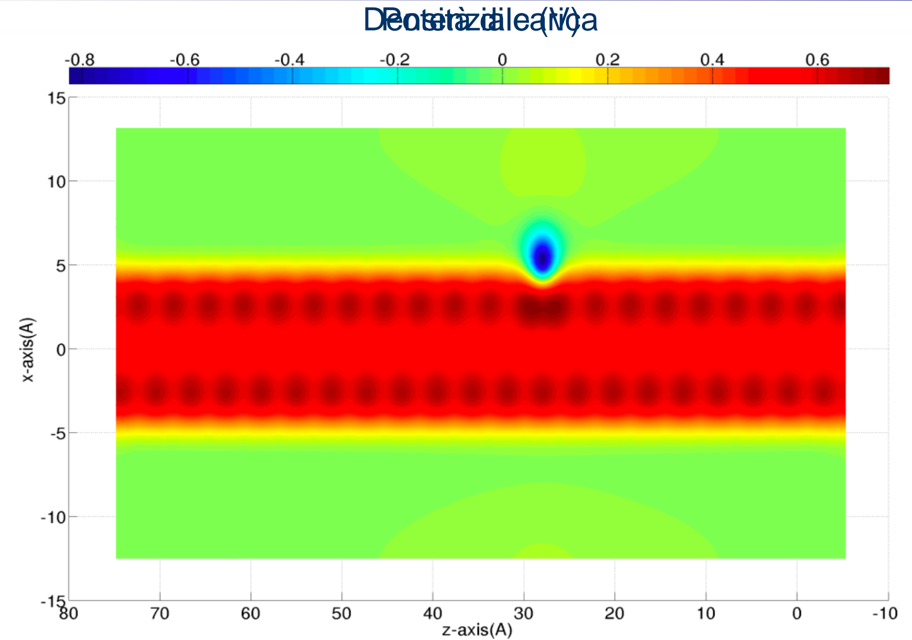


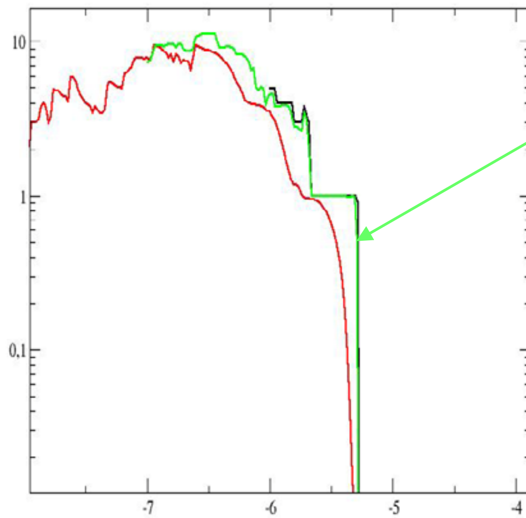


Nanowire	$G(E_f)$ [Ω^{-1}]	Δ%
SiNW Ideal (7.72 nm)	5.04×10^{-5}	-
SiNW 1DB (7.72 nm)	5.08×10^{-6}	90.69%
SiNW 2DB (15.22 nm)	4.27×10^{-6}	91.53%

