Bridging Technology and Design for Beyond CMOS

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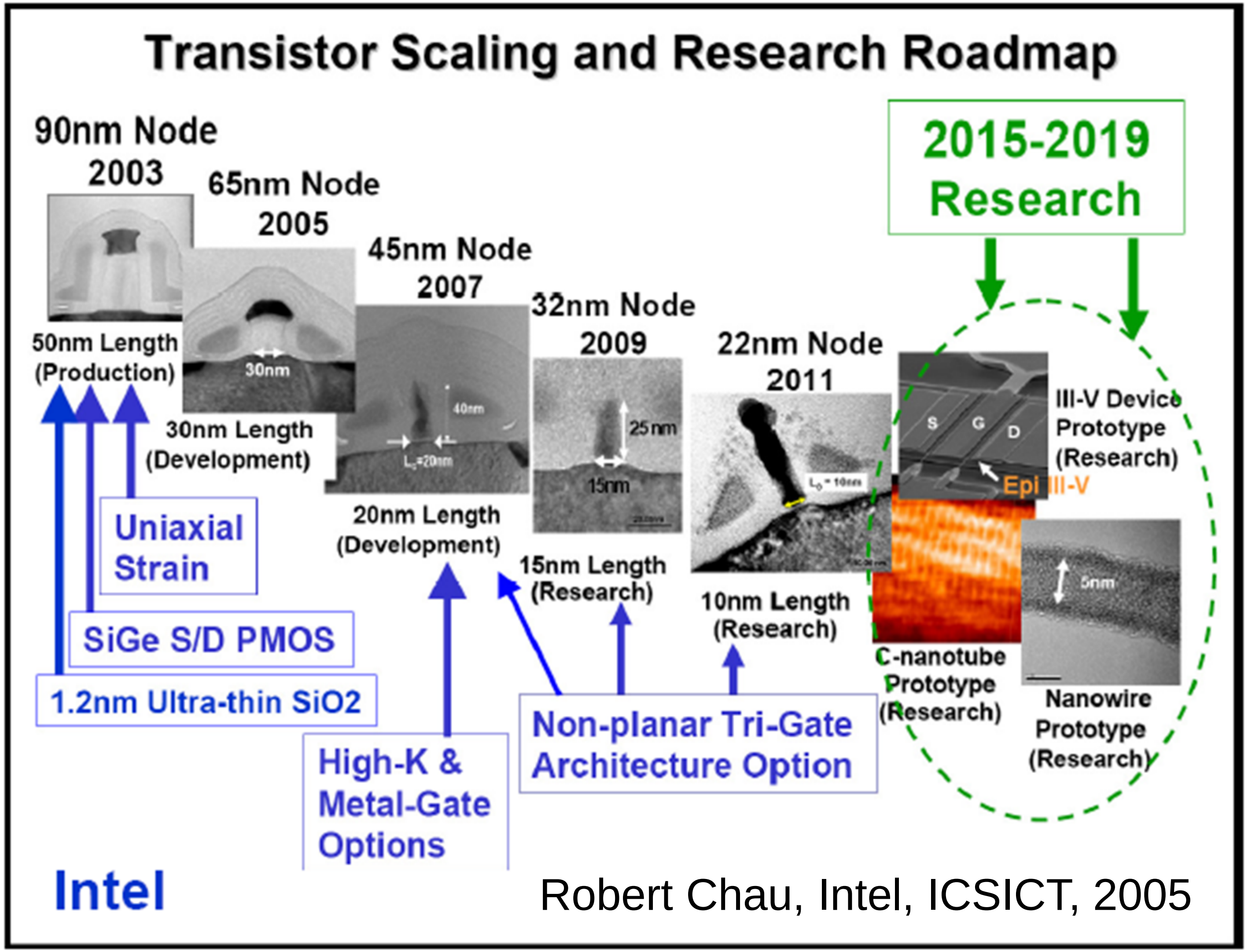
Outline

- **Beyond Moore: devices and technology**
  - **Nanowires and nanotubes**
  - **Single Molecules**
  - **Nanomagnets**

- **Simulation and Design Beyond Moore**
  - **Device modelling**
  - **Novel architectures**

- **Conclusions**

More Moore -> Beyond Moore



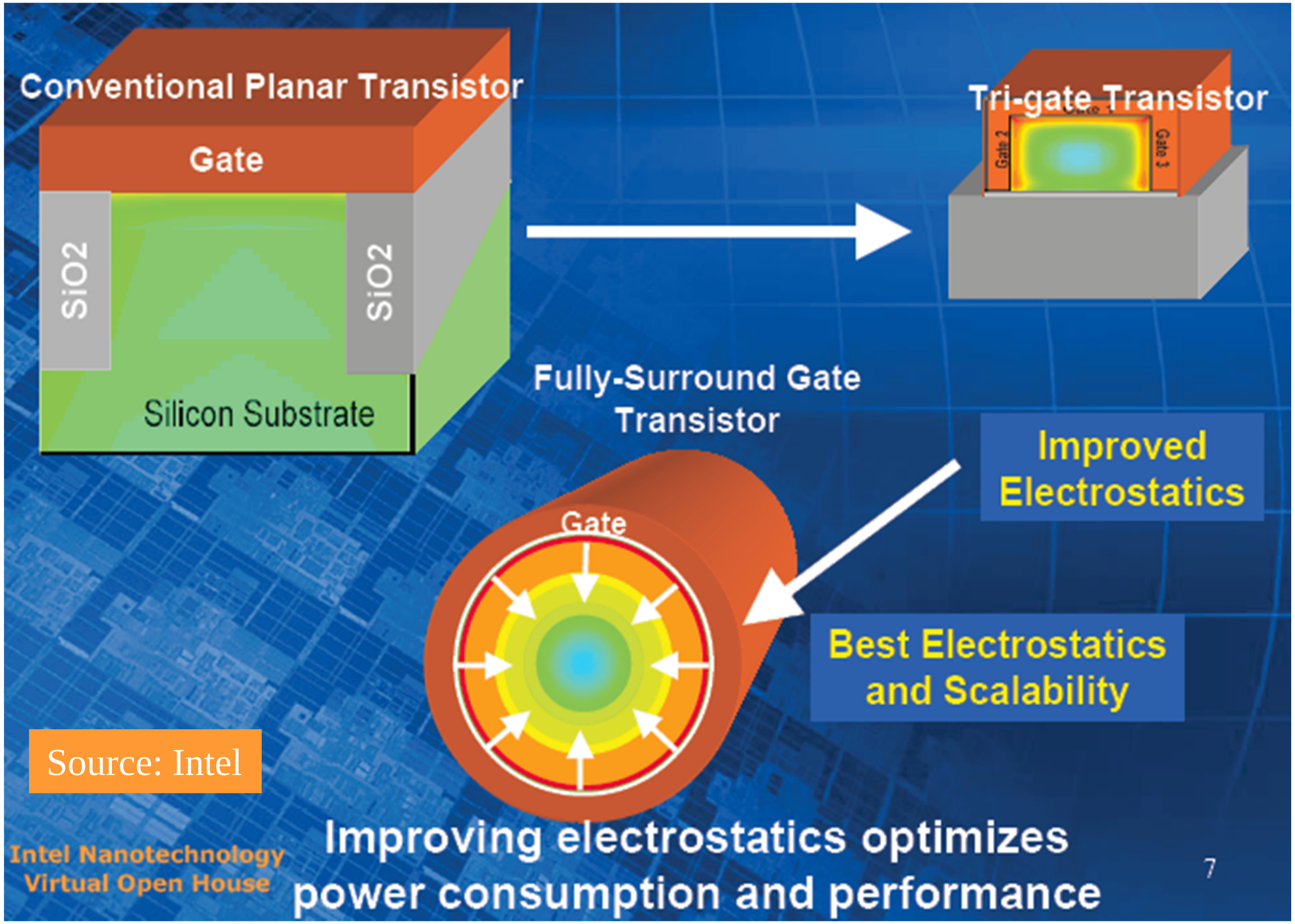
Beyond Moore

Beyond CMOS logic and memory device candidates:

- **Nanowire transistors**
- **CNT transistors**
- **Resonant tunneling devices**
- **NEMS devices**
- **Single electron transistors**
- **Molecular devices**
- **Spintronic devices**

