The bridge to design

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Outline

- Multiscale approaches for nanostructures
  - Simulation of nanostructures
  - Cross Bar Architectures
  - Simulation of organic FETs and organic inverters
- Field coupling in Quantum Cellular Automata
  - Quantum Cellular Automata
  - Magnetic logic gate
- Conclusions

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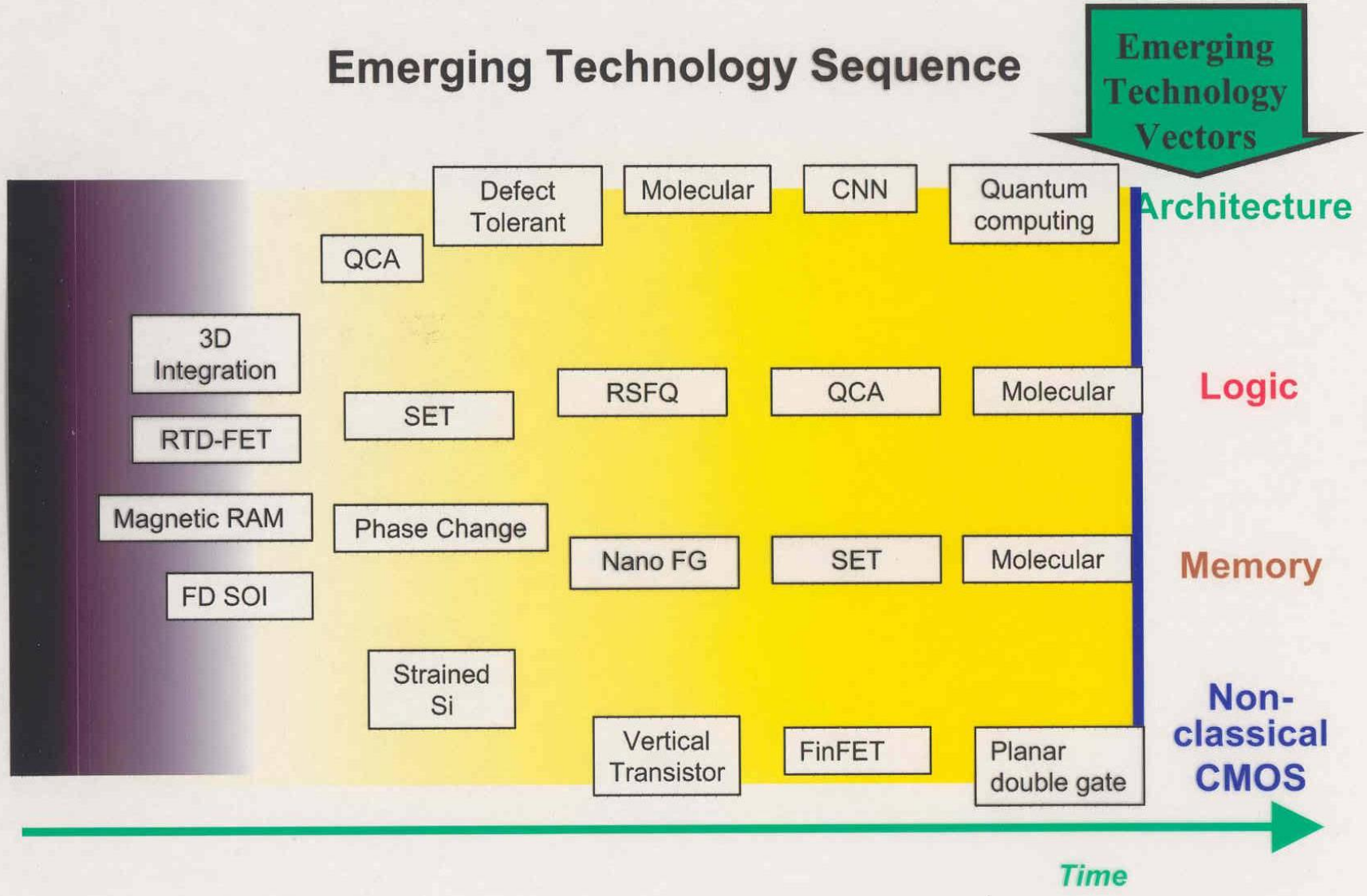
International Technology Roadmap for Semiconductors