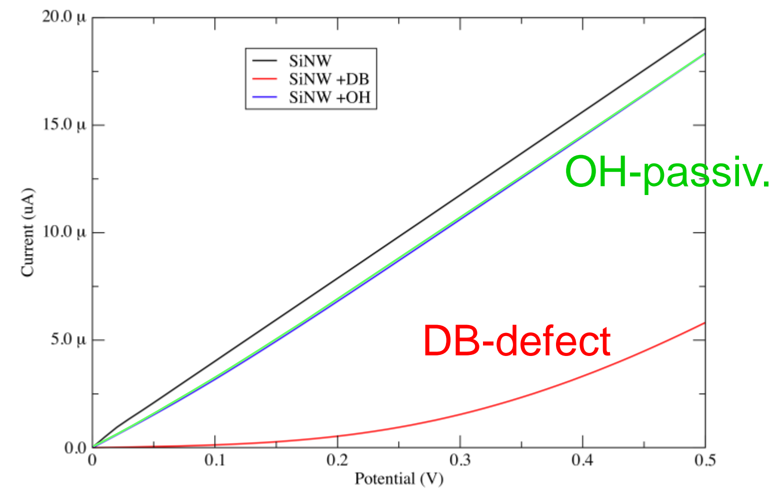
OH passivated bond



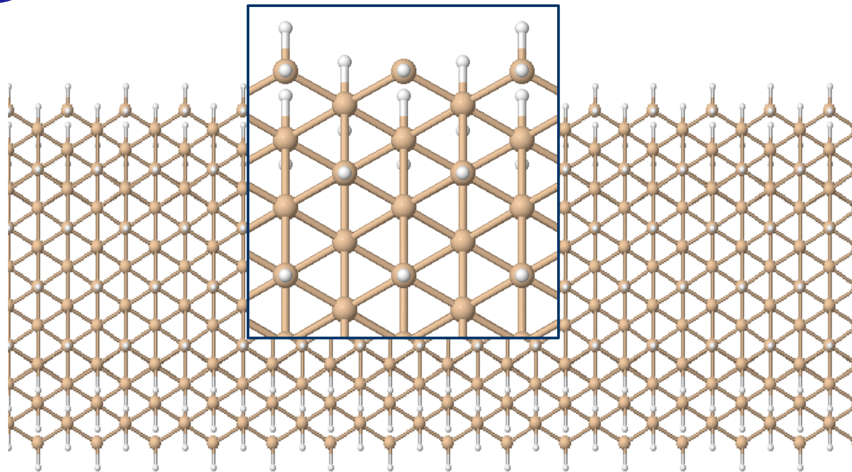


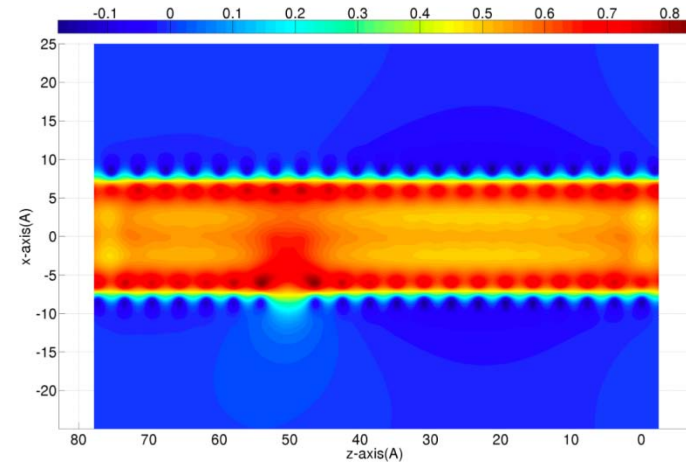


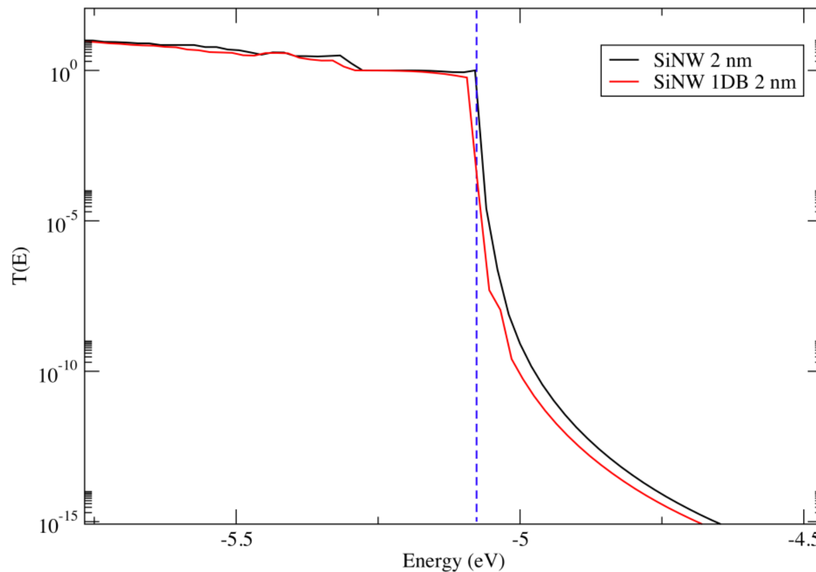
OH passivated