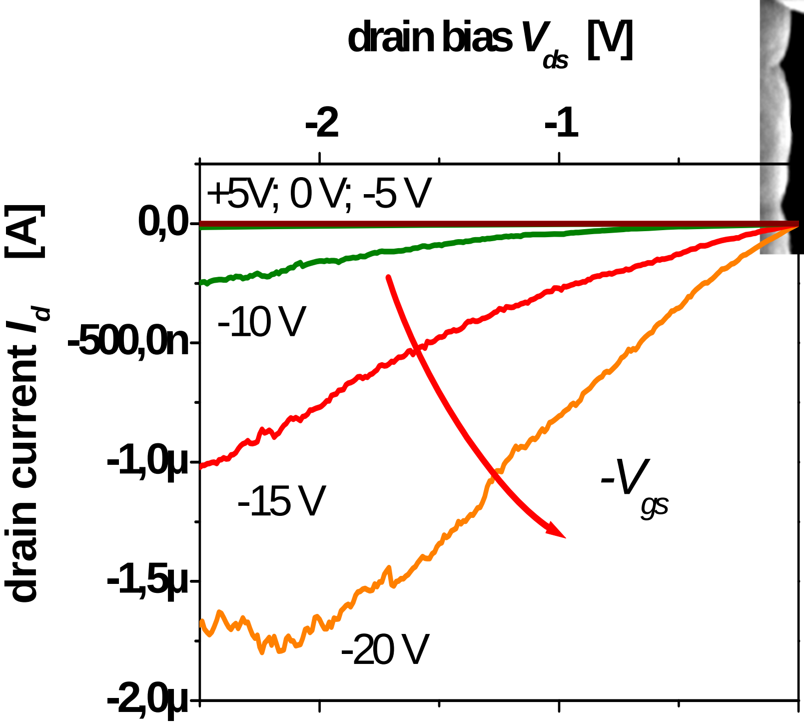
All those candidates (some of which not yet demonstrated) still suffer from major reliability and stability problems

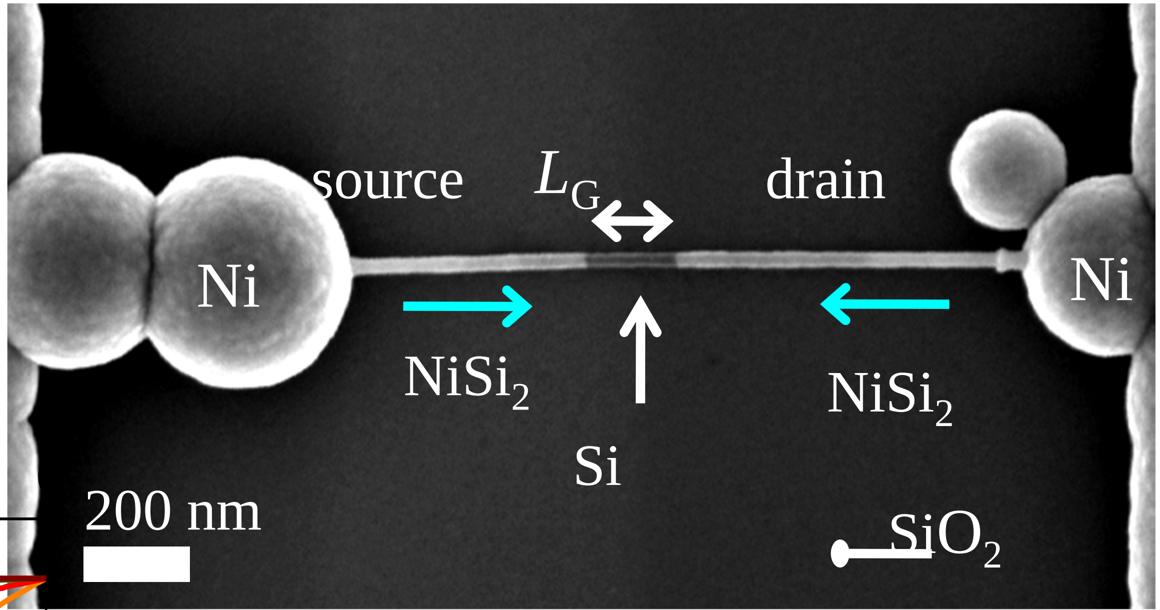
Nano-Device Structure Evolution



Silicon nanowire transistors

L_g = 1.3µm; Ø = 26 nm;
t_{ox} = 300nm SiO_2

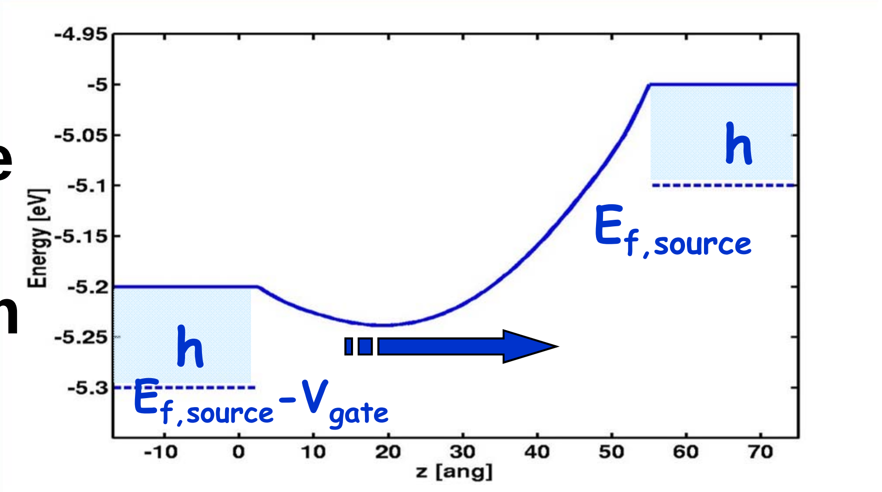




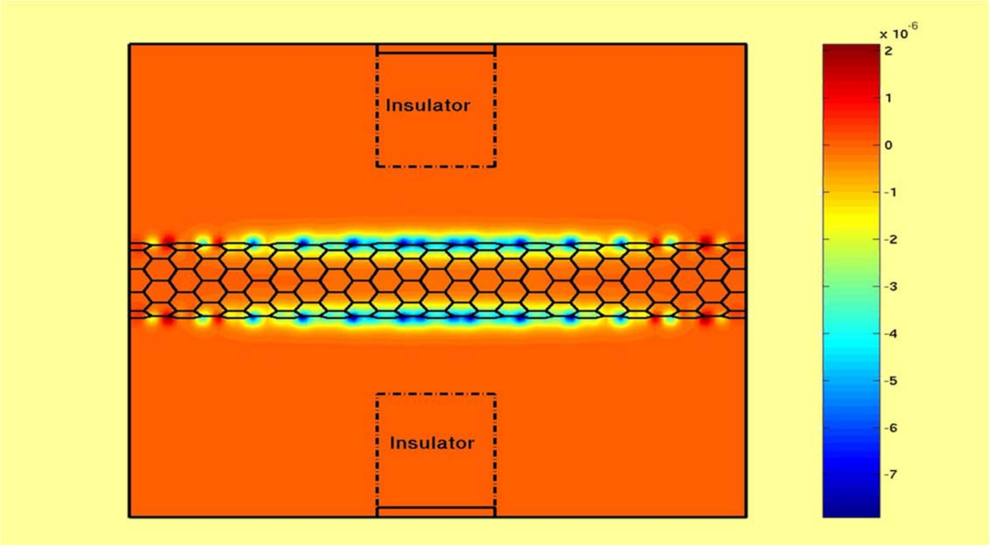
Weber W. M. et al. *Nano Lett.* 6, 2660 (2006)

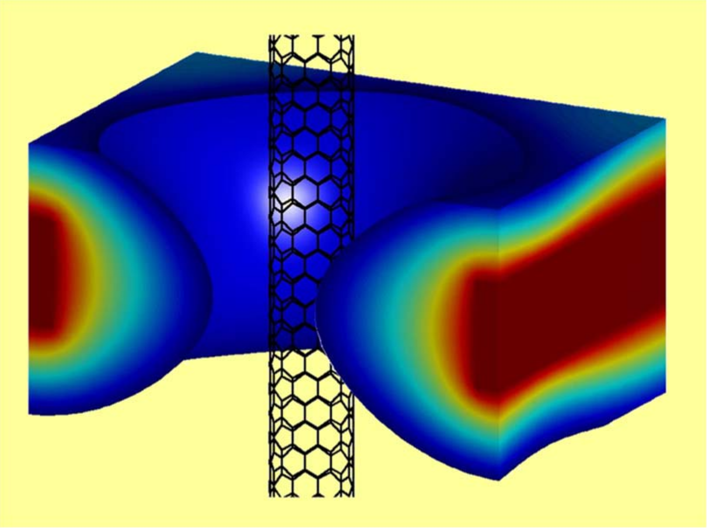
QM Simulation of CNT-Transistors

The CNTs behave like ideal p-type nanowires. The gate voltage modulates the transmission of the holes which are injected from the source contact.