Beyond Moore

Beyond CMOS logic and memory device candidates:

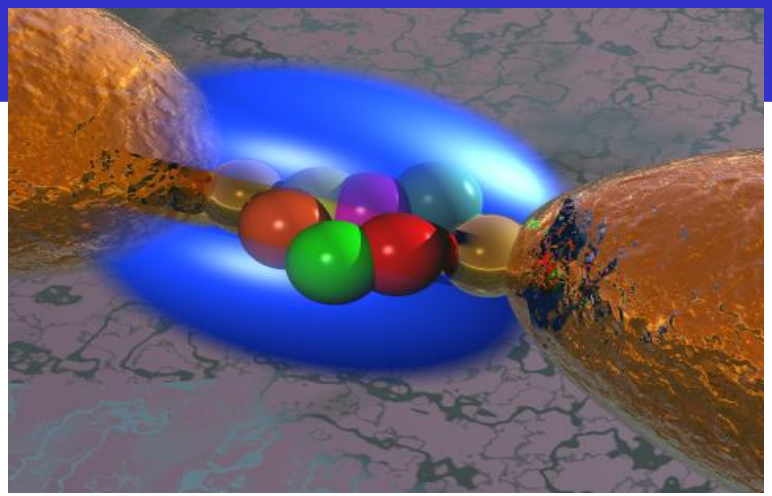
- **Nanowire transistors**
- **CNT transistors**
- **Resonant tunneling devices**
- **NEMS devices**
- **Single electron transistors**
- **Molecular devices**
- **Spintronic devices**

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

Simulation and modeling tools

- Circuit-based modeling (SPICE)
- Drift-diffusion device simulation (OTFT, MOSFET, HEMT,..)
- Monte Carlo device simulation (HEMT, QCL, …)
- Ab-initio and quasi-ab-initio modeling of molecules
- NEGF calculation of carrier transport in molecules
- Tight binding calculation of electronic properties of nanostructures