2nm p-SiNW





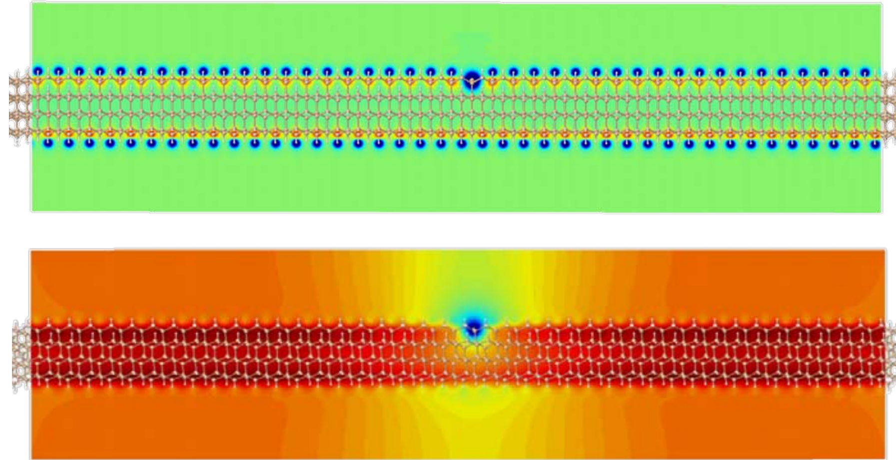


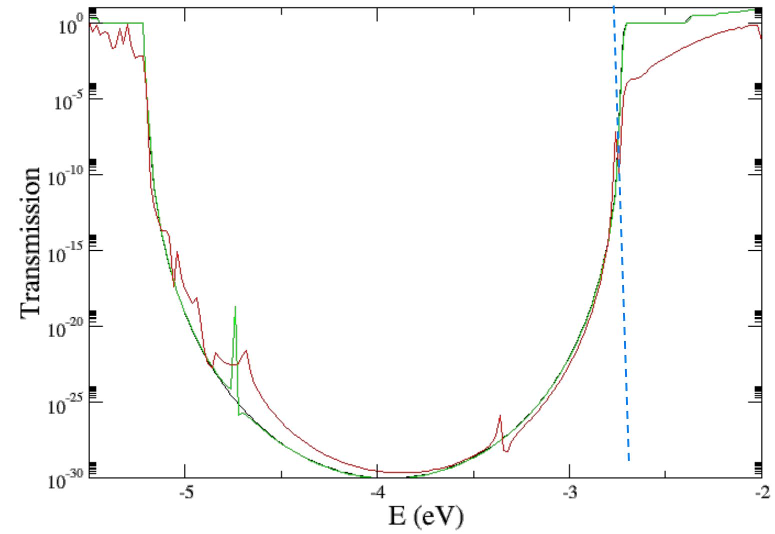
Less severe effect: 32% reduction

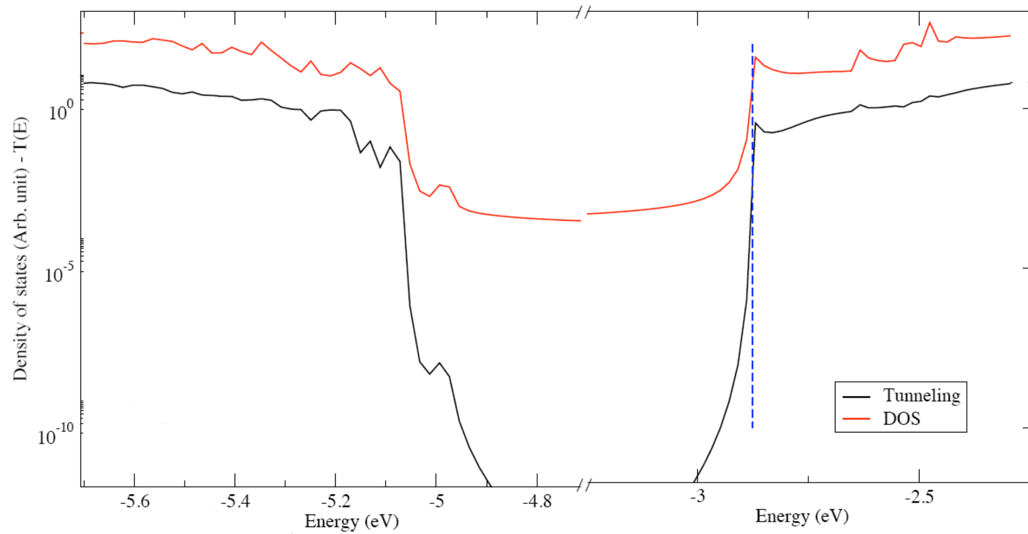
The DB defect is practically **neutral**

