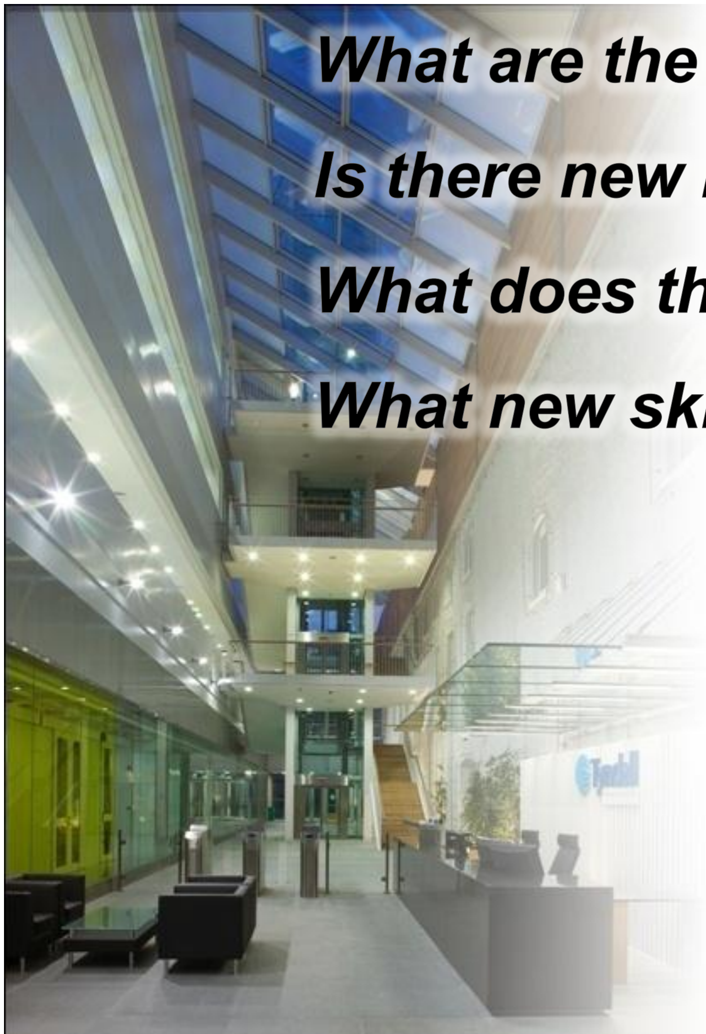
Breakthrough Materials & Methods



What are the key enabling materials and methods?

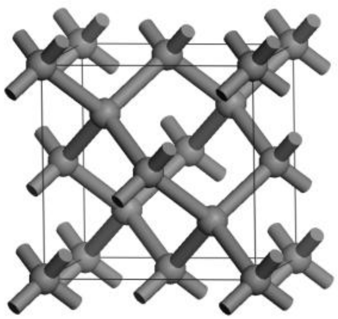
Is there new magic at the interfaces?

What does the nano world enable?

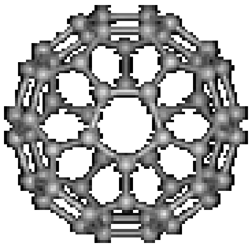
What new skills will be required?

Jim Greer

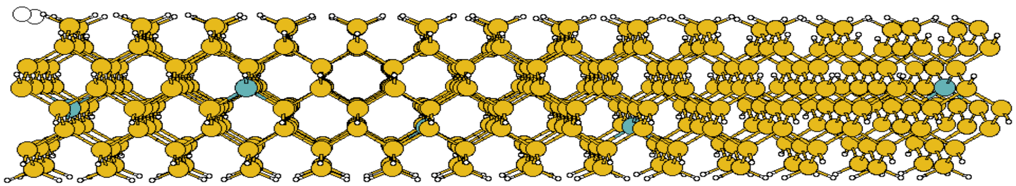
What are the key enabling materials and methods?



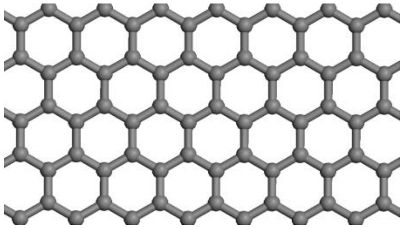
0D quantum dots,
molecules

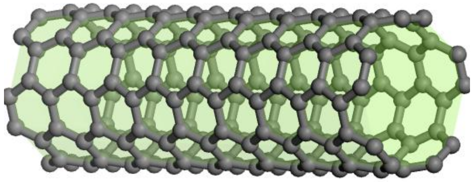


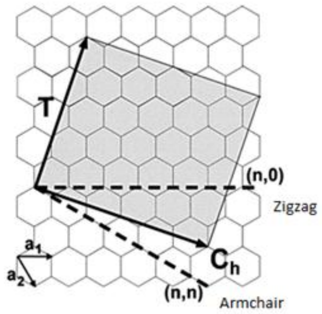
1D semiconductor nanowires,
carbon nanotubes

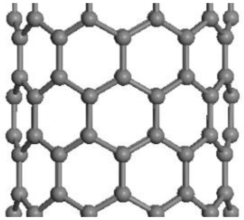


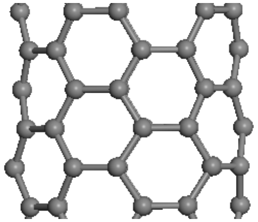
2D quantum wells,
graphene







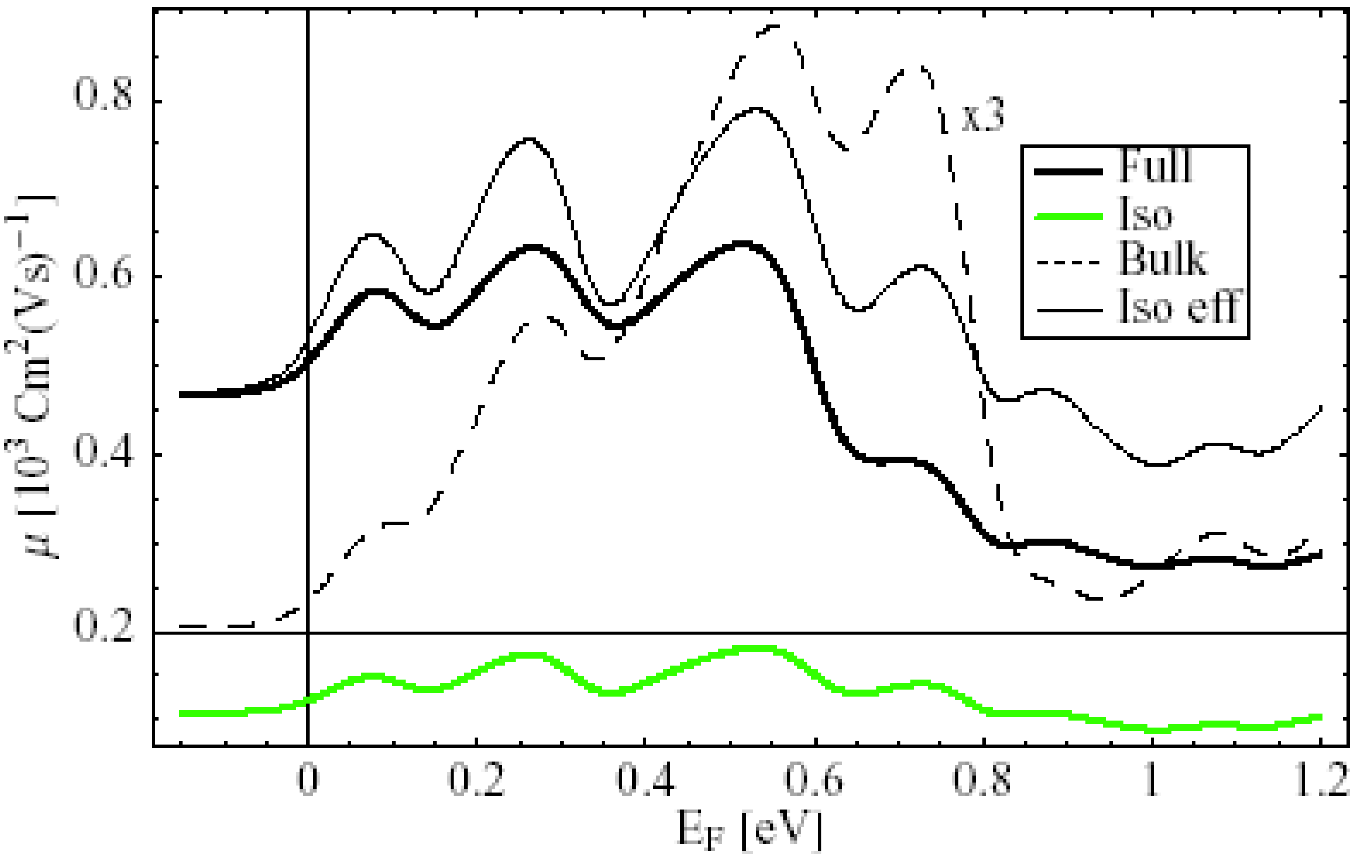


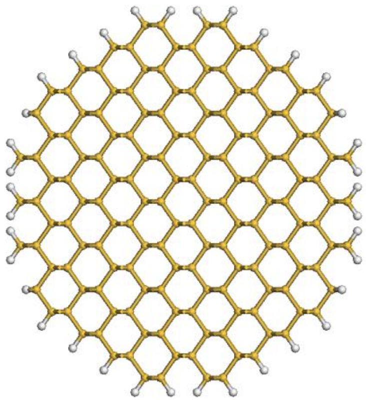


Zigzag – semiconducting
Armchair – metallic
Open challenge: controlled chirality

electron-phonon coupling in Si nanowires

What works in bulk fails on the nanoscale





<110> 3 nm

Full – NW def pot
Iso – isotropic bulk
Bulk – bulk def pot
Iso eff- isotropic NW

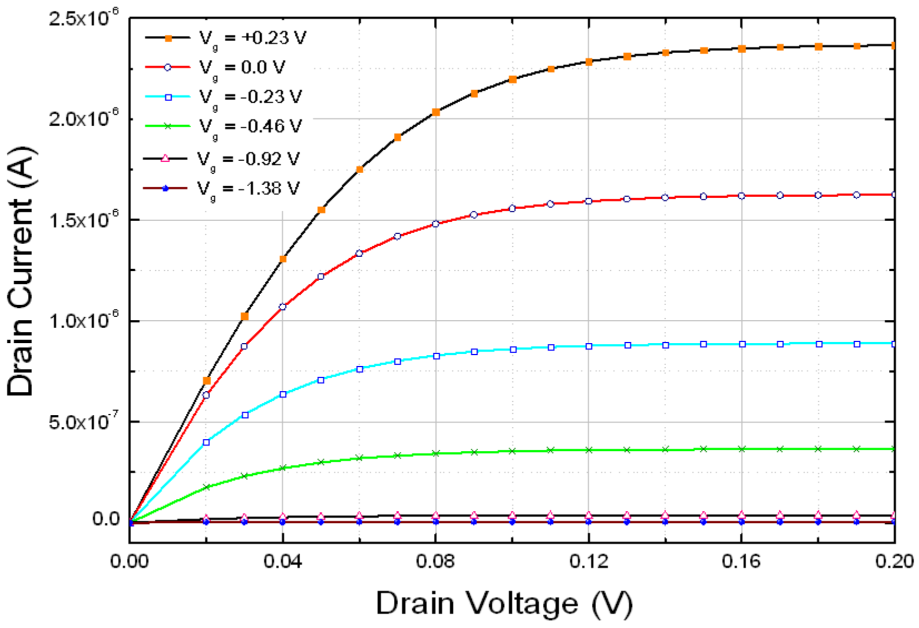
[110] grown mobility is 6x times larger than for [100]
Sensitive to details of deformation potential