Conduction through Single Molecules



An electronic structure problem

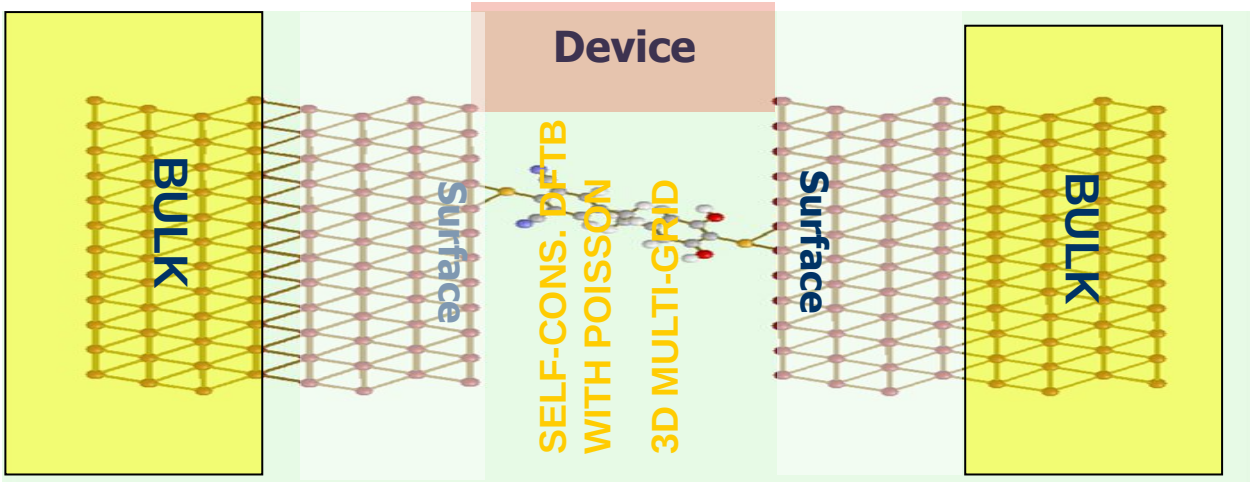
Self-consistent solution

Efficient Density Functional Theory codes

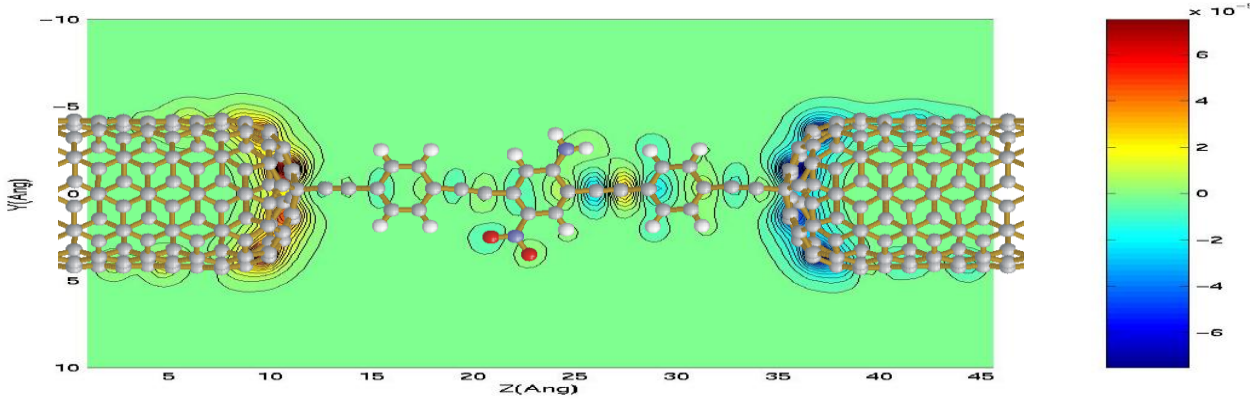
SIESTA (Soler et al.)
→Numerical basis functions, *O(n)* scaling → **TranSIESTA**