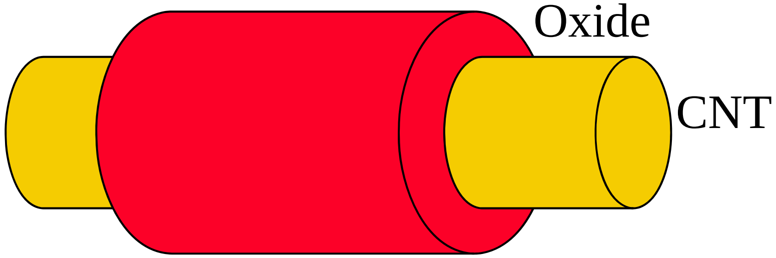
The energie-erofile of the highest valence-subband in a (10,0) CNT for V_{DS} = 0.2 V and V_{GS} = 0.6 V.

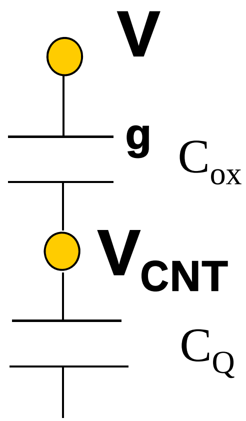




CNT quantum capacitance

Gate is a Macroscopic metal





$$\frac{1}{C_{tot}} = \frac{1}{C_Q} + \frac{1}{C_{ox}}$$

$$\frac{1}{C_Q} = \frac{1}{C_E} + \frac{1}{C_D}$$

$$C_D = e^2 D\left(E_f\right)$$

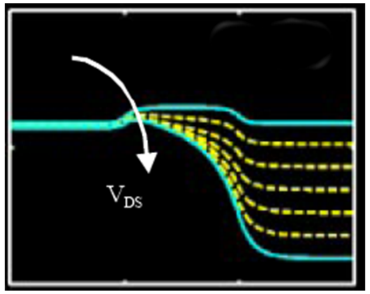
$$C_E = \left(-\frac{\partial E_l}{\partial Q}\right)^{-1}$$

In a classic MOS $C_Q >> C_{ox}$ => modulation depends on C_{ox}

In a well-tempered MOS $C_G >> C_S, C_D$

In 1D systems C_Q is small

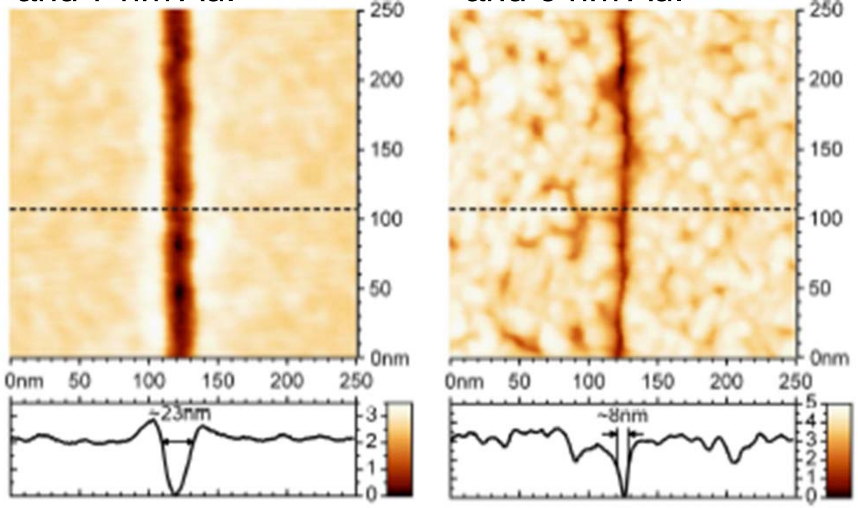
V_{ds} can influence the channel charge and barrier

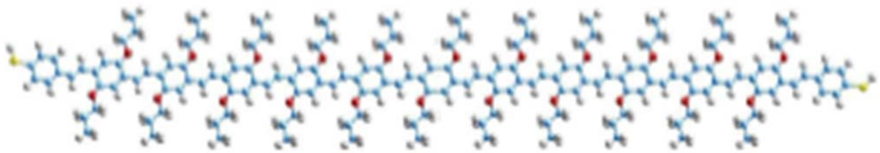


Molecular components

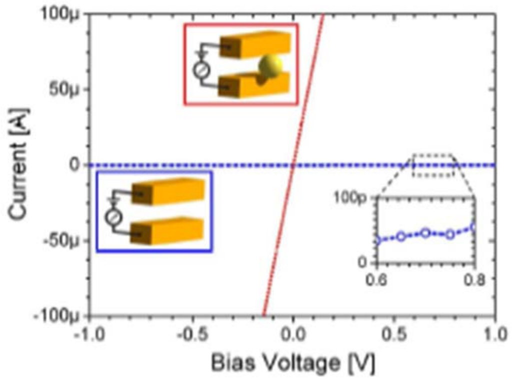
20 nm embedded GaAs layer after etching and deposition of 3 nm Ti and 7 nm Au.

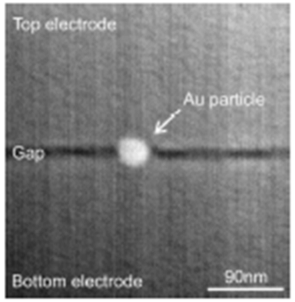
5 nm embedded GaAs layer after etching and deposition of 2 nm Ti and 6 nm Au.

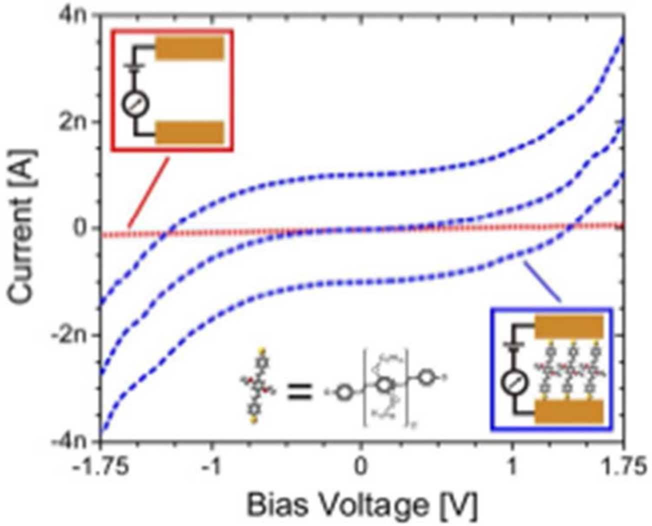




OPV11 molecules with simplified phenyl side chains synthesized by the group of Prof. Dr. E. Thorn-Csányi at the University of Hamburg)