n-doped SiNW

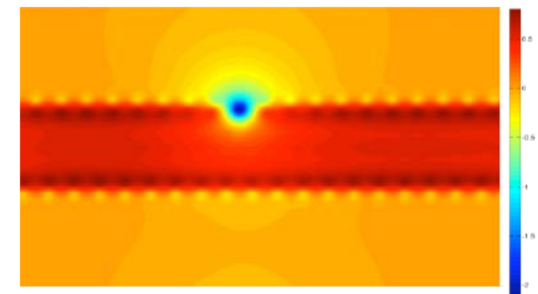
1.2 nm



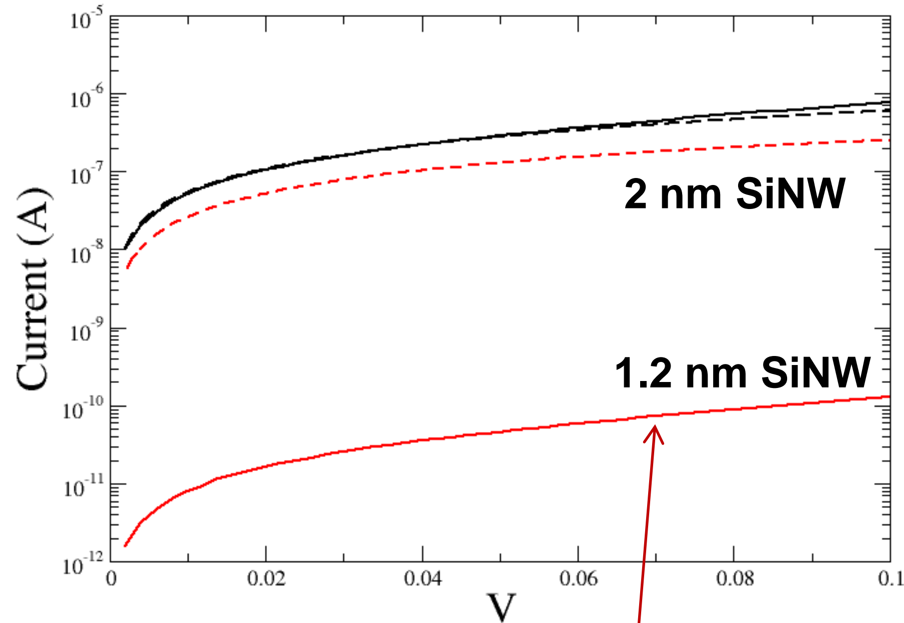


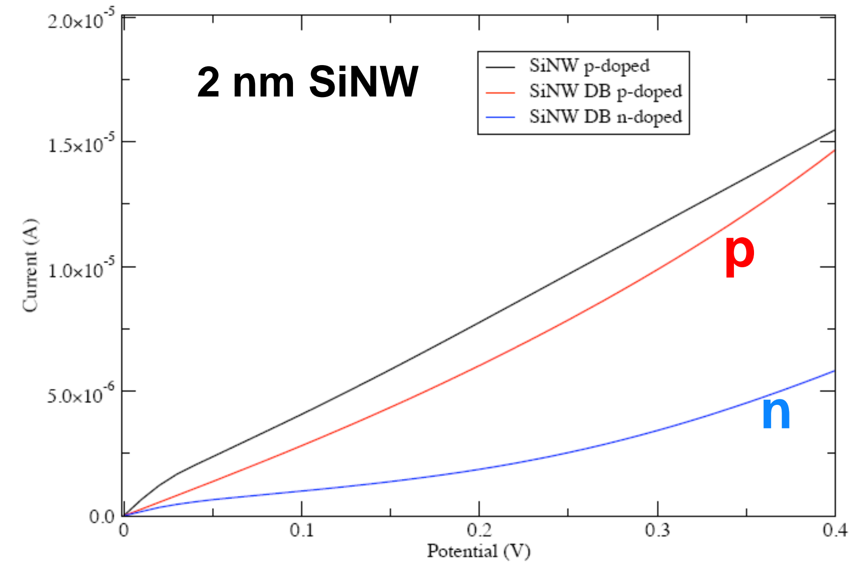


2 nm



I-V n-SiNW





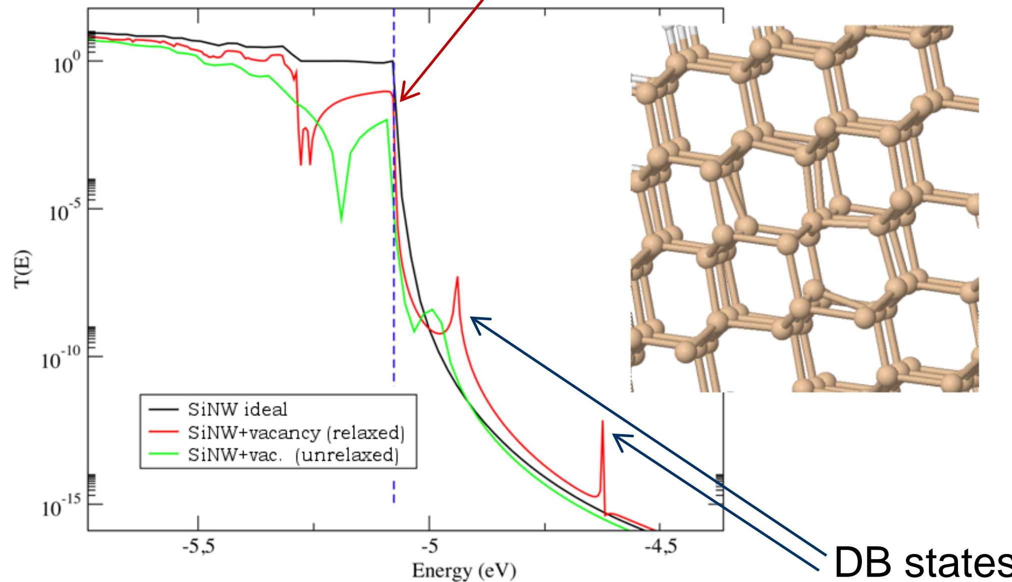
Severe reduction of current

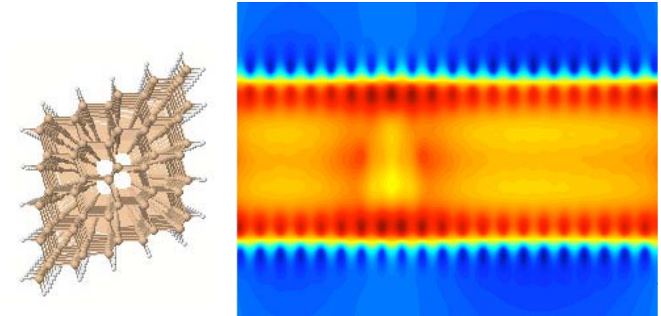
Conductance can be severely affected in ultra-narrow n-doped SiNW

The effect is much smaller on larger NW.