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

Self-Consistent Quantum Transport

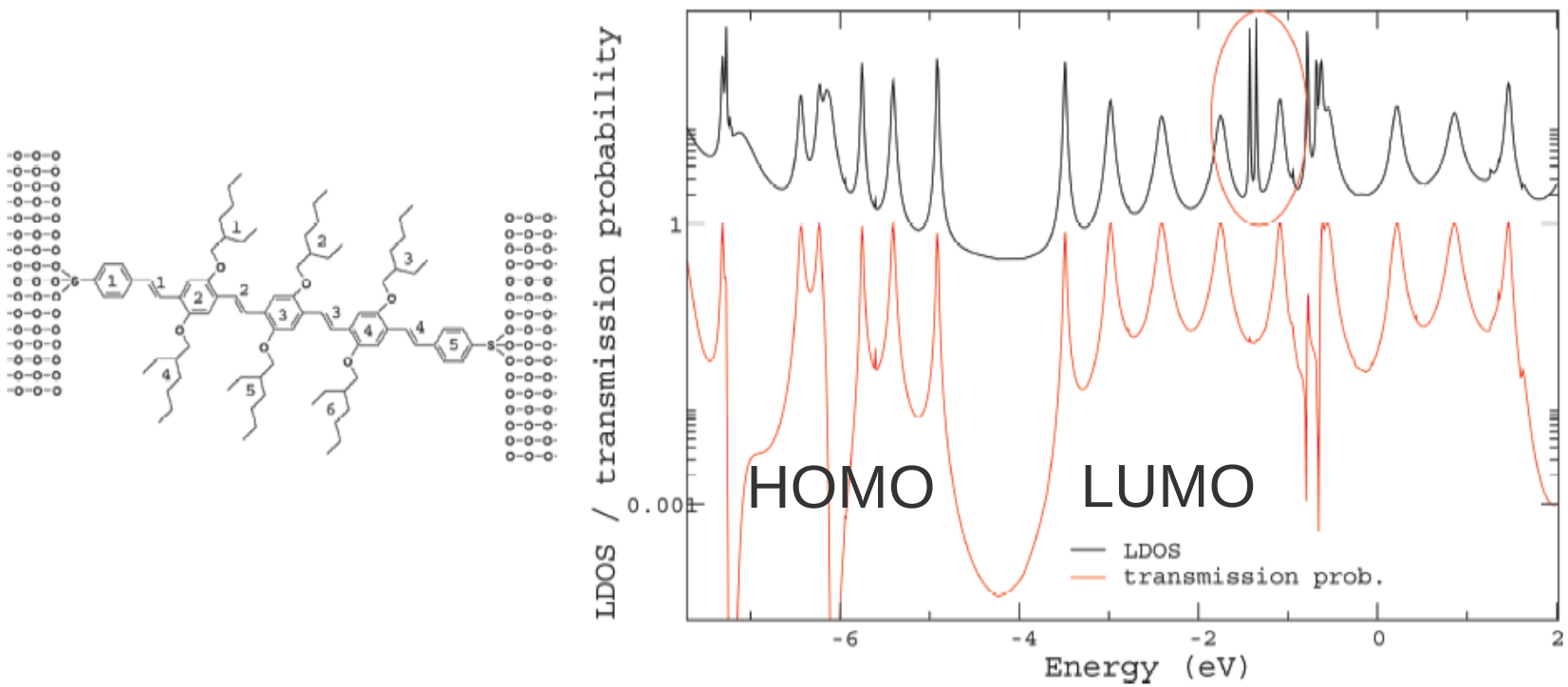


The simulated structure is divided into ‘bulk’ and ‘device regions’



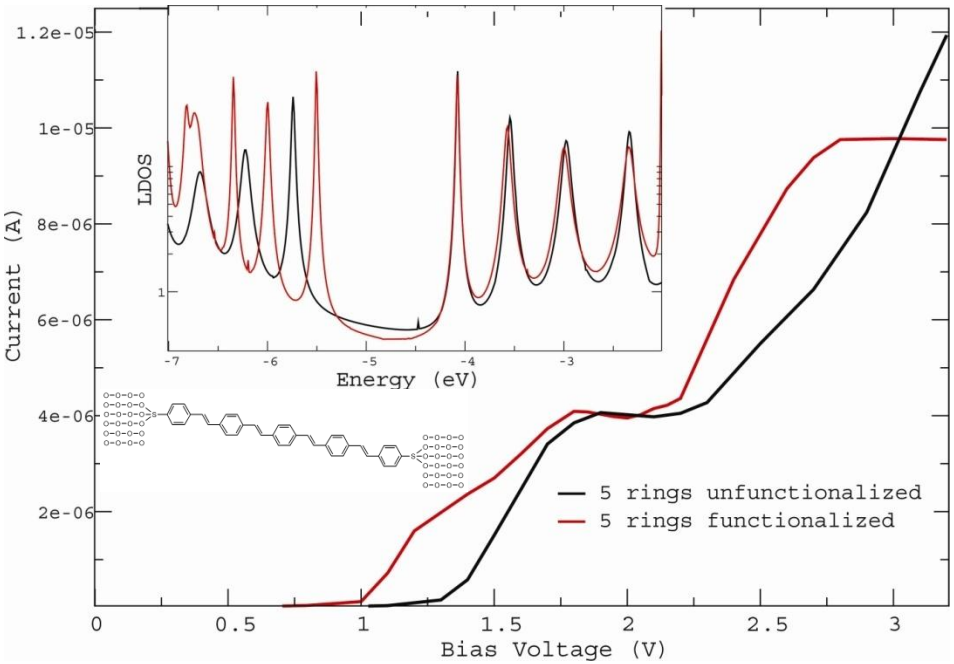
Self-consistent potential of molecule contacted to carbon nanotubes