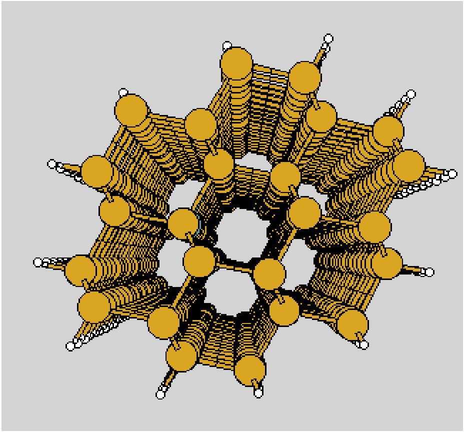
Murphy-Armando, Fagas and Greer, Nano Lett. (2010)

SiNW Gate-all-around junctionless transistor

Relaxed H-saturated [110] SiNW

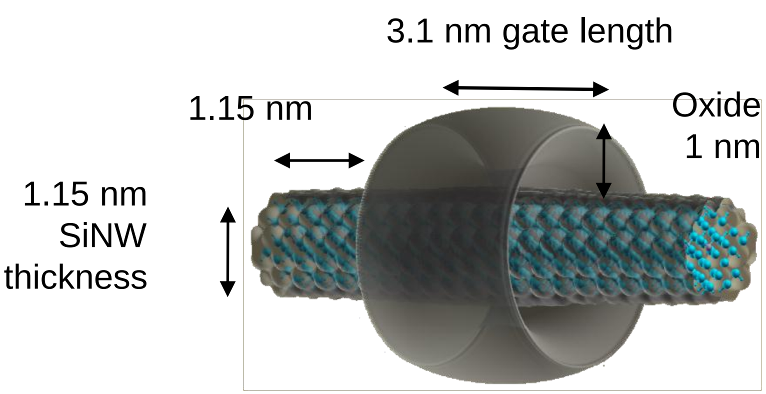
- Diameter = 1.15 nm
- Dopant atoms: As or P





Cross section

Dimensions of gated simulated device



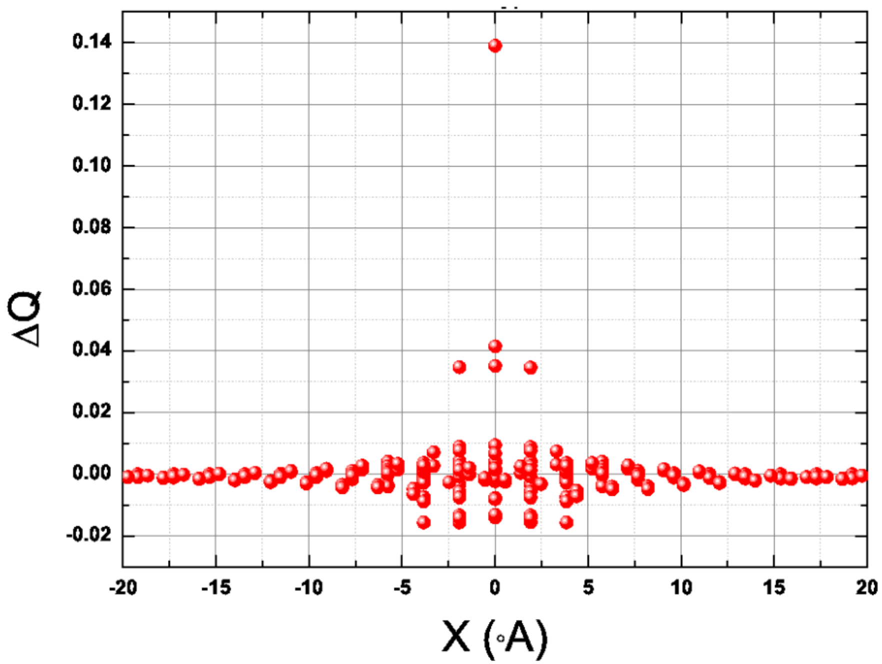
Simulated GAA junctionless transistor (right):

Oxide thickness 1 nm – continuum dielectric κ

Gate length = 3.1 nm

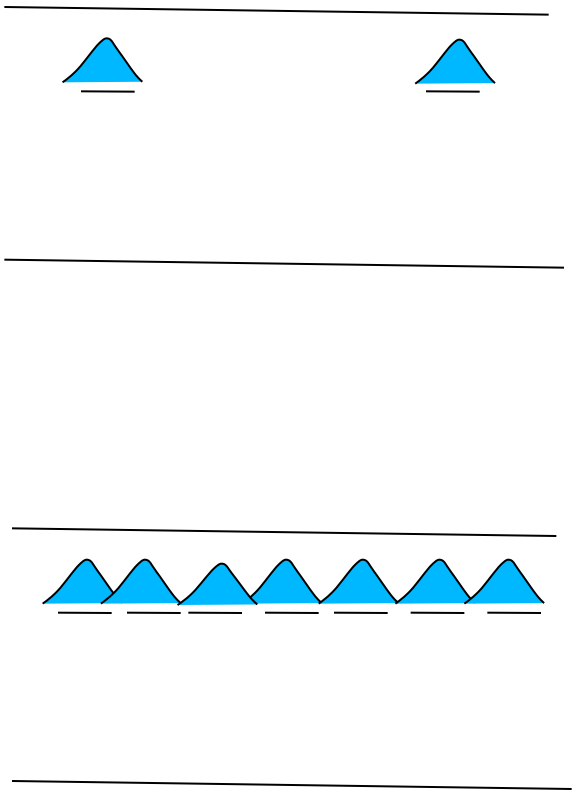
Ansari, B. Feldman, Fagas, Colinge, Greer
Appl. Phys. Lett. (2010)

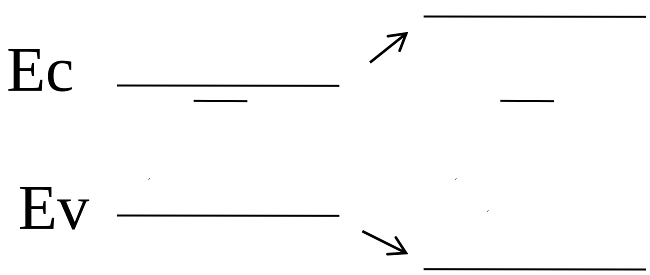
At these scales, requires a highly doped device?



Mulliken charge difference, ΔQ^M
Charge de-localizes over ~2 nm !

Comparable to gate length

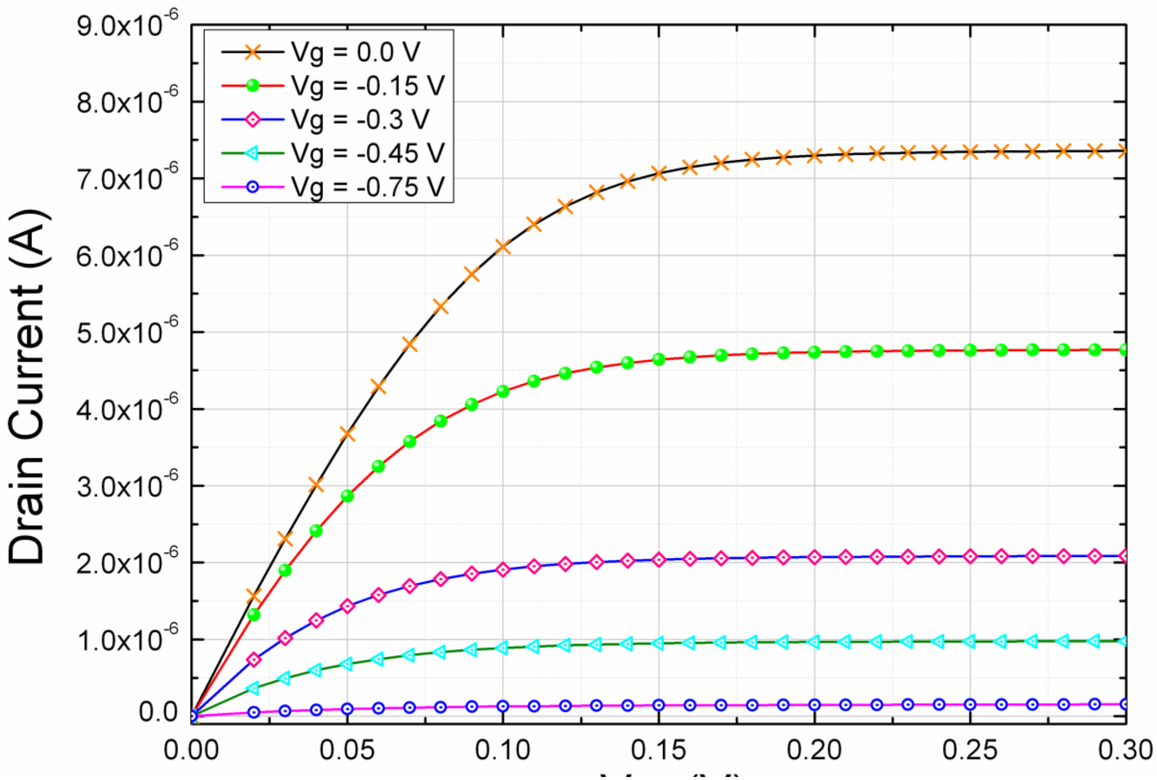




Half filled band ➔ metal

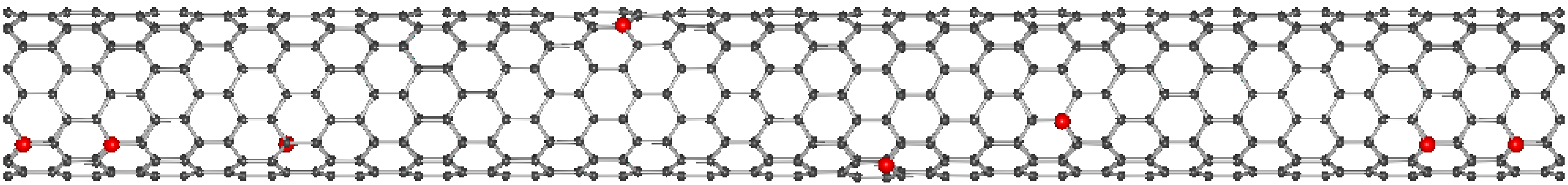
Mott insulator to metal transition

CNT Gate-all-around junctionless transistor



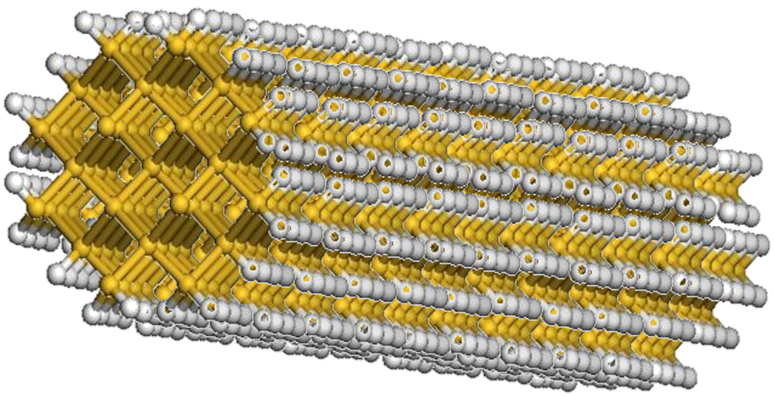
- N-type
- Comparable to similar SiNW devices
- Dopant profiles influence device operation