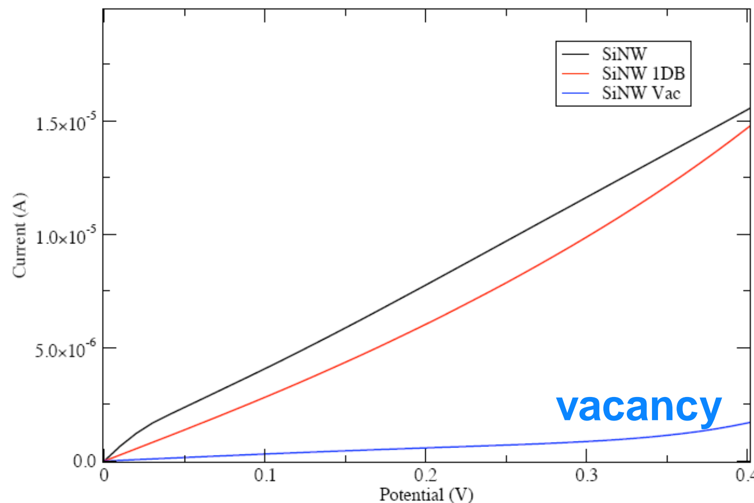
Si vacancy

Relaxation decreases Si-Si distance, increasing tunneling





DB states

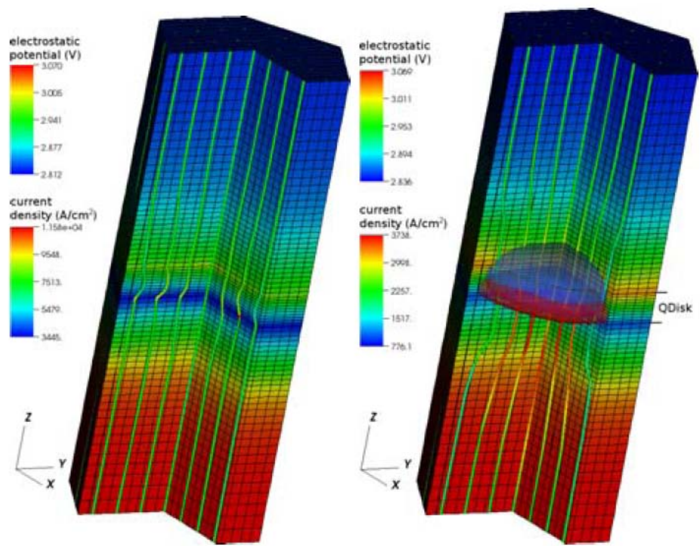


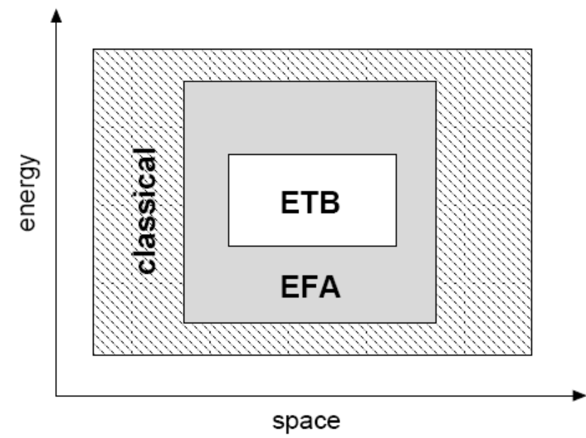
- A Si vacancy can have a large impact on p-doped NW.
- The effect is similar in magnitude to a DB in a n-doped NW.