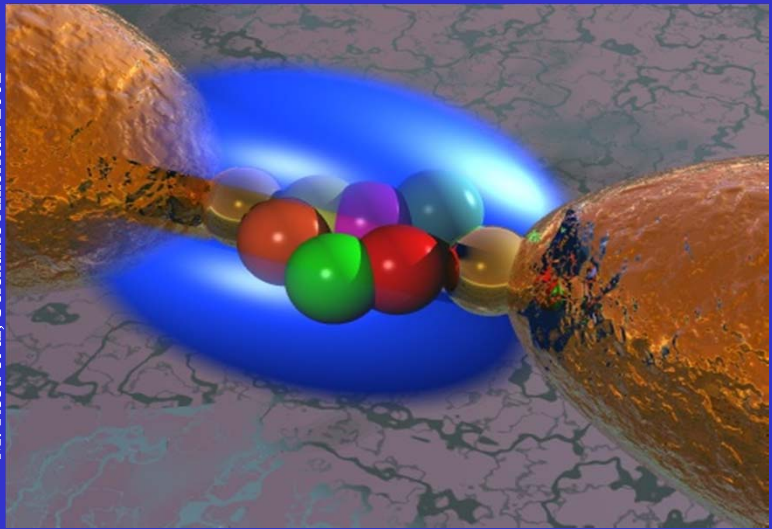






In collaboration with G. Abstreiter, WSI, M. Tornow, TU Braunschweig

Molecular Conduction



M. Reed et al, Scientific American 2002

An electronic structure problem

Self-consistent solution

Transmission – electron flow

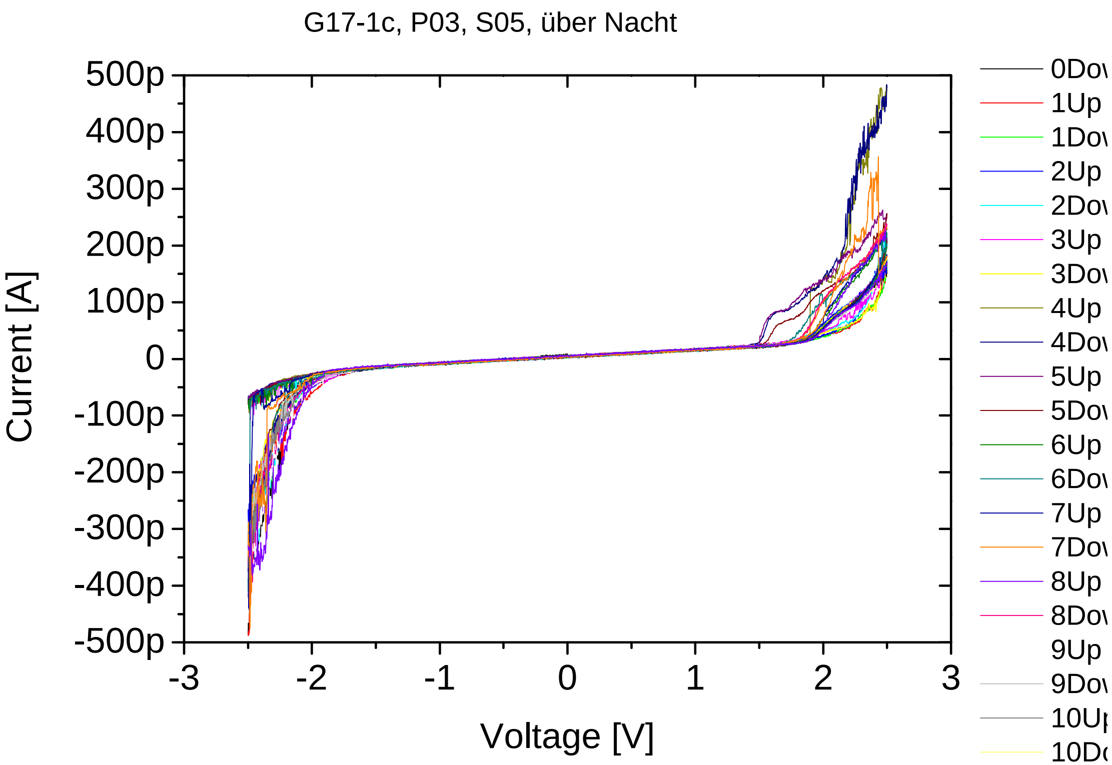
Efficient Density Functional Theory codes

SIESTA (Soler et al.)
→Numerical basis functions, *O(n)* scaling → **TranSIESTA**

DFTB (Frauenheim et. al.)
→DFT parameterized tight-binding → **gDFTB**

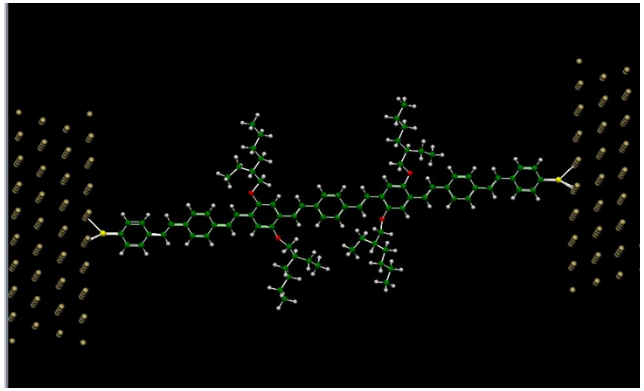
Single molecule devices

A large variation is found in the IV characteristics between succesive sweeps.



Reasons can be due to:

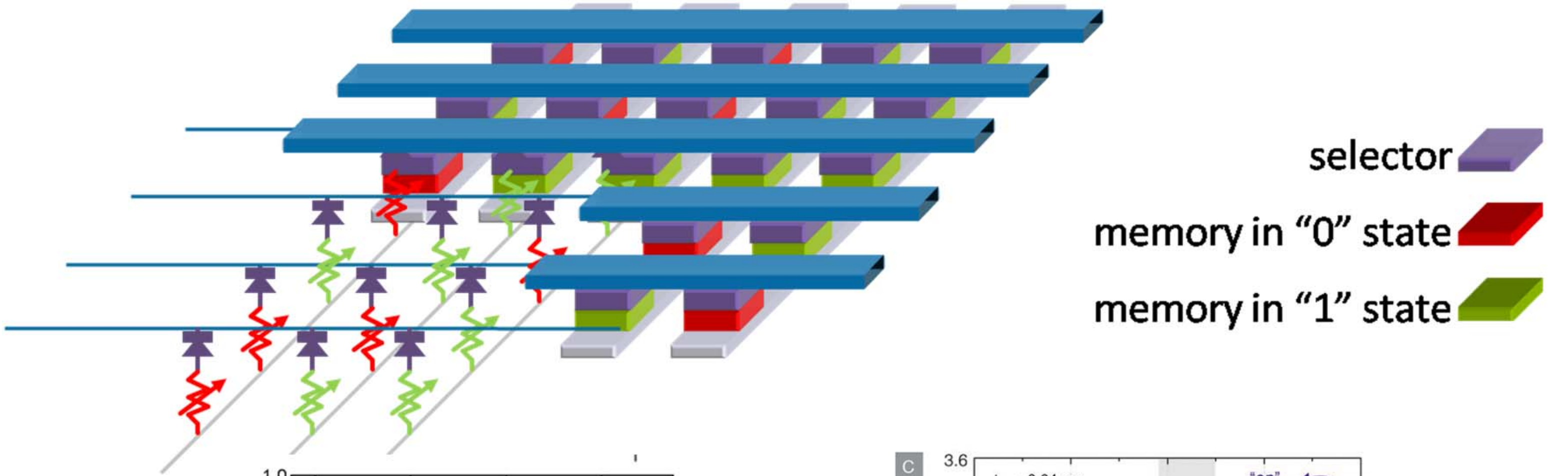
- Configurational changes in single molecules
- Variation in the number of molecules attached to the electrodes
- Changes in the bond of a single molecule to the metal contact
- …

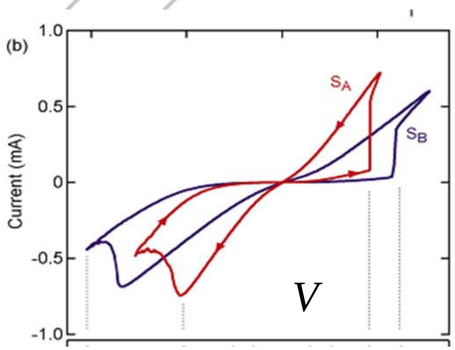


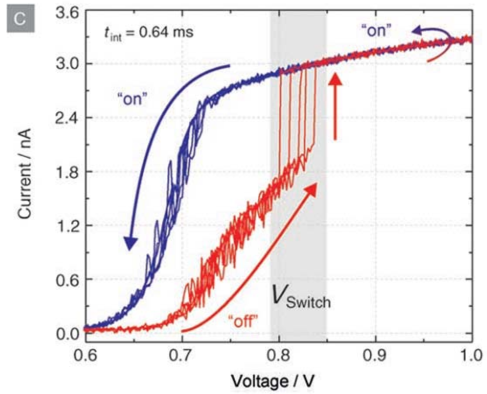
Such variability has to be dealt at a circuit/architecture level

Cross bar non volatile memory

A crossbar memory – probably the simplest possible functional circuit – is one of the proposed application of single molecule electronics







The current-voltage characteristics of molecules is typically hysteretic, with step-like nonlinearities and possibly non-symmetric (rectifying) behavior.