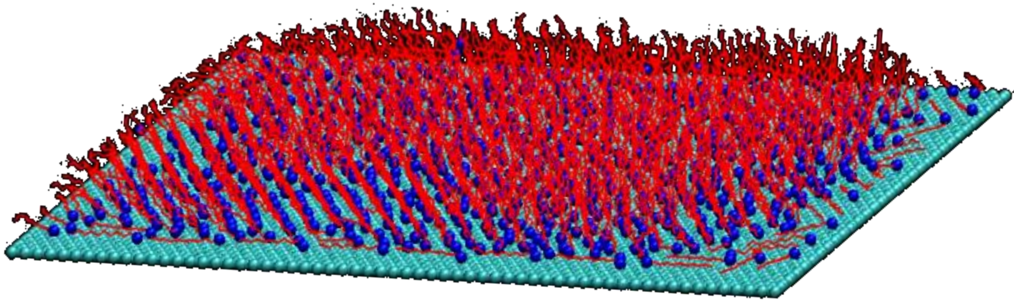
Doping levels > 1% achievable



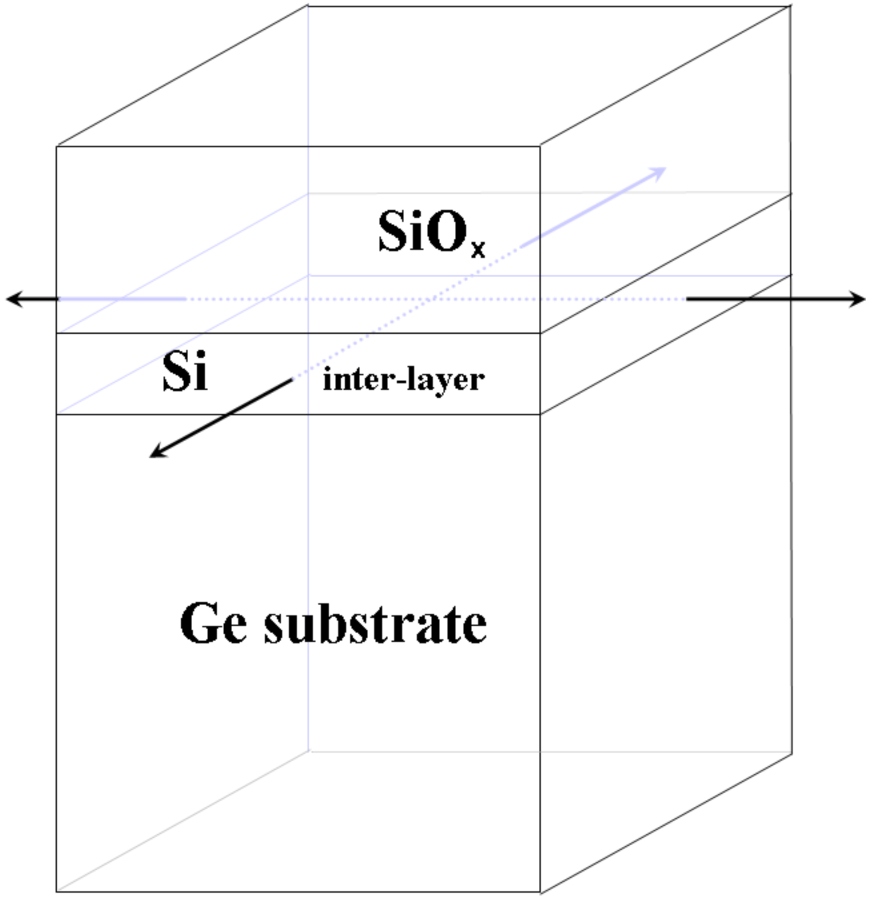
Is there new magic at the interfaces?

$$\frac{surface}{volume} = \frac{\pi r^2}{4\pi r^3/3} \propto \frac{1}{r} \Rightarrow$$ Nanostructures are mostly surface





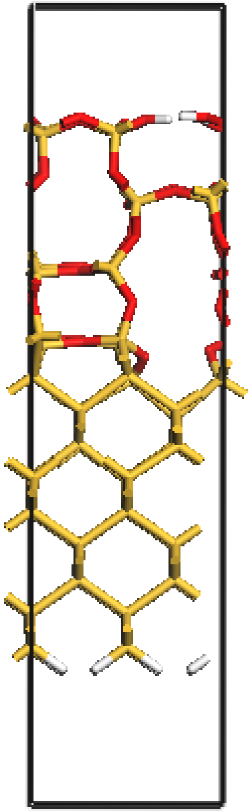
Strain in Si interlayers at SiOx/Ge interface



Substitute Ge substrate atoms with Si to form interlayer

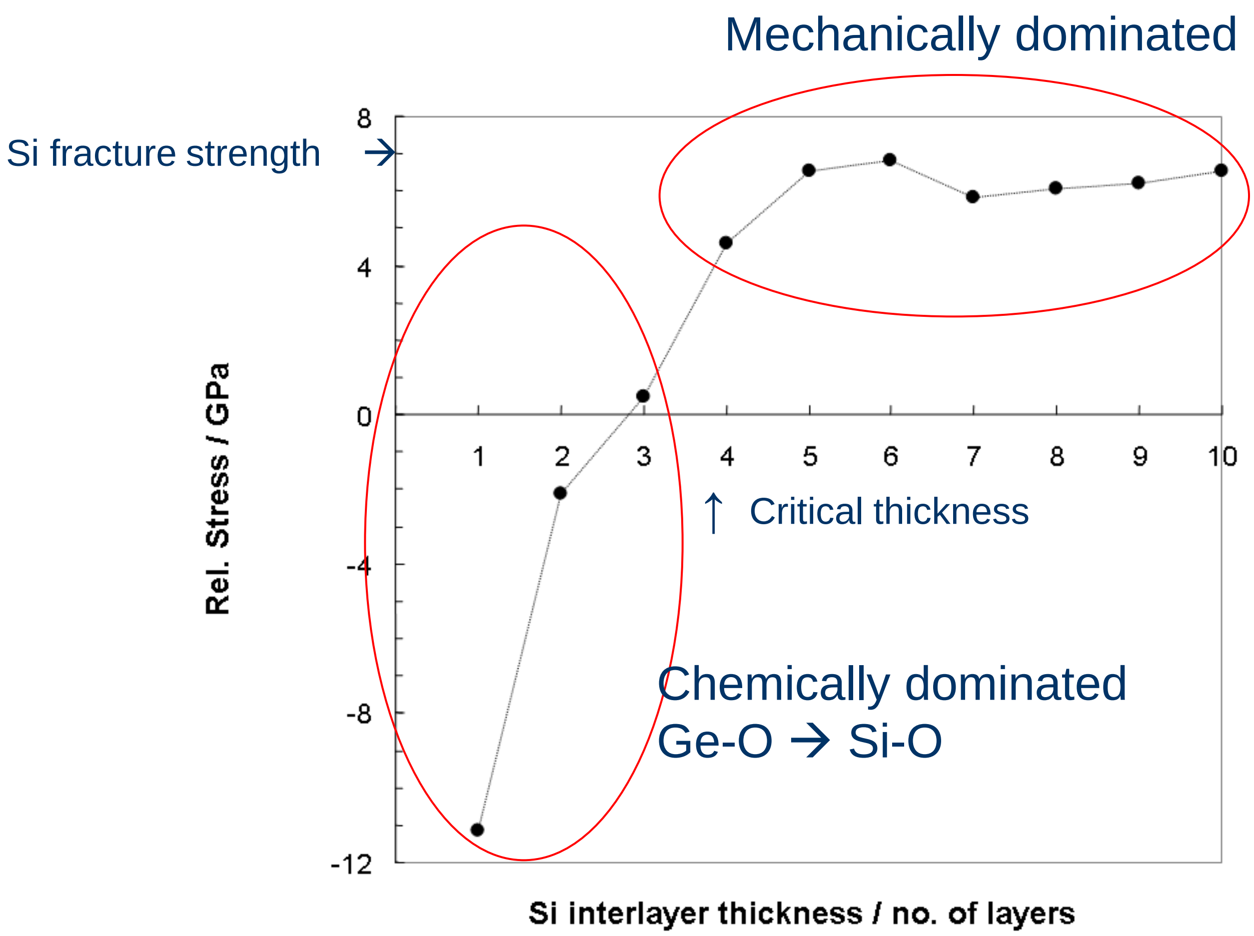
High mobility substrate with ideal Si/SiO_x interface

From continuum and atomic simulation – strain resides in interlayer



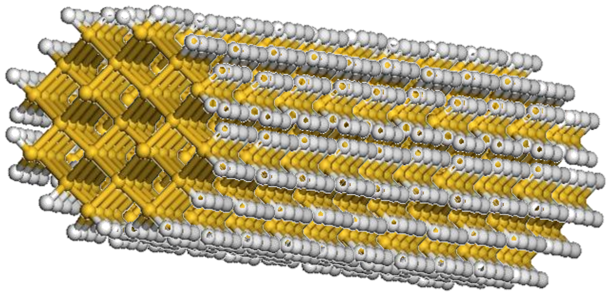
O'Callaghan, Monaghan, Elliott, and Greer
Appl. Phys. Lett. **90**, 143511 (2007)

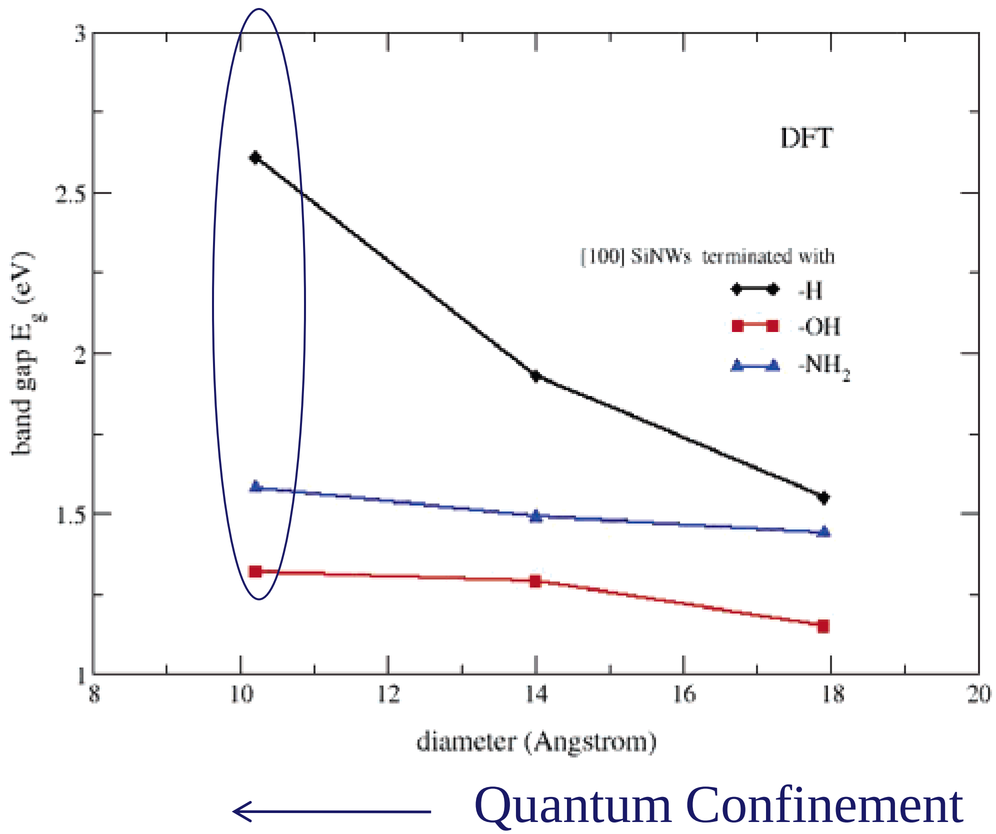
Stress in interlayer with increasing thickness



Increasing surface-to-volume yields new effects

Band gap control by surface chemical modification

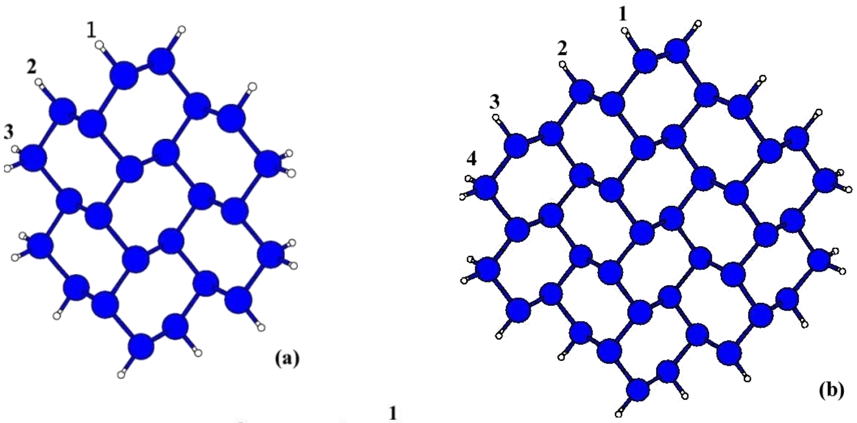


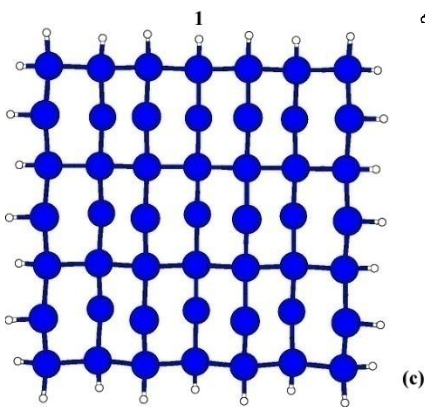


Leu, Shan, Cho, Phys, Rev. B (2006)
Nolan, O'Callaghan, Fagas, Greer, Frauenheim, *Nano Lett.* (2007).