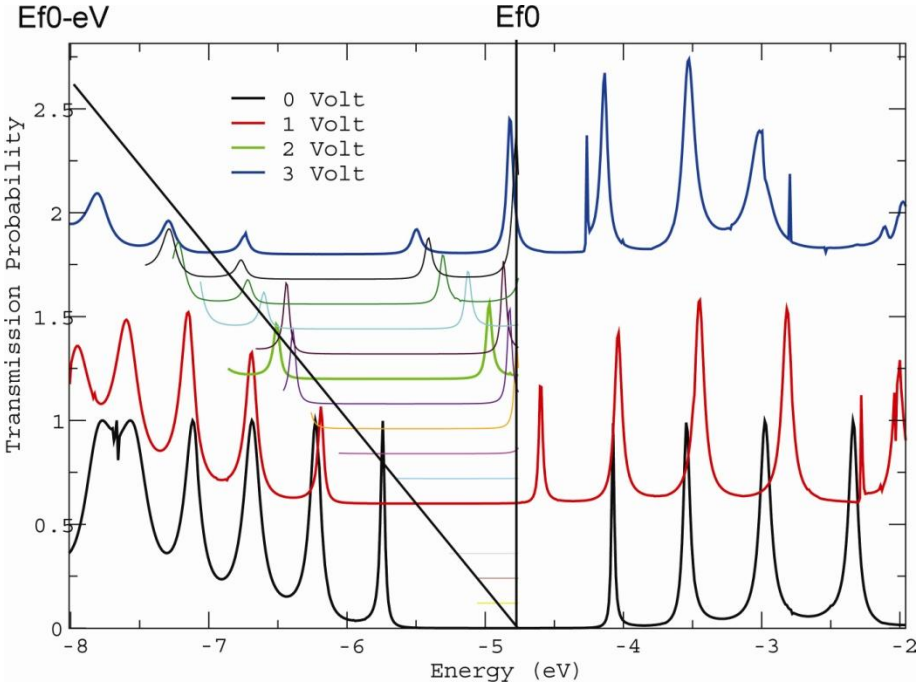
Transmission function



The current-voltage characteristics can be calculated from the so called Landauer equation as an integral of the transmission function T(E)

I-V characteristics in OPVs

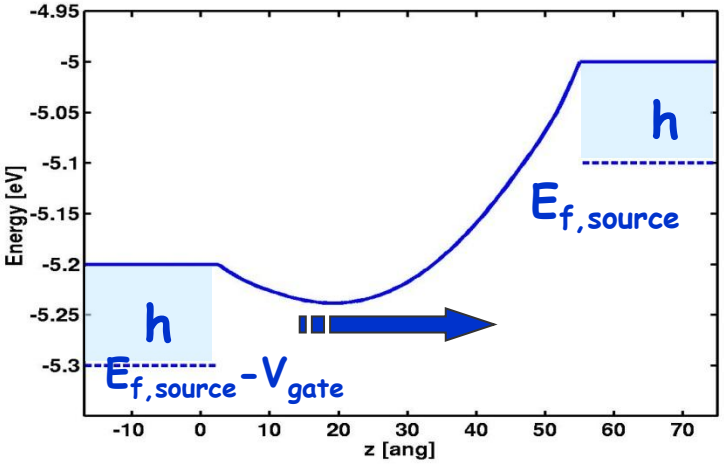




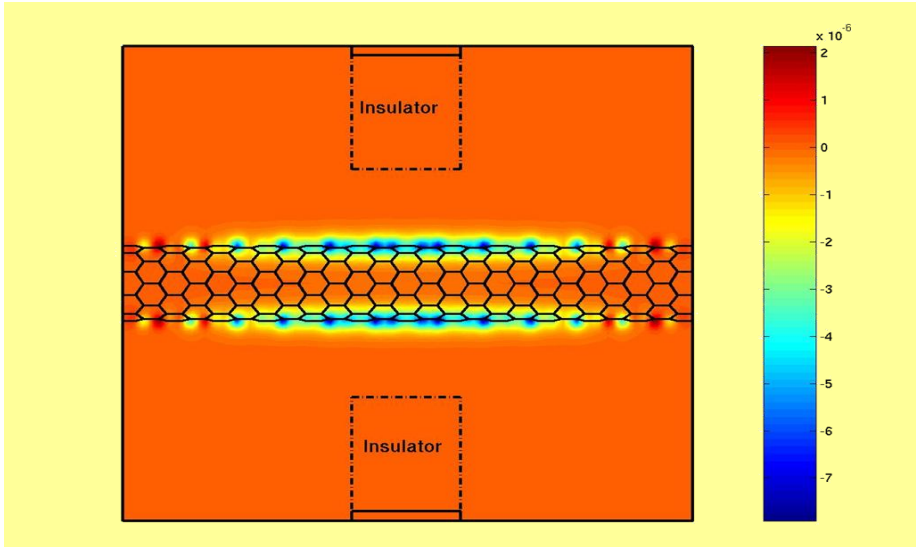
Al long as no resonances are included in the transmission window (low bias), the current is negligible (*tunneling regime*). The threshold voltage occurs when the HOMO-LUMO states enter such window. The terrace is due to the fact that the transmission peaks broaden and shrink at increasing voltage