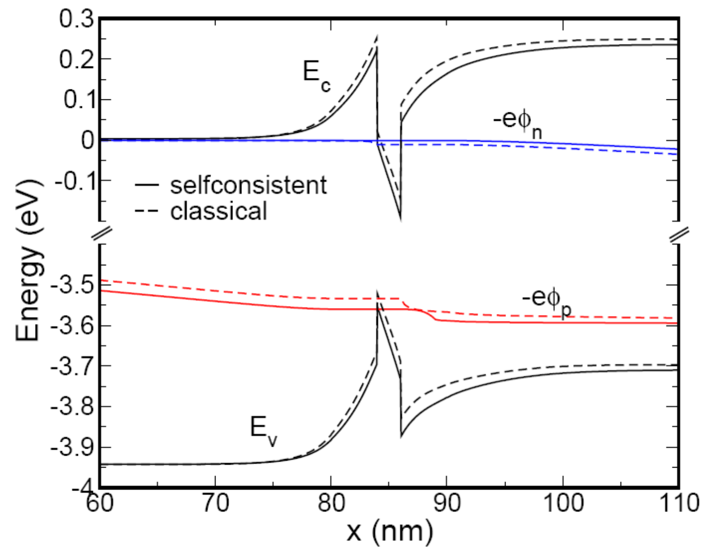
Conclusions

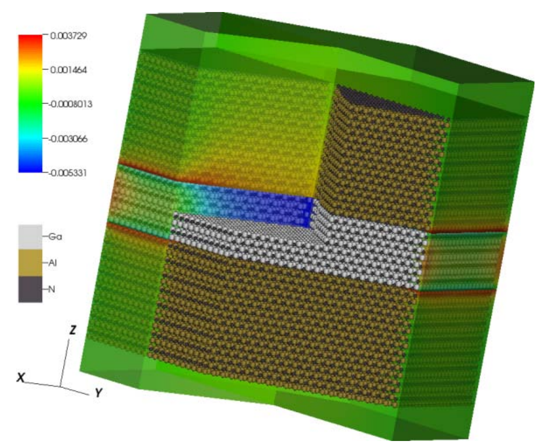
- Negatively charged DB are possible in (110)SiNW
- These defects can significantly affect transport of ultra narrow wires
- The effect of DB defect is less important in p-doped (110)SiNW
- In both *p&n*- doped NWs the effect of Si-vacancies is non-negligible

http://www.tibercad.org









$sp^3d^5s^*$ Empirical TB

POSTER SESSION !!

Prof. Aldo Di Carlo

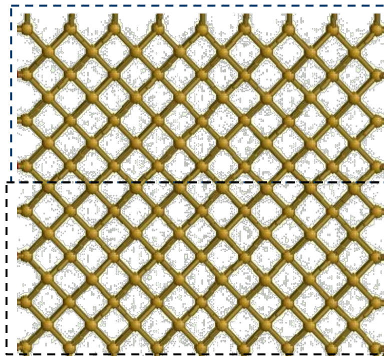
Gabirele Penazzi, PhD
Marco Pacini, Student
Luca Salvucci, Student

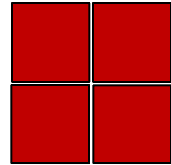
Matthias Auf Der Maur, Post Doc
Fabio Sacconi, Post Doc
Alessio Gagliardi, Post Doc

Dr. Bàlint Aradi
Prof Th. Frauenheim @ BCCMS, Bremen

Thank you

Sub-partitioning of each layer



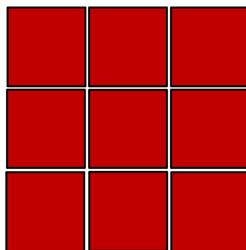


$$G_{11}(E) = \left(ES_{11} - H_{11} - H_{12}g_{22}H_{21}\right)^{-1}$$

$$g_{22}(E) = \left(ES - H_{22}\right)^{-1}$$

$G_{11}(E)$	$G_{12}(E) = -G_{11}H_{12}g_{22}$
$G_{21}(E) = -g_{22}H_{21}G_{11}$	$G_{22}(E) = g_{22} + g_{22}H_{21}G_{11}H_{12}g_{22}$

2 O(m^3)/8 + MM mult $\approx$ O(m^3)/3



O(m^3)/9 + MM mult $\approx$ O(m^3)/6

LibNEGF

- General Sparse Matrices (CSR)
- Automatic partitioning (METIS)
- Parallel computations (MPI/OpenMP)
- GPU acceleration (?)

… work in progress…