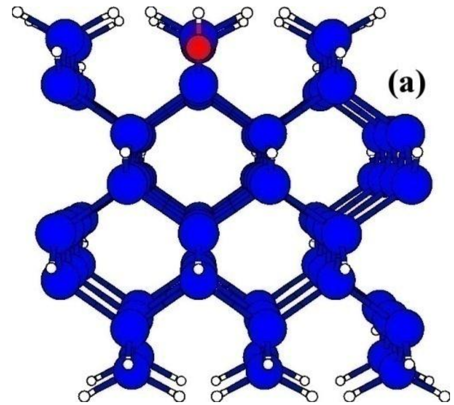
Scattering off surface oxide in quasi-1D wires

<110> Si nanowire
W = 1.15 nm and 1.54 nm





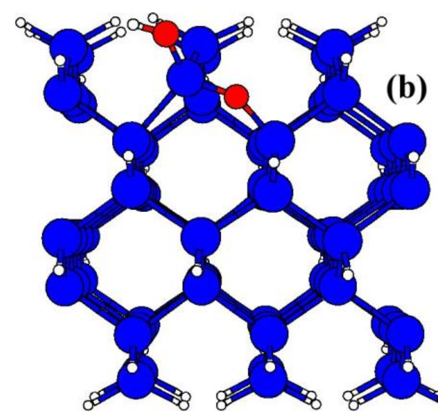
<100> SiNW
W = 1.63 nm



Si at oxidation state Si^{+1}

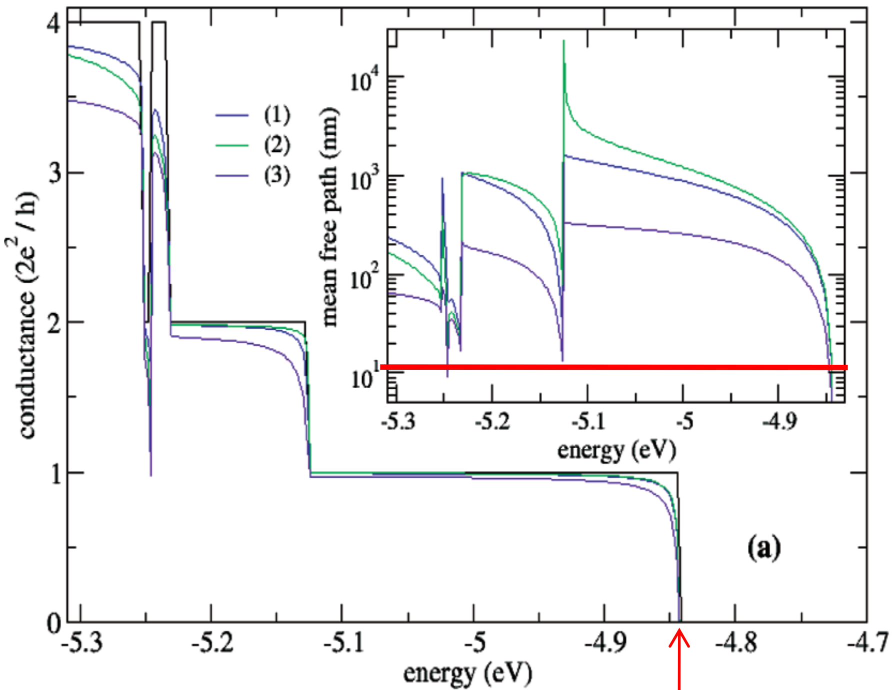
and Si^{+2}

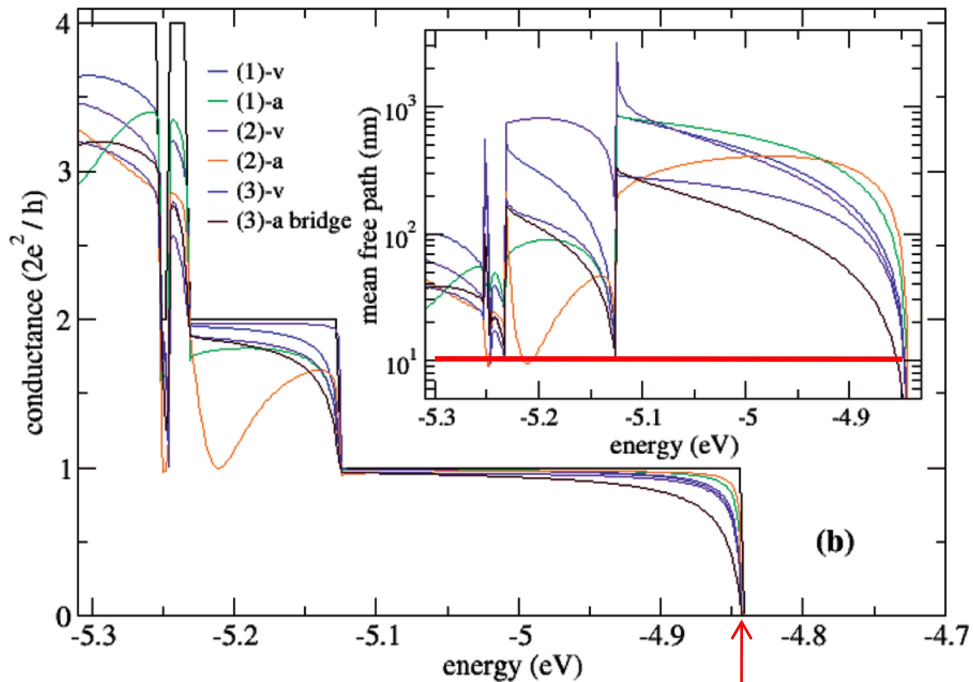
Si-O-Si backbond



Fagas and Greer, Nano Letters (2009)

Hole scattering in [110] Si nanowires



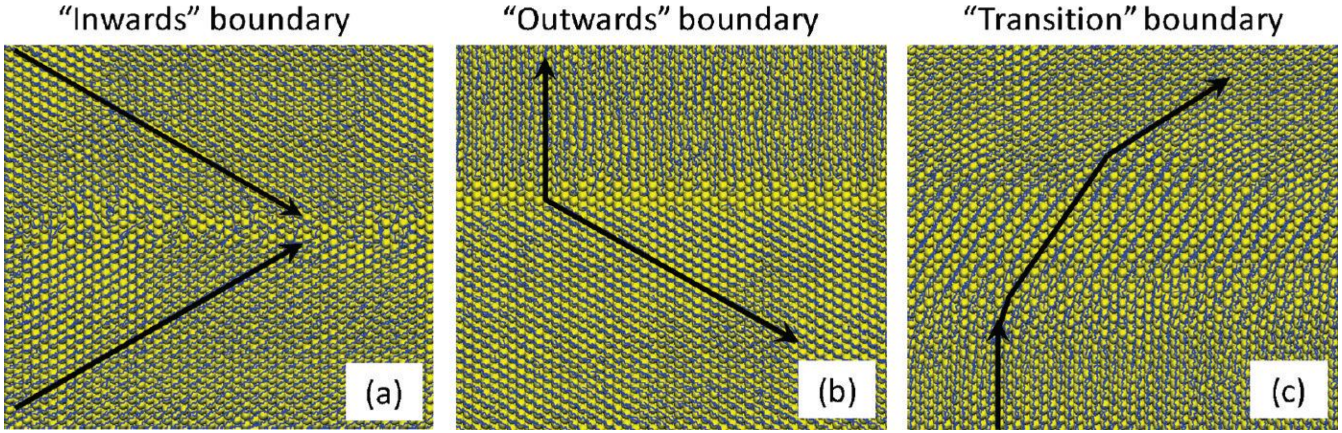


[110] oxidation varied with surface hydroxyl groups
W = 1.15 nm
Defect density n = $5 \cdot 10^{19}$ cm^{-3}

[110] oxidation varied with surface hydroxyl groups and O backbonds
W = 1.15 nm
Defect density n = $5 \cdot 10^{19}$ cm^{-3}

Scattering lengths calculated from method of :
Markussen, Rurali, Jauho and Brandbyge, PRL (2007)

Different materials and approaches?