Computing with single molecules

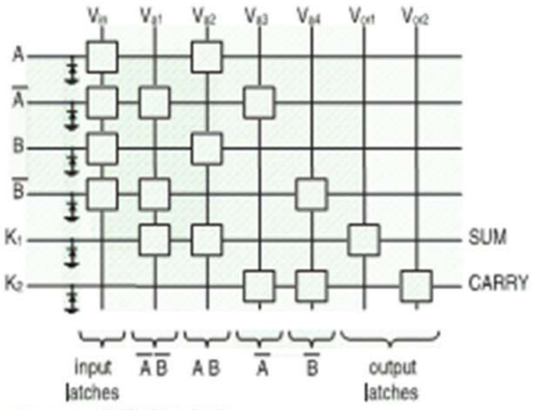


FIGURE 16 Half-adder circuit

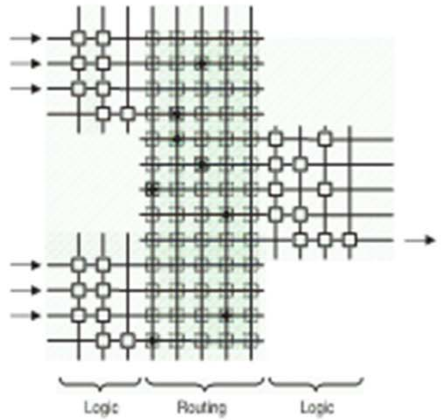
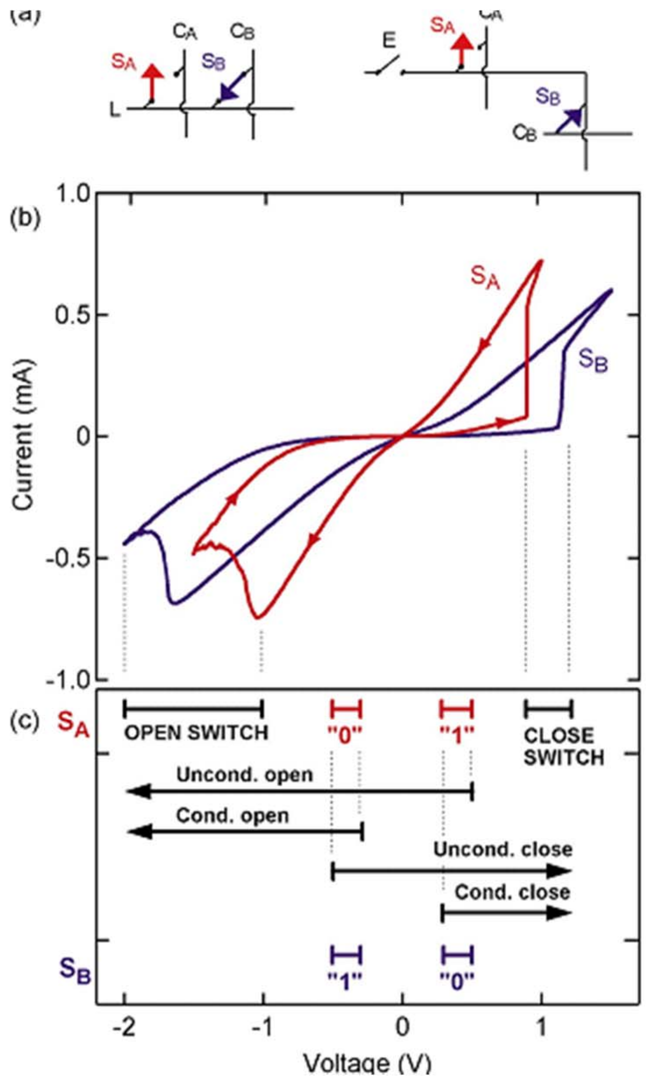


FIGURE 17 Combining multiple crossbars to implement more complex logic functions. The crossbar in the *middle* is used strictly for routing – the closed junctions there are configured once and left to route signals from the output of the logic blocks *on the left* to the logic block *on the right*



Self-organized computation with unreliable, memristive nanodevices

G S Snider

Computing with hysteretic resistor crossbars

Hewlett-Packard Laboratories, 1501 Page Mill Road, Palo Alto, CA 94304, USA

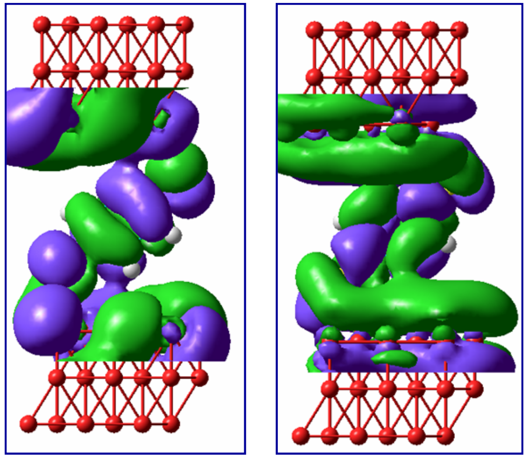
From modelling to design

We can simulate transport in molecular and semiconducting nanostructures quite reliably, accounting for charging effects, dissipation, screening as long as the molecular systems consist of a sufficiently small number of atoms,

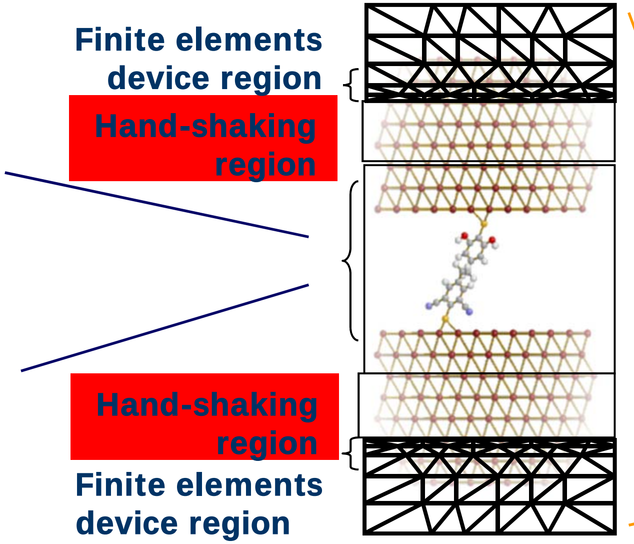
but

the simulation of realistic systems, especially in terms of the contacts and in general the coupling with the external environment is still a problem

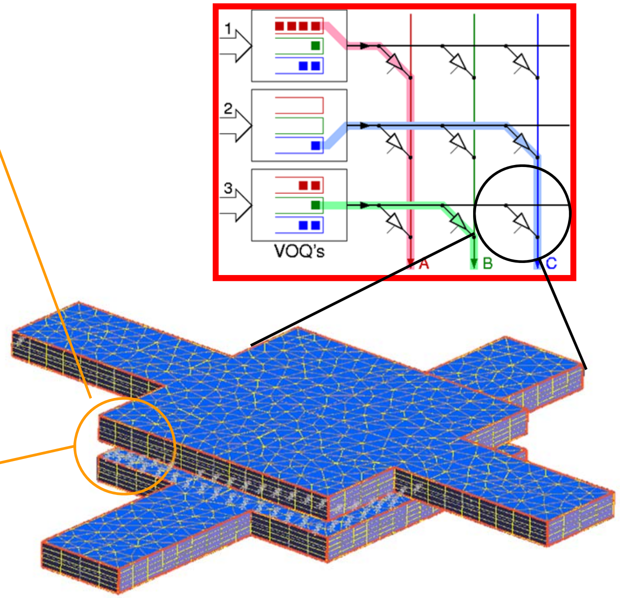
Multiscale modelling



DFTB + quantum-transport approaches using Non-equlibrium Green Functions.



Well-established drift diffusion simulator codes are used to simulate contacts and devices surrounding the molecules.