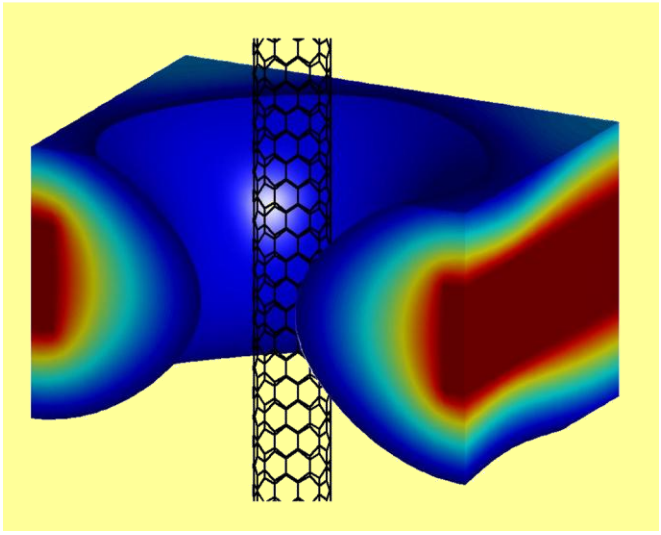
Vertical CNT-transistor

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



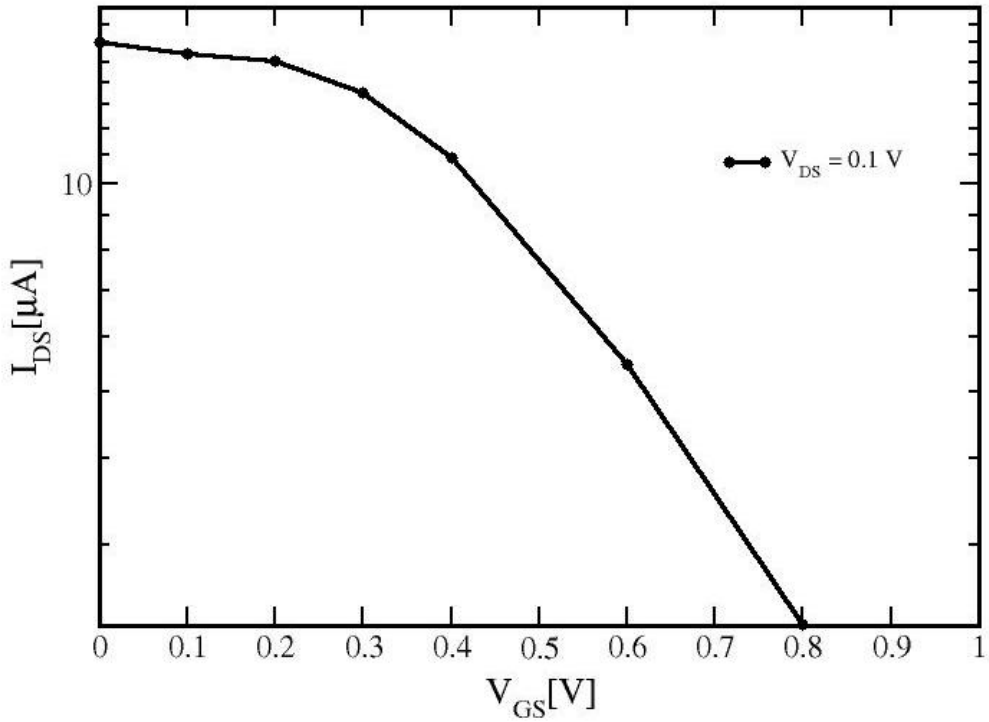
The energie-profile of the highest valence-subband in a (10,0) CNT for V_{DS} = 0.2 V and V_{GS} = 0.6 V.