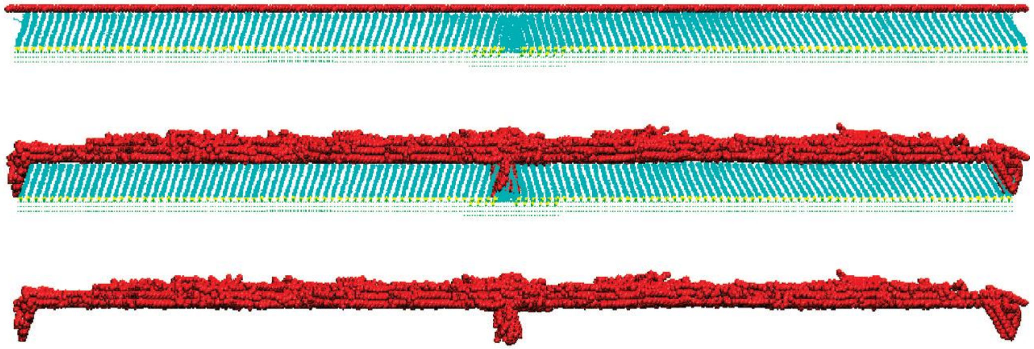
MD: "easy" to explore machine use

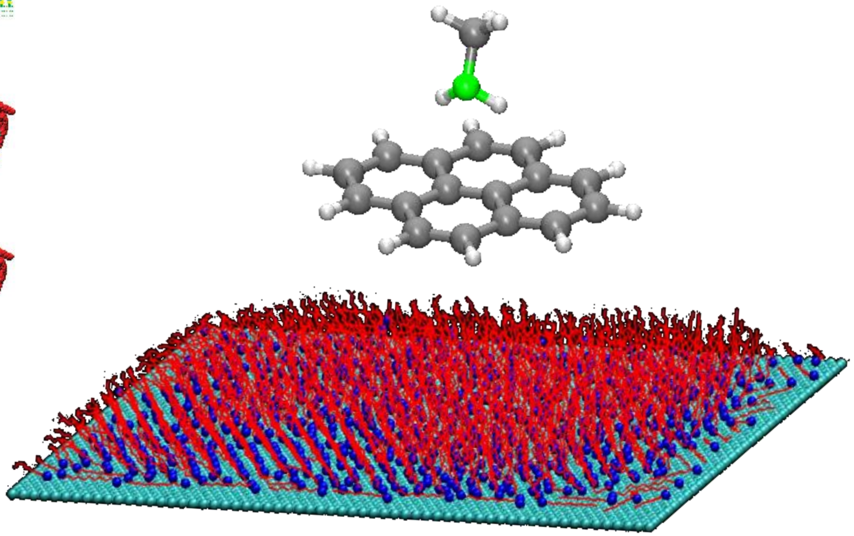
O(10^{6}) atoms

512 compute cores

approaching 0.1 µsec

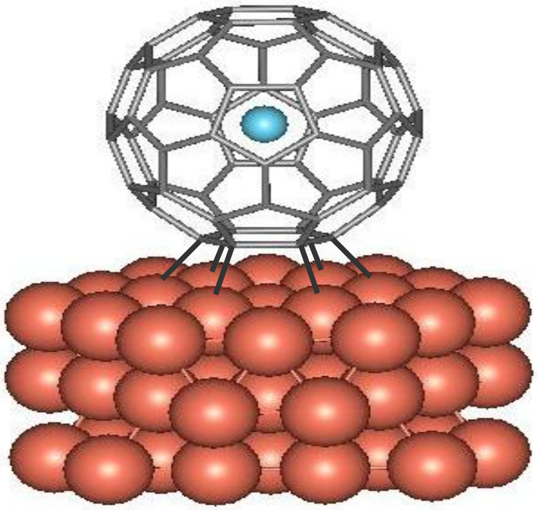
4096 cores on IBM Watson's USA based BG



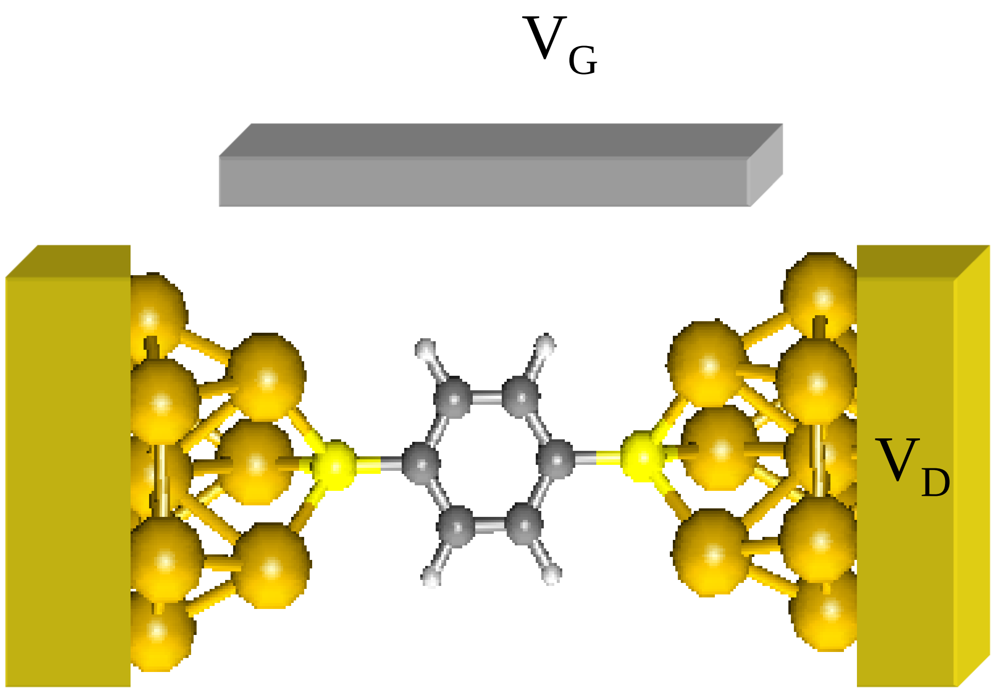


Gannon, Greer, Larsson, Thompson, *Langmuir* (2009)
Gannon, Greer, Larsson, Thompson, *Nano* (2010)

What does the nano world enable?

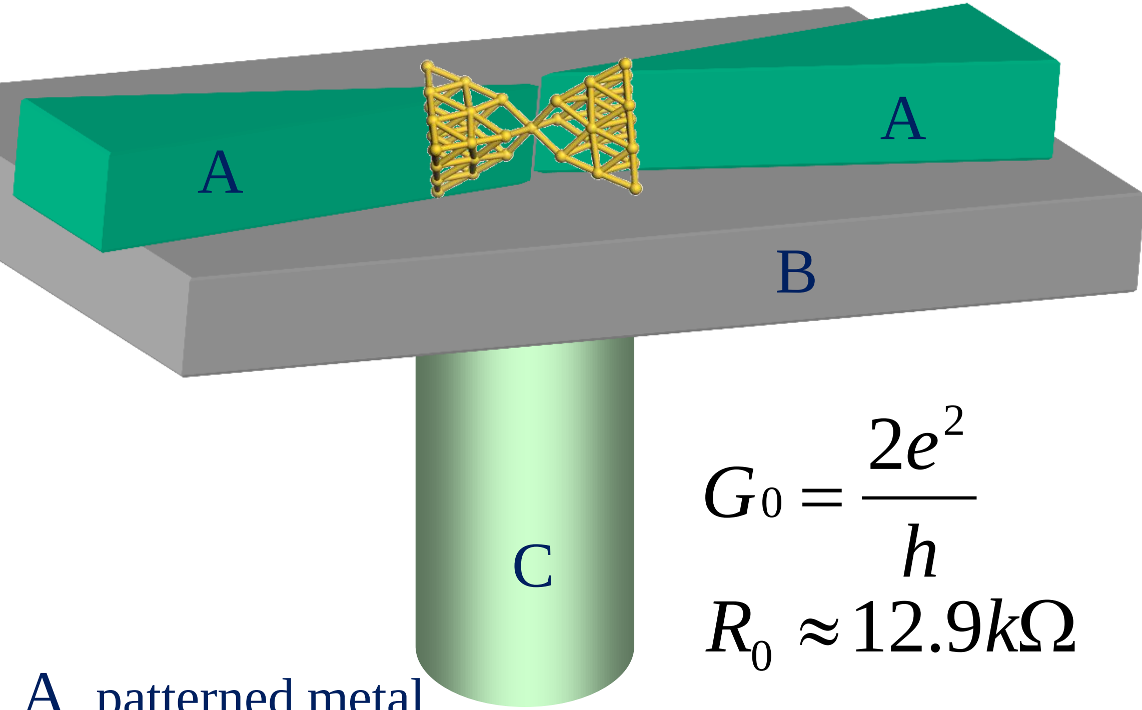


10 to 15 years ago we didn't know if Si transistors would work below 10 nm



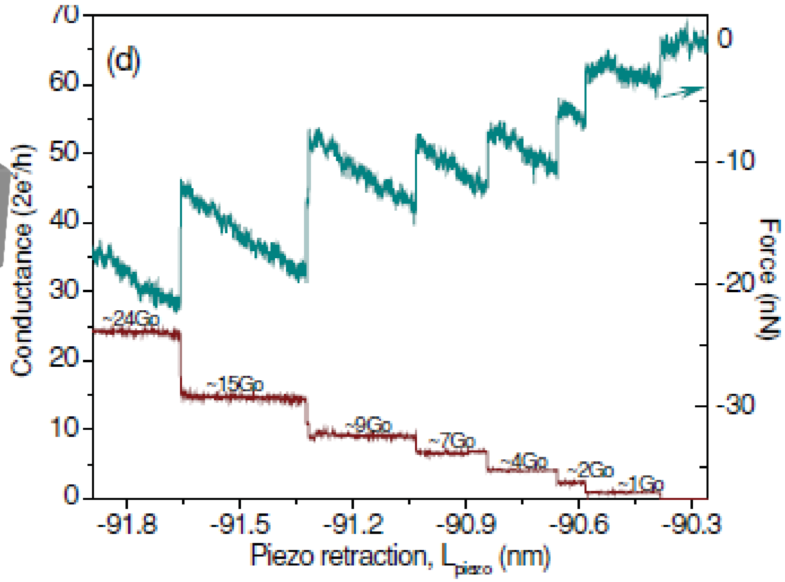
Molecular electronics is still a great opportunity to explore electron transport on the 1 nm scale

Mechanical break junctions



$$G_0 = \frac{2e^2}{h}$$

$$R_0 \approx 12.9 k\Omega$$



Armstrong et al, PRB 2011

A patterned metal

B polymer substrate

C piezoelectric piston

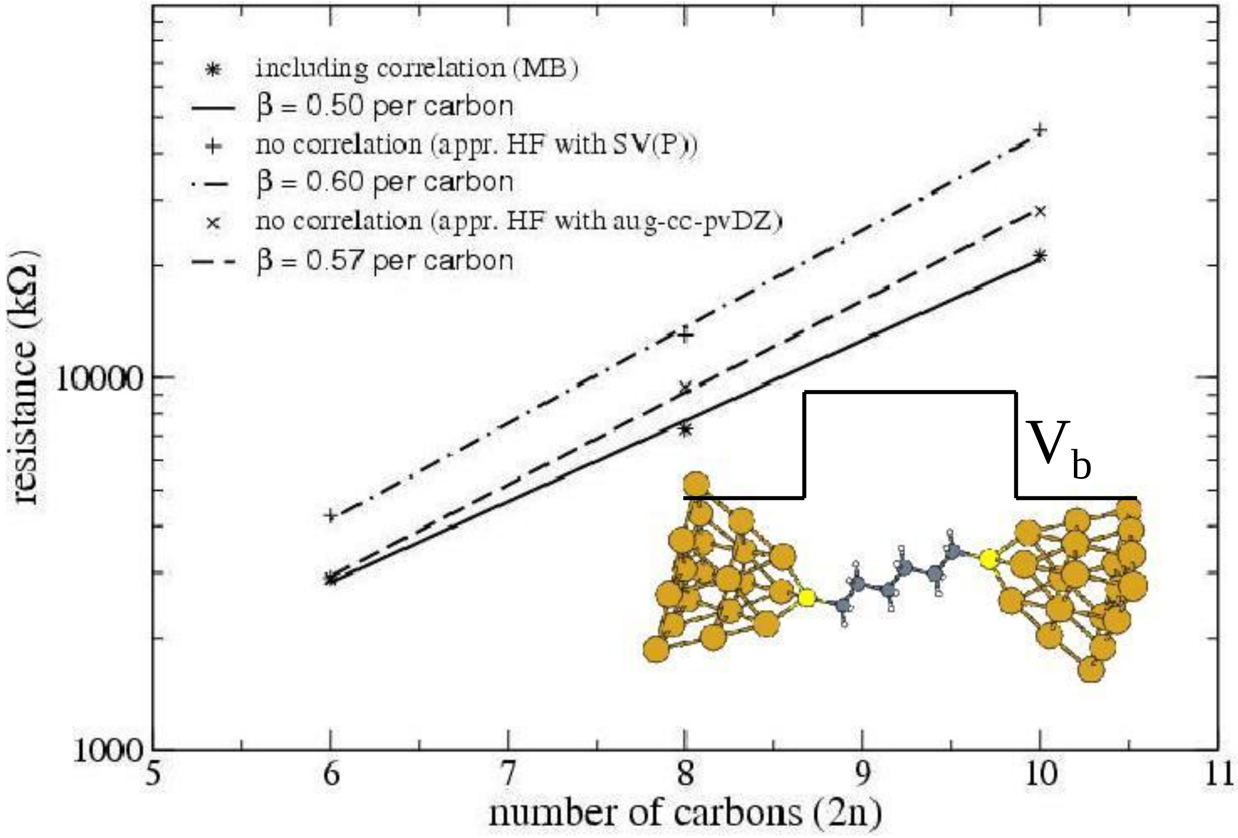
A single conducting channel has an intrinsic quantised resistance

For macroscopic conductors, many parallel channels, intrinsic conductance is low

In nanoscale conductors, this resistance is unavoidable

Exponential decay in resistance with length

Conductance across Au-S-$(C_2H_4)_n$-S-Au molecular junction



Agrees well *some* measurements:

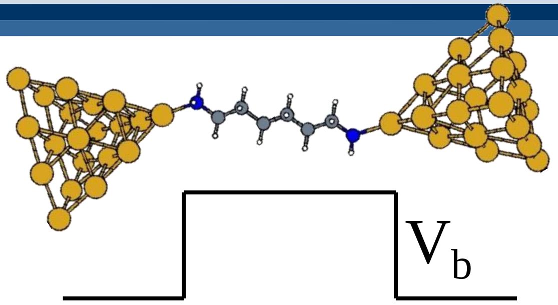
- β =0.57 / n
  [Cue et al., J. Phys. Chem B 106, 8609 (2002)]