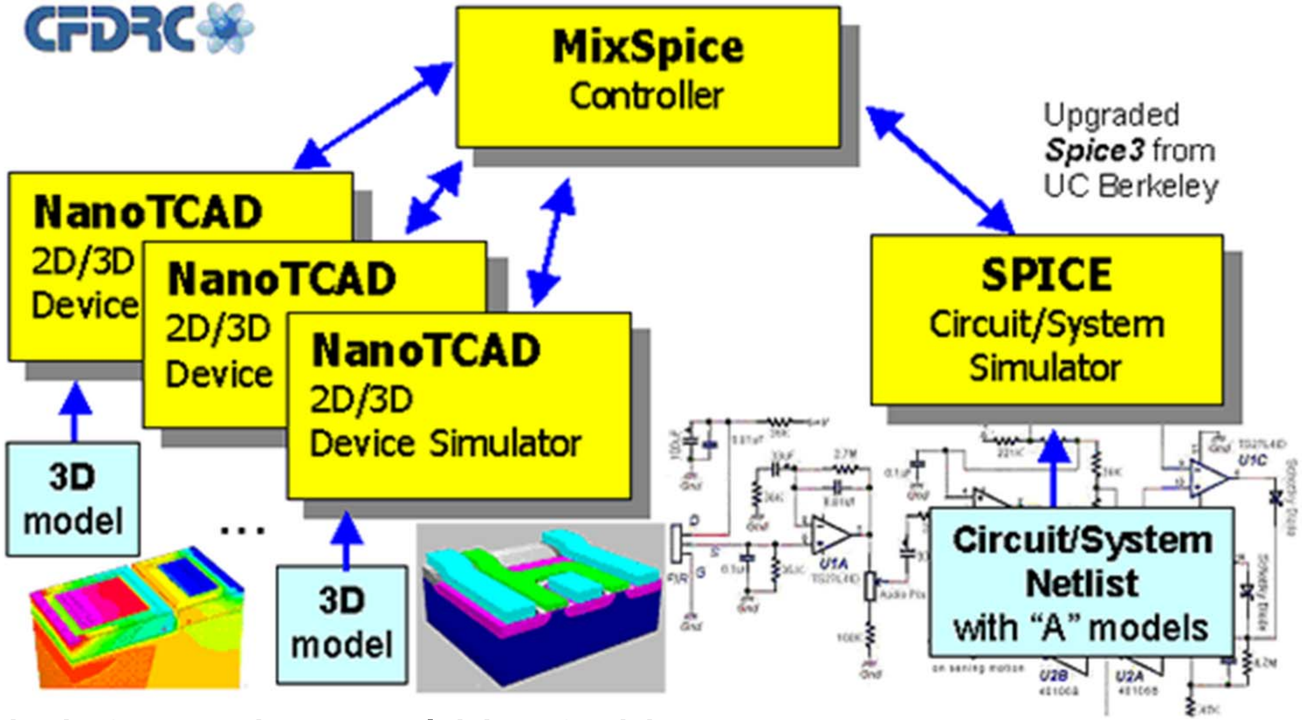


Circuit level

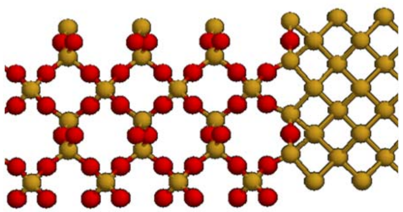
nanometer region	submicron to micron region	Micron to millimeter regions
Ab initio models	Quantum-classical interfaces	Continuum-based and circuit models

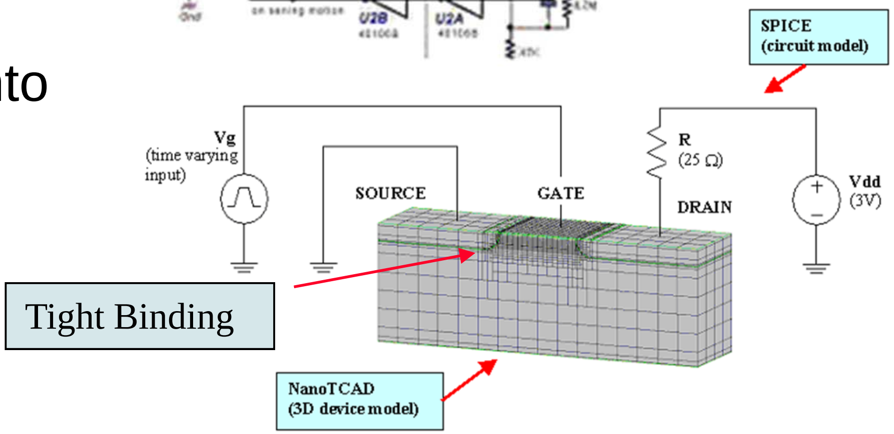
Physics ⟷ Engineering

Mixed-Mode Simulation

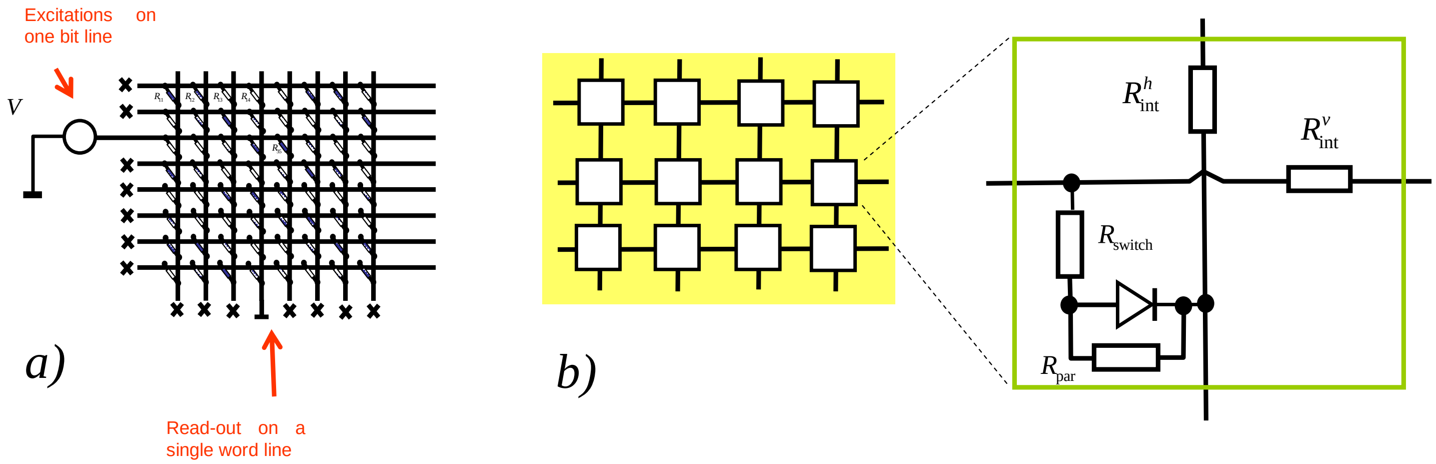


Atomistic information could be fed into the NanoTCAD simulator

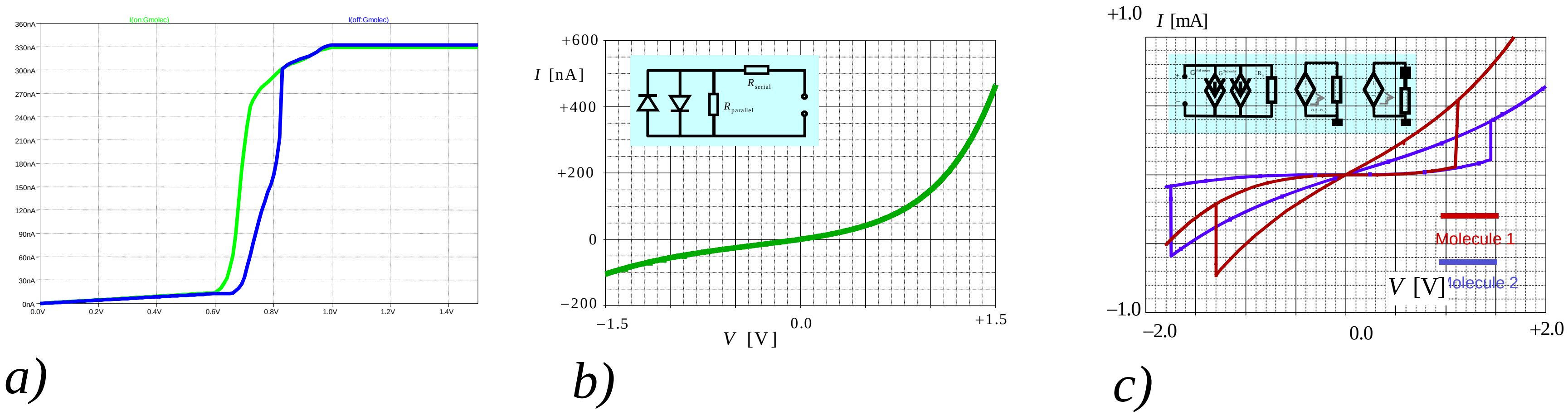




Modelling a cross bar memory

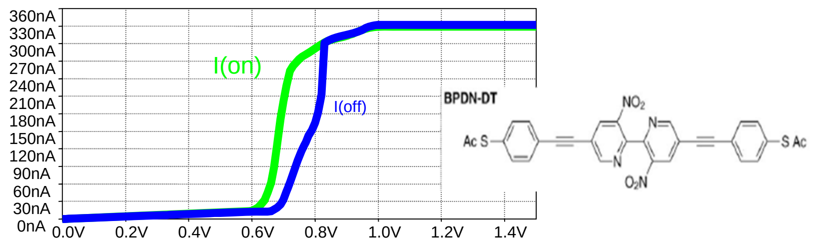


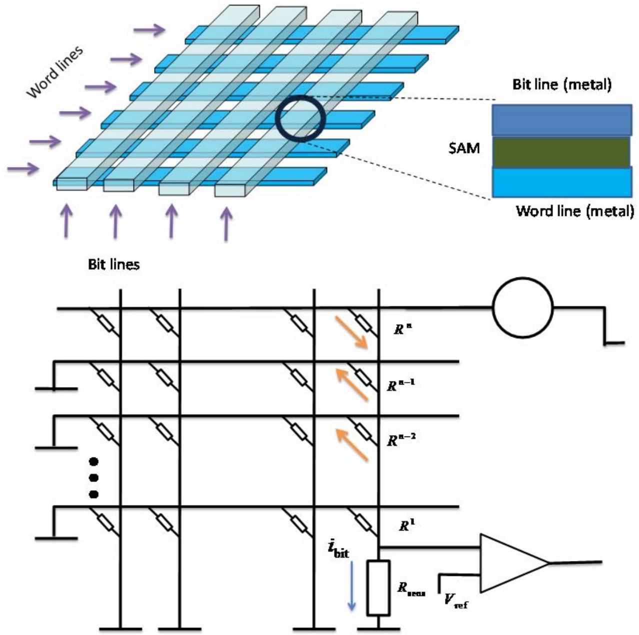
We use SPICE circuit simulations to investigate such circuits. We built the model of the junction using published (molecular) I-V curves and then generated SPICE netlists of large circuits using a Matlab script.