Landauer Formalism is used to calculate the current between souce and drain

$$I = \frac{2e}{h} \int \overline{T}\ E \left[f_1^+\ E\ - f_2^-\ E\ \right] dE$$

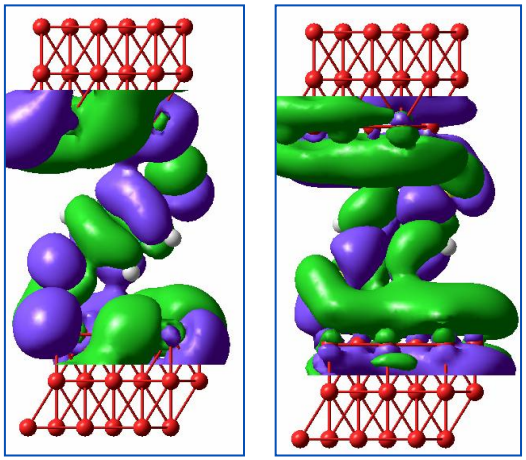


We can simulate transport in molecular structures quite reliably, accounting for charging effects, dissipation, screening as long as the molecular systems consist of a sufficiently small number of atoms,

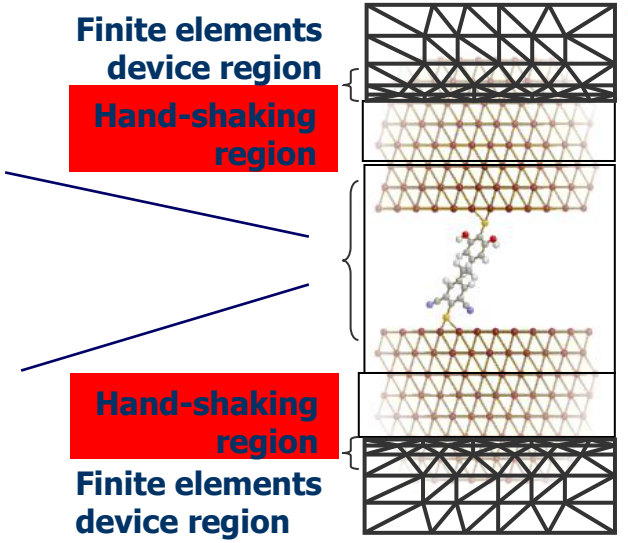
but

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

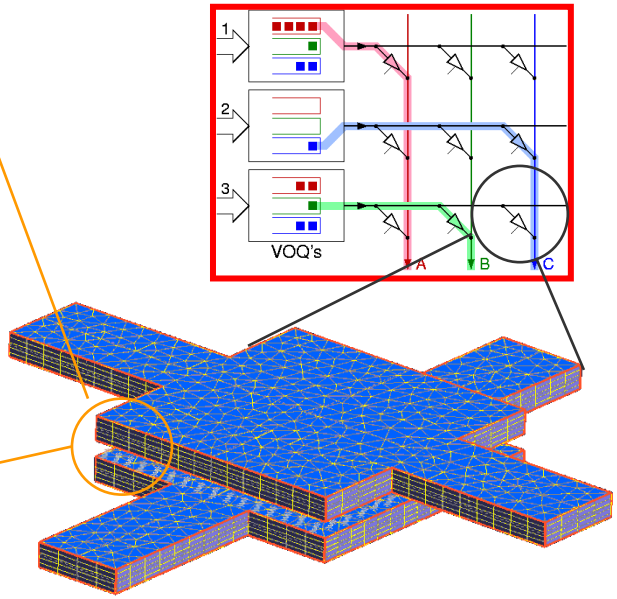
Multiscale modeling



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.