- β= 0.52 / n
  [Haiss et al., PCCP 6, 4330 (2004)]

- β= 0.68 – 0.79 / n
  [Akkerman et al., Nature 441, 69 (2006)]

G. Fagas, et al, *Phys. Rev. B* (2006).

Different linkers: well defined conductances



“Quantitative” agreement with well-defined measurements of molecular conductances

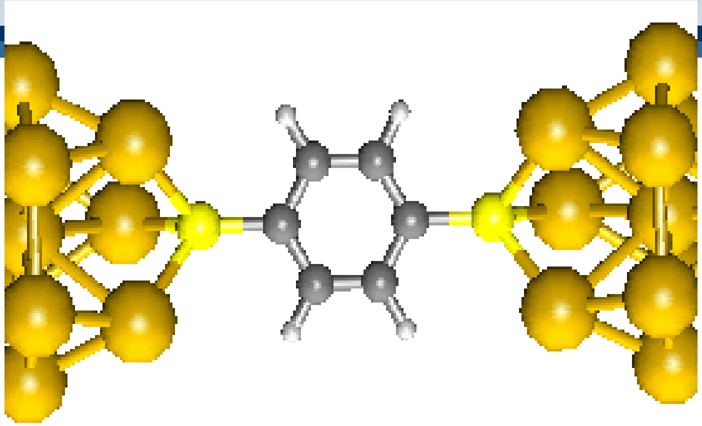
	Conductance (ns)			
	NH-anchoring	NH2-anchoring	L. Venkataraman et al, Nano Letters **6**, 458 (2006)	F. Chen et al, JACS **128**, 15874 (2006)
Pentane	34.52±16.51	51.99±24.10	27.12±0.77	-
Hexane	12.96±2.98	30.64± 6.07	11.62±1.16	20.79
Heptane	4.27±1.03	4.91± 3.26	5.66±1.55	-
Octane	3.65	4.33± 3.26	2.32±2.32	3.85

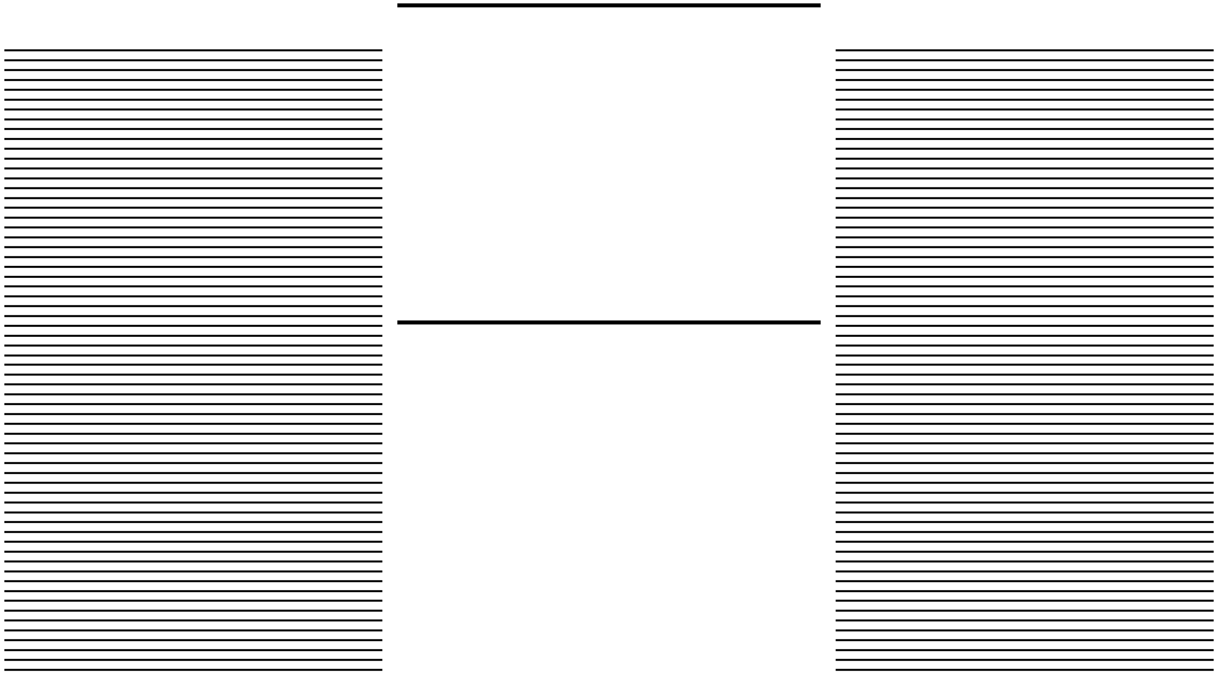
… additionally

direct comparision to NEGF+DFT, complex band structures, and analytical tunnel barrier models

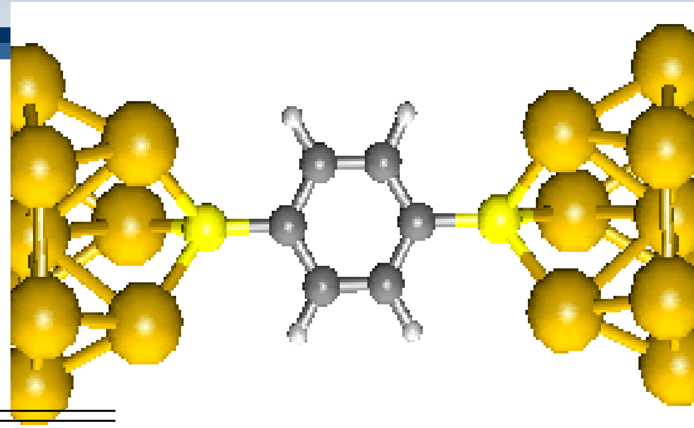
McDermott *et al* (2009)

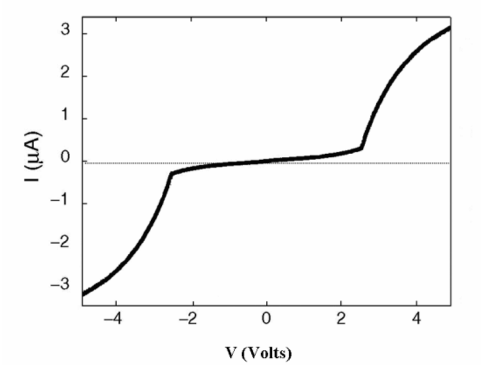
Molecular Quantum Dot

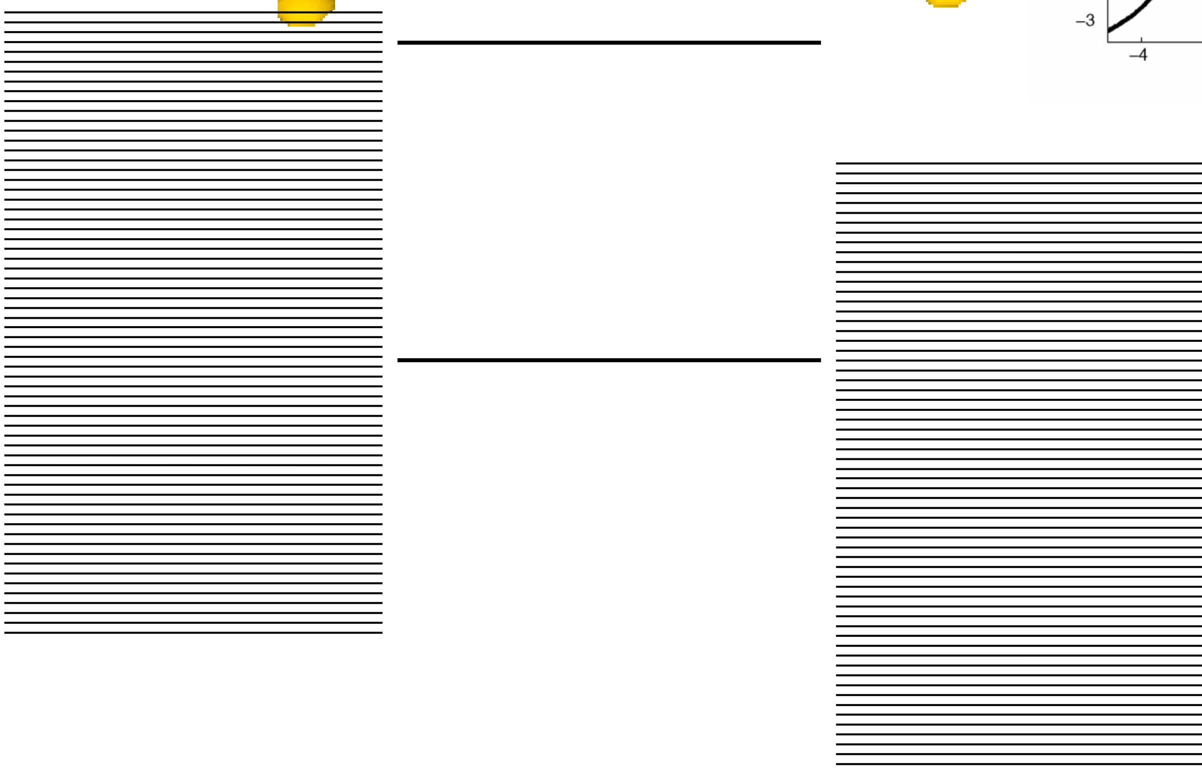




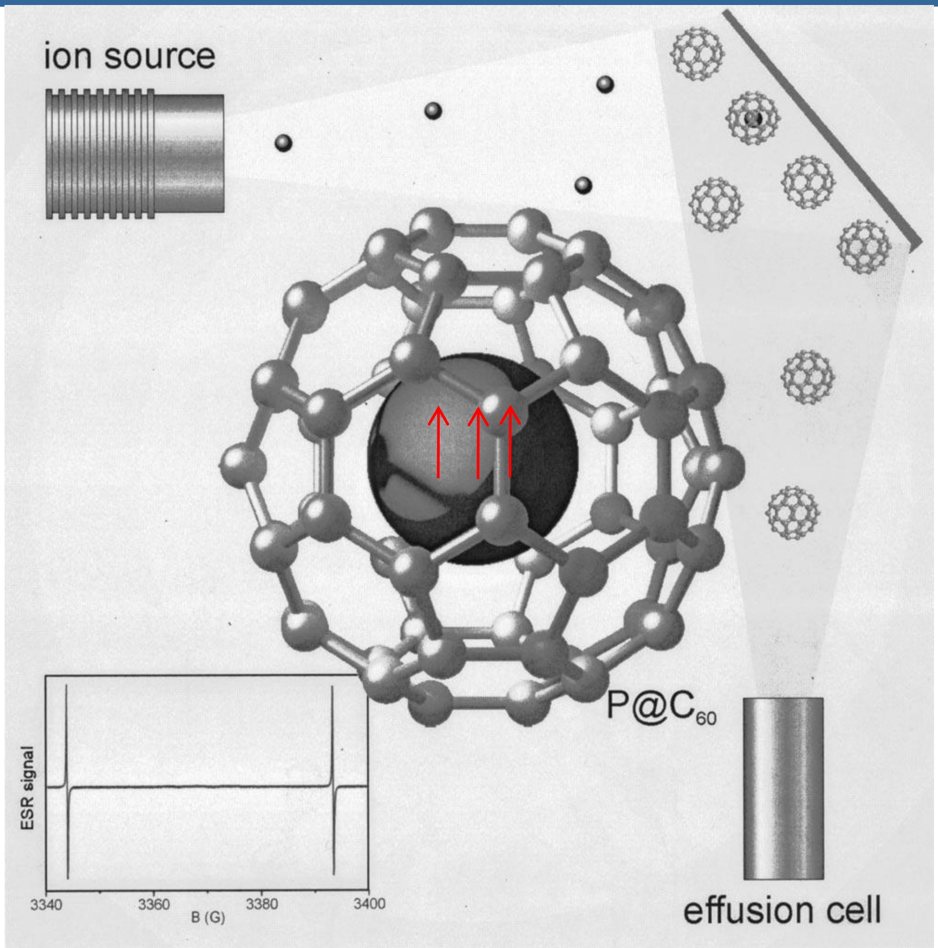
Molecular Quantum Dot

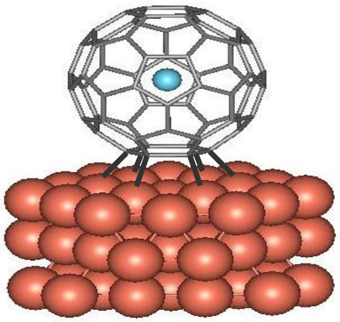






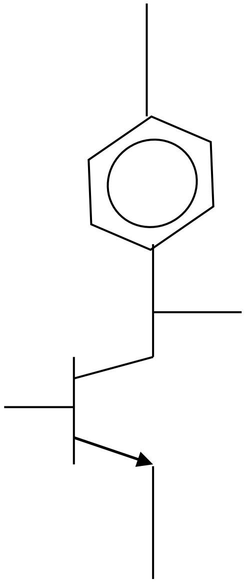
Group V Atoms Trapped in C_{60}





Weidinger et al, 2002
Extremely long spin coherence times (order of ms)

What new skills are required?