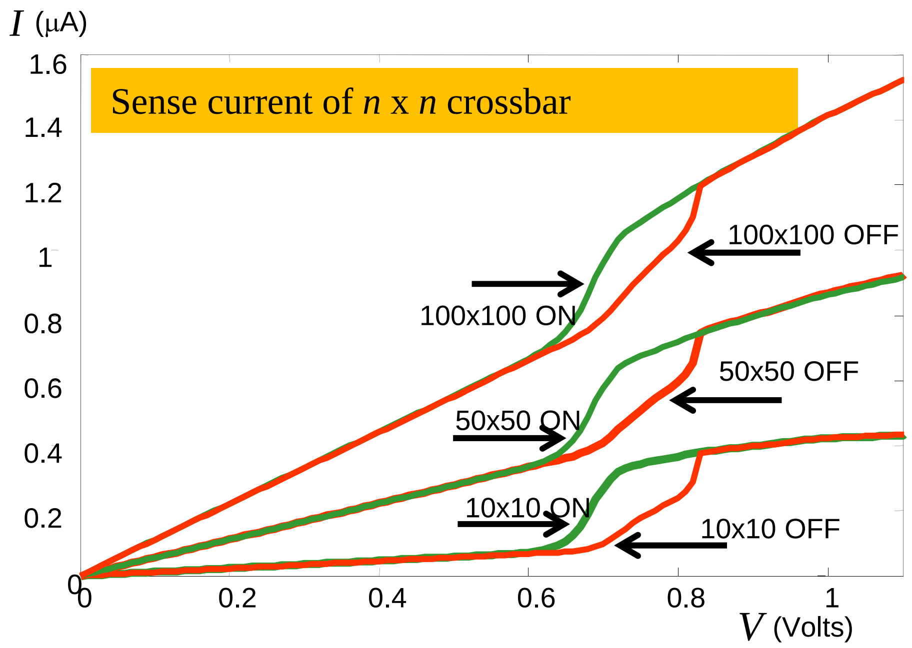
Cross-point arrays

We have set up a circuit model for molecular cross bar arrays to address the performance and the scalability of such systems. The IV characteristics for the SPICE model taken from: E. Lortscher, J. W. Ciszek, J. Tour, H. Riel: *Reversible and Controllable Switching of a Single-Molecule Junction*, Small 2, No. 8-9, 973 (2006)



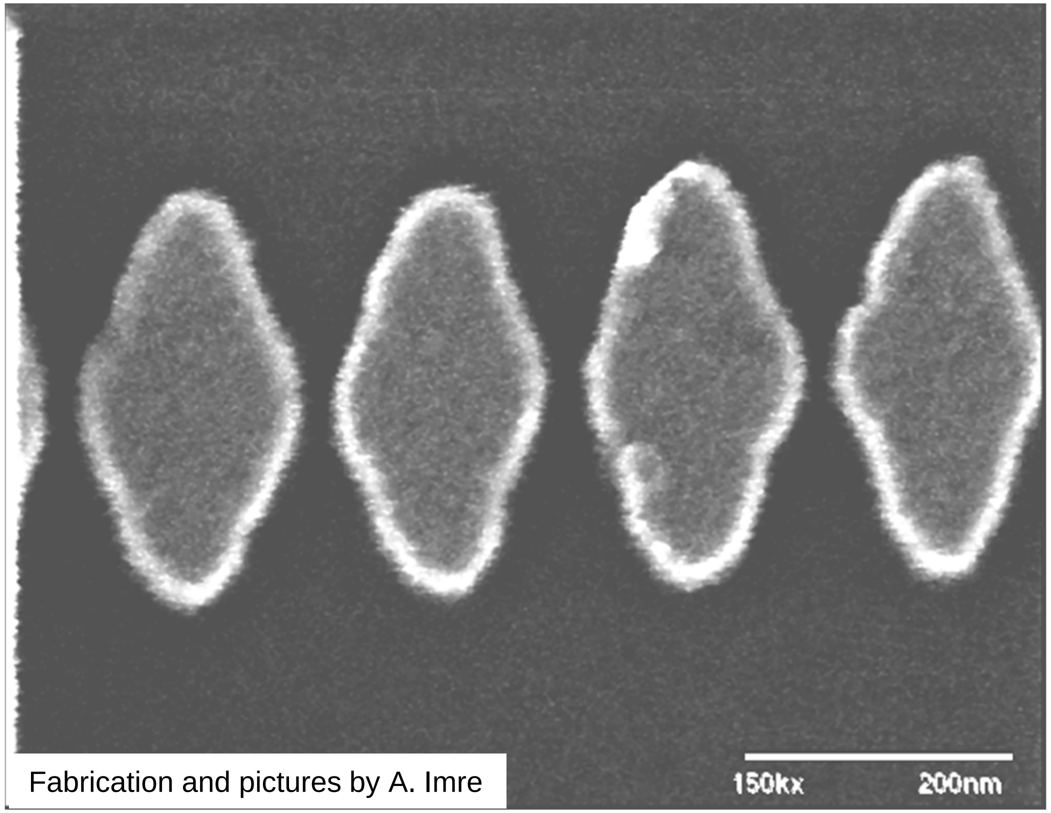


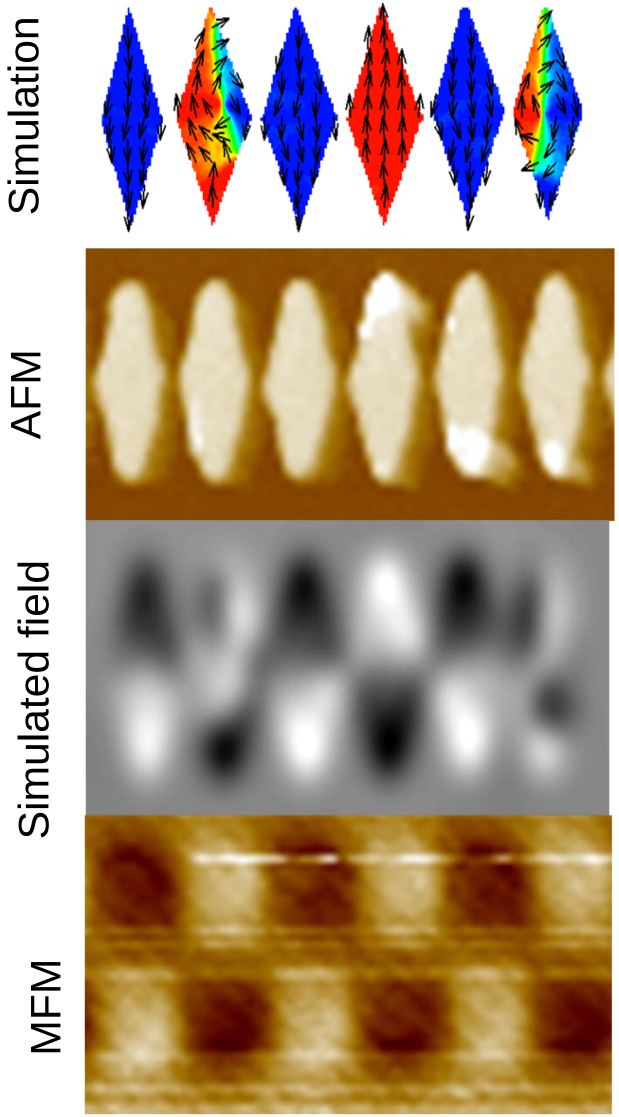
G. Csaba and P. Lugli, IEEE Trans. Nanotechn. (2009)



- Nonlinearity of the molecule IV characteristics enhances read-out margin
- Coupling molecular layer with solid-state diodes enables large-scale circuits

Coupled nanomagnets

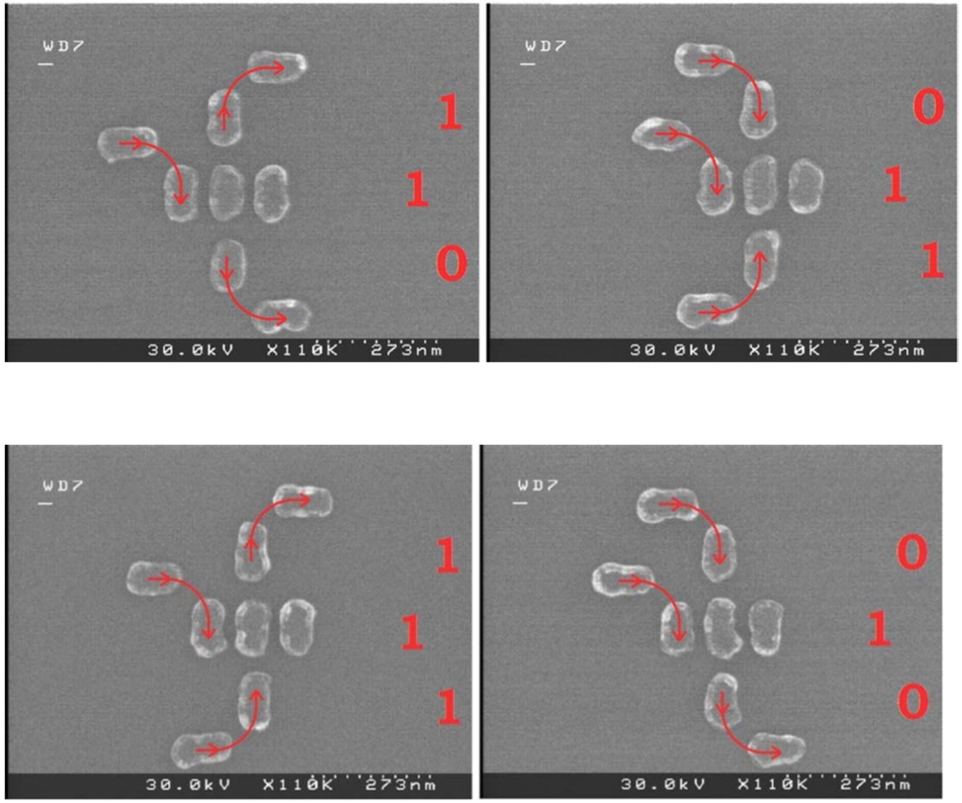


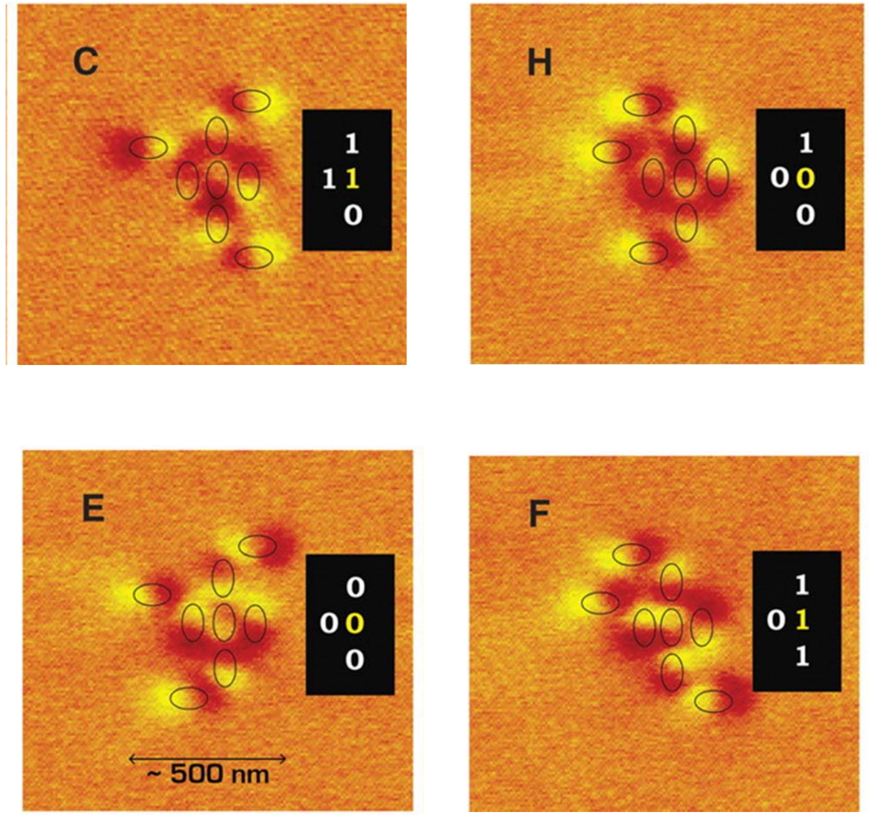


Investigations of permalloy nanomagnets (thermally evaporated and patterned by electron beam lithography) confirm the simulation results

Courtesy of W. Porod, Notre Dame University

Working majority gate



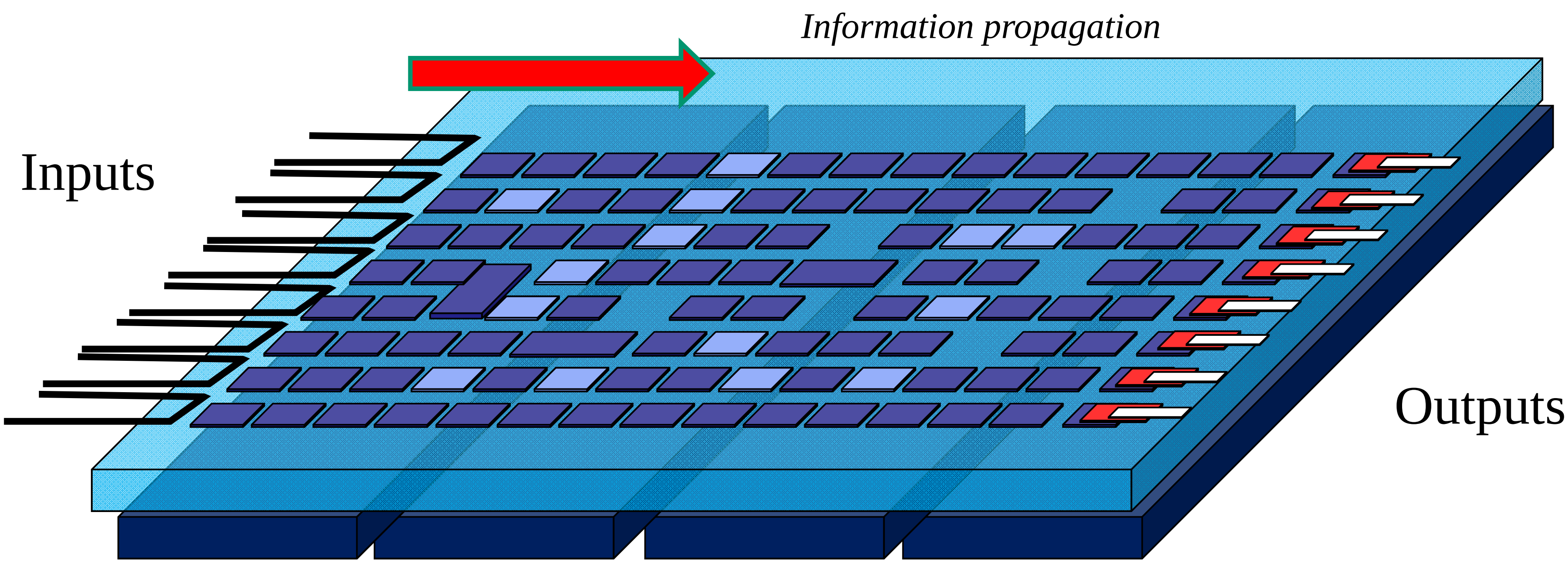


SEM images

MFM images

Imre et. al. *Science* 2006

Logic with nanomagnets



The challenges:

How to make signals propagating?	→	Integrated clocking
How to write in the magnets?	→	Localized field from wires
How to read out the magnets?	→	Hall sensor

In collaboration with M. Becherer and D. Schmit-Lansiedel (TUM) , W. Porod (Notre Dame)

Conclusions

- **Nanotechnology provides a variety of interesting and promising nanostructures**
- **Critical issues such as reliability, stability and lifetime are going to become routine and will have to be addressed at a circuit/architecture level**
- **Quantum mechanical device modelling must be matched to circuit simulations**
- **Novel circuits and architectures are going to be needed for a full exploitation of nanocomponents**


nano
Thanks for your attention!