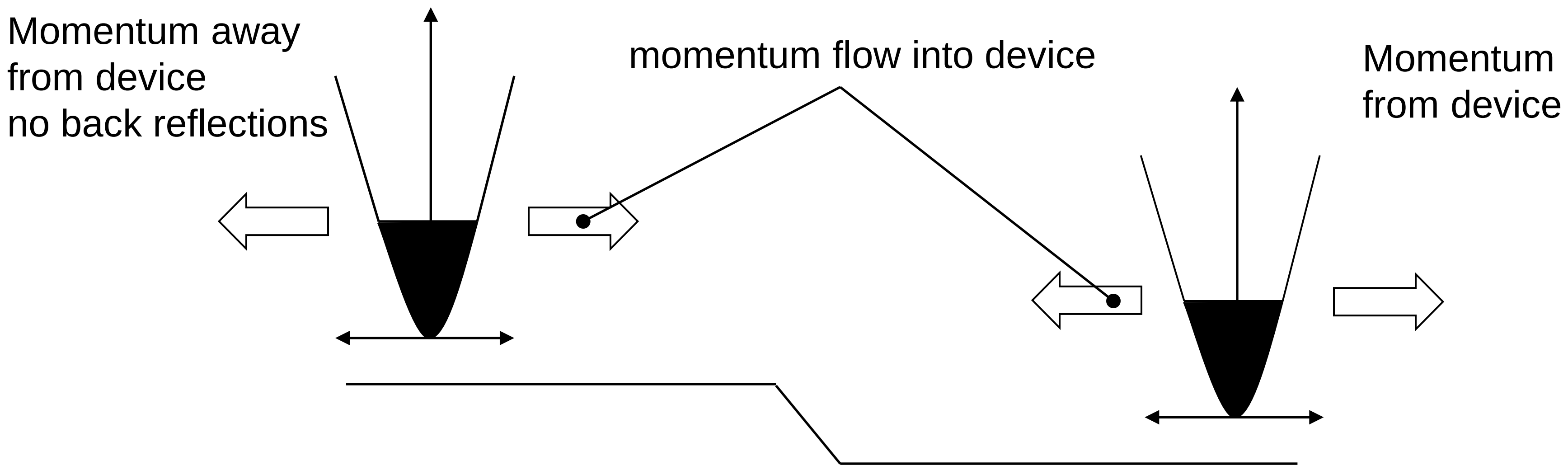


How to design

- Classical circuits working near quantum limits

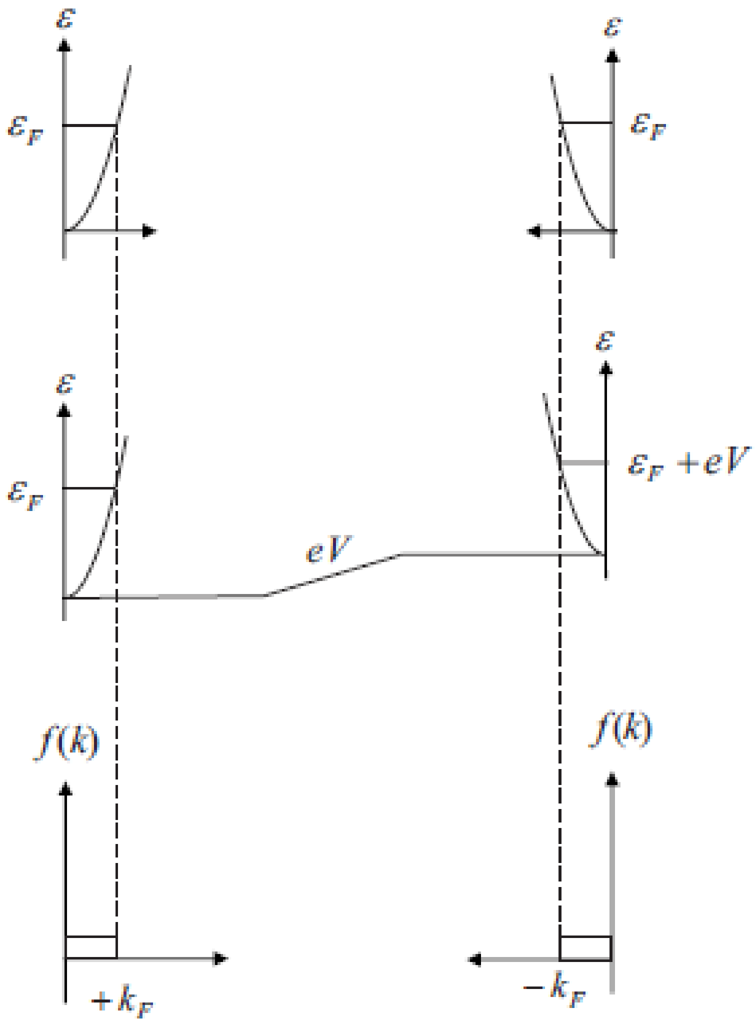
- interface between quantum and classical worlds

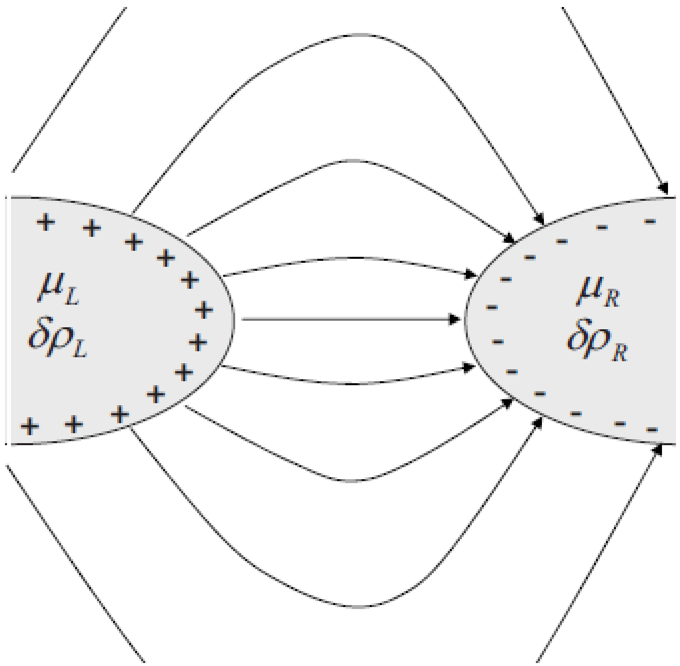
Quantum electronic transport



$$I = \frac{2e}{h} \int_{-\infty}^{+\infty} [f(E+\mu_L) - f(E-\mu_R)] T(E)\, dE$$

How does a battery work?





Density matrices

Quantum mechanical *system* average for *O*

$$< O > = < \Psi | \hat{O} | \Psi >$$

Quantum mechanical *subsystem* average for *O*

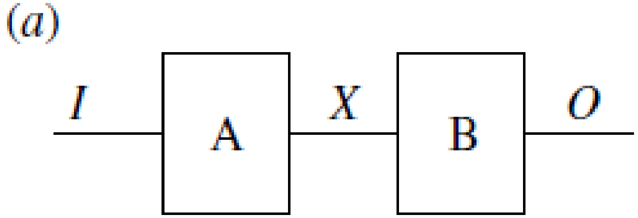
$$< O > = Tr[\hat{O}\rho]$$

How do we define O as outputs and what are the inputs?

$$O_k = \langle \hat{O}_k \rangle = f(I_1, I_2, \ldots, I_n)$$

Delaney and Greer, Proc Roy Soc A (2006)

Can we write quantum to “classical” circuit laws?



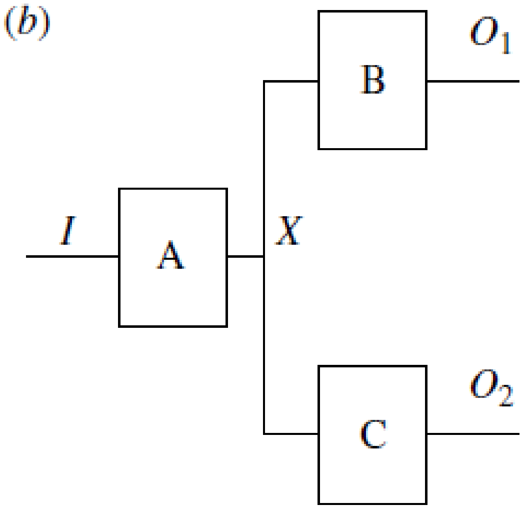
Input and output should correlate

$$\langle \hat{I}\,\hat{O}\rangle \neq \langle \hat{I}\rangle\langle \hat{O}\rangle$$

Density matrices between subsystems should factorize

$$\langle \hat{O}\rangle = \mathrm{Tr}_{\mathrm{AB}}\,\hat{O}\hat{\rho}(I) = \mathrm{Tr}_{\mathrm{A}}\hat{\rho}_{\mathrm{A}}(I)\mathrm{Tr}_{\mathrm{B}}\,\hat{O}\hat{\rho}_{\mathrm{B}}(X) = \mathrm{Tr}_{\mathrm{B}}\,\hat{O}\hat{\rho}_{\mathrm{B}}(X).$$

Fan-out:
The two outputs should
not correlate
(operations B and C independent)



$$\langle \hat{O}_1\hat{O}_2\rangle = \mathrm{Tr}_{\mathrm{ABC}}\,\hat{O}_1\hat{O}_2\hat{\rho}(I) = \mathrm{Tr}_{\mathrm{A}}\,\hat{\rho}_{\mathrm{A}}(I)\mathrm{Tr}_{\mathrm{B}}\,\hat{O}_1\hat{\rho}_{\mathrm{B}}(X)\mathrm{Tr}_{\mathrm{C}}\,\hat{O}_2\hat{\rho}_{\mathrm{C}}(X) = \langle \hat{O}_1\rangle\langle \hat{O}_2\rangle$$

We know how to calculate density matrices

Canonical ensemble

$$< E > = Tr[\hat{H}\hat{\rho}]$$

$$\hat{\rho} = \exp[-\beta\hat{H}]$$

Grand canonical ensemble

$$< E > = Tr[\hat{H}\hat{\rho}]$$

$$< N > = Tr[\hat{N}\hat{\rho}]$$

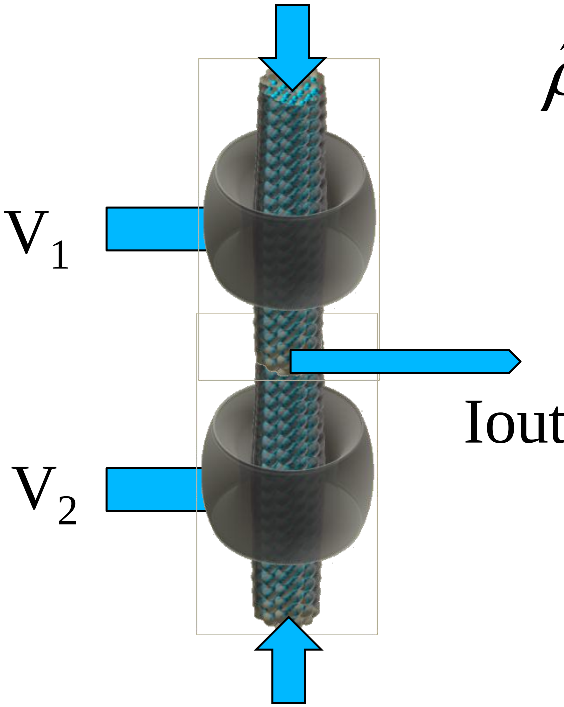
$$\hat{\rho} = \exp[-\beta\hat{H} + \mu\hat{N}]$$

Maximize entropy: yields best estimate to subsystem density matrix

MaxEnt (Jaynes 1957)

Information Theory (Shannon 1948)

Interacting quantum sub-systems as circuits



$$\hat{\rho} = \exp[-\beta(\hat{H} + \hat{V}_1 + \hat{V}_2) + \lambda_D \hat{F}_D + \lambda_s \hat{F}_S]$$

Inputs

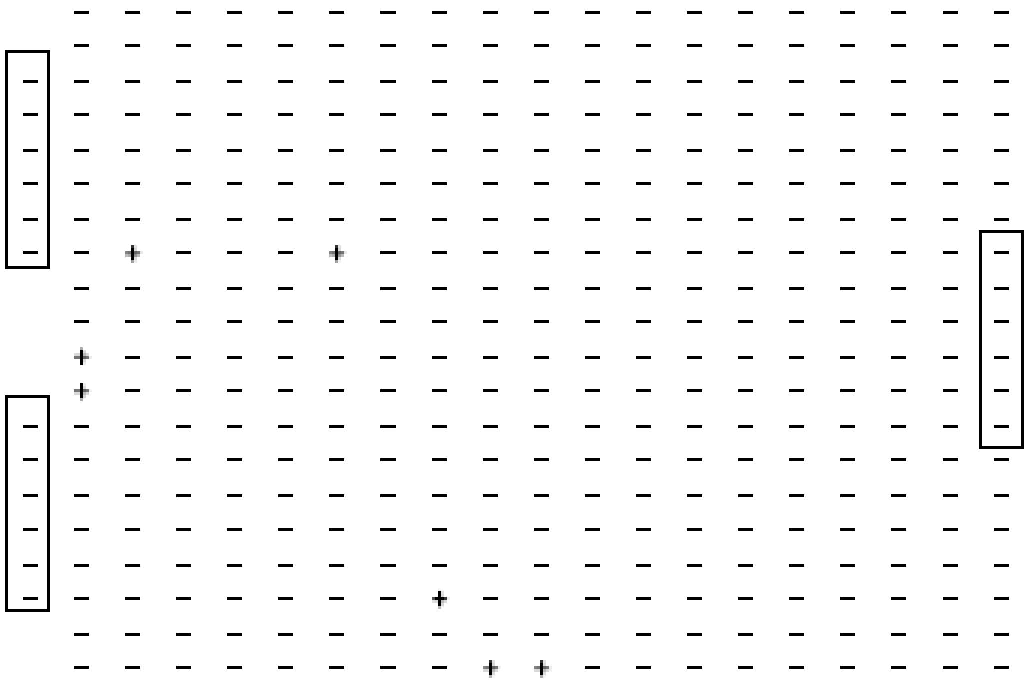
Operation

Power supply

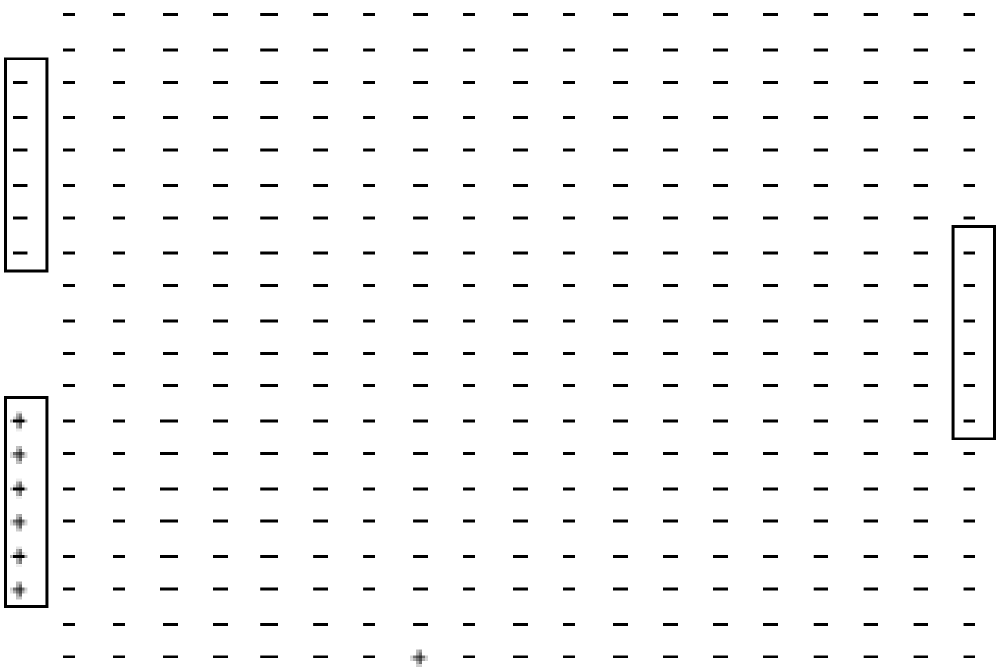
$$< I >= Tr[\hat{I}_{out} \exp[-\beta(\hat{H} + \hat{V}_1 + \hat{V}_2) + \lambda_D \hat{F}_D + \lambda_s \hat{F}_S]]$$

Output

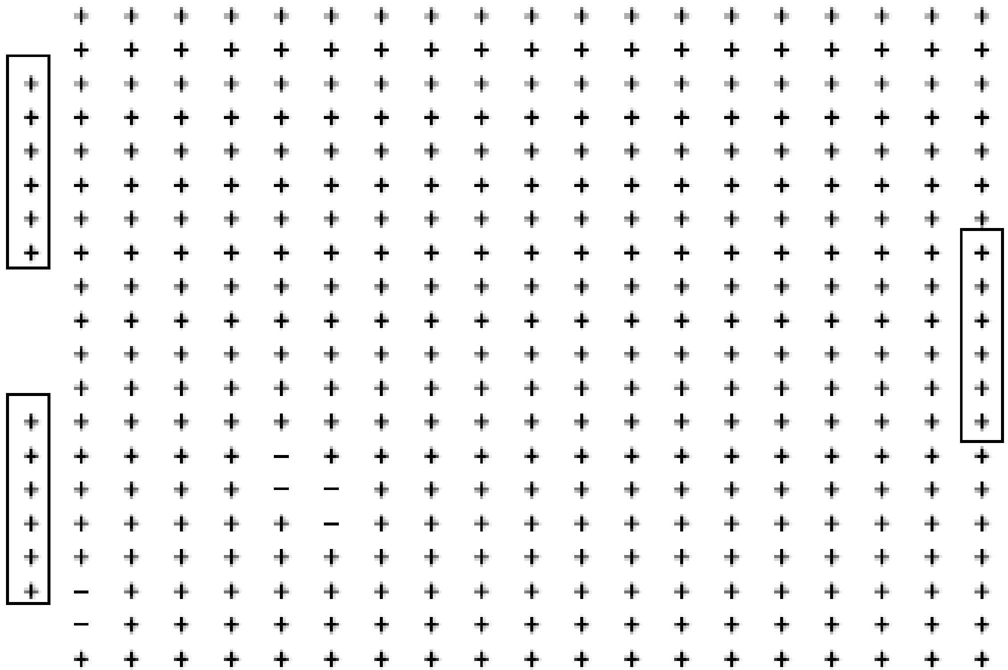
A simple example: spin gate



A simple example: spin gate

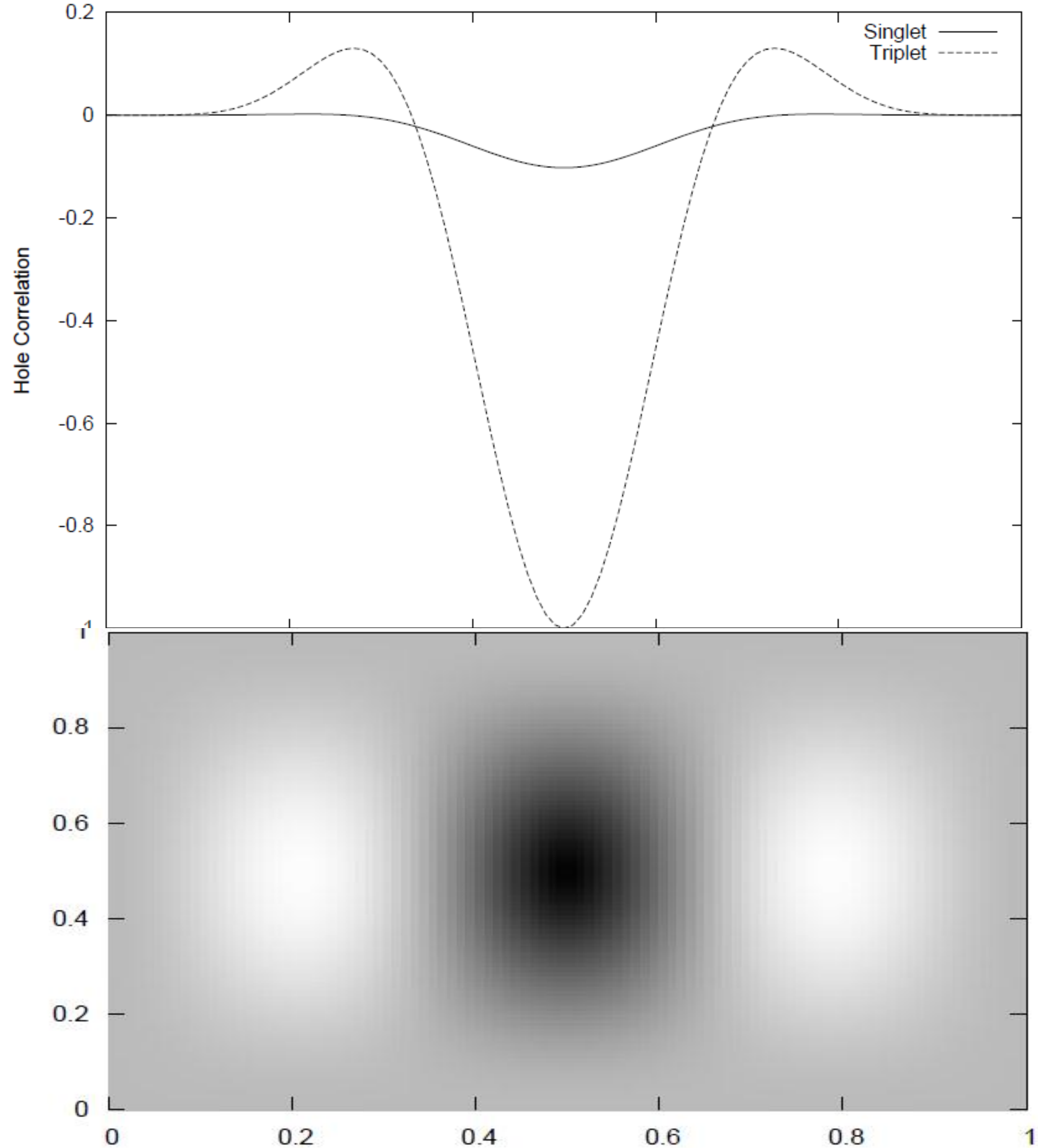


A simple example: spin gate



“AND”

Correlations in nanowires



The end is nigh

… but what the heck does nigh mean?