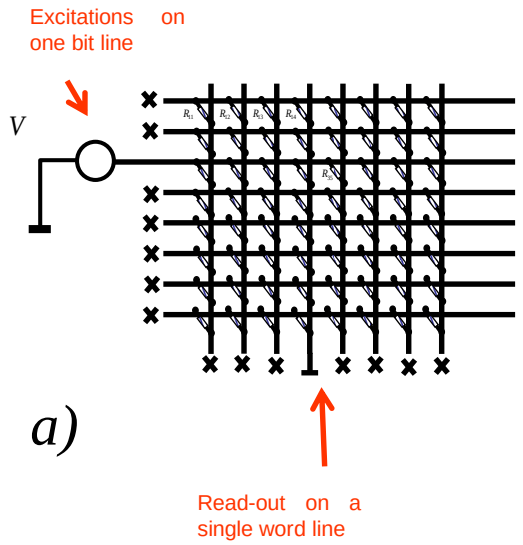
Circuit level

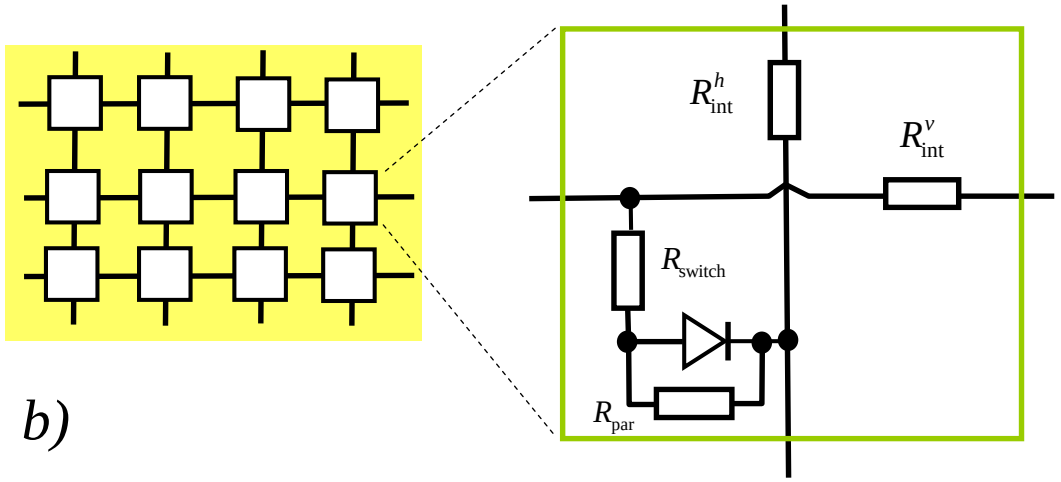
nanometer region | submicron to micron region | Micron to millimeter regions

Ab initio models | **Quantum-classical interfaces** | **Continuum-based and circuit models**

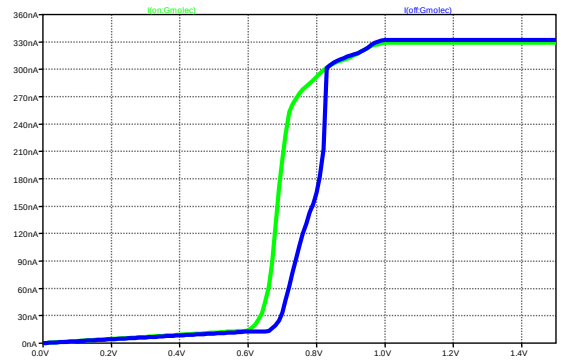
Physics — Engineering

Modelling a cross bar memory

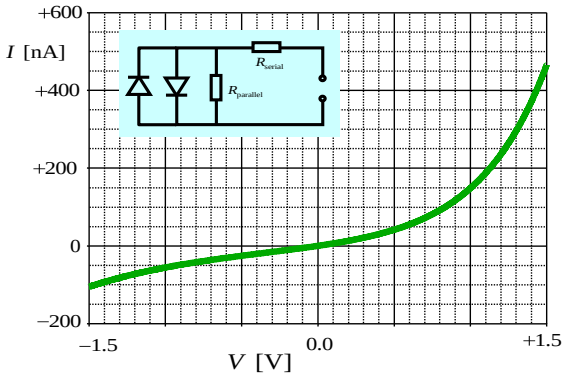




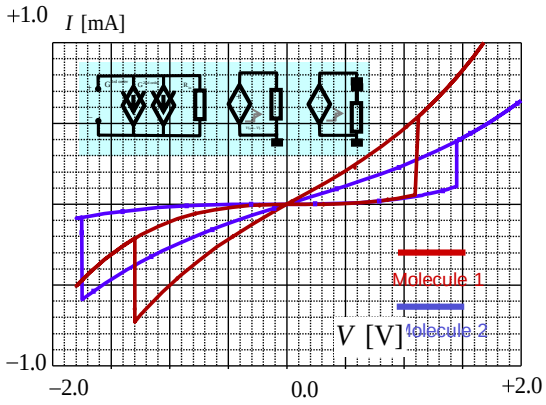
We use SPICE circuit simulations to investigate such circuits. We built the model of the junction using published (molecular) I-V curves and then generated SPICE netlists of large circuits using a Matlab script.



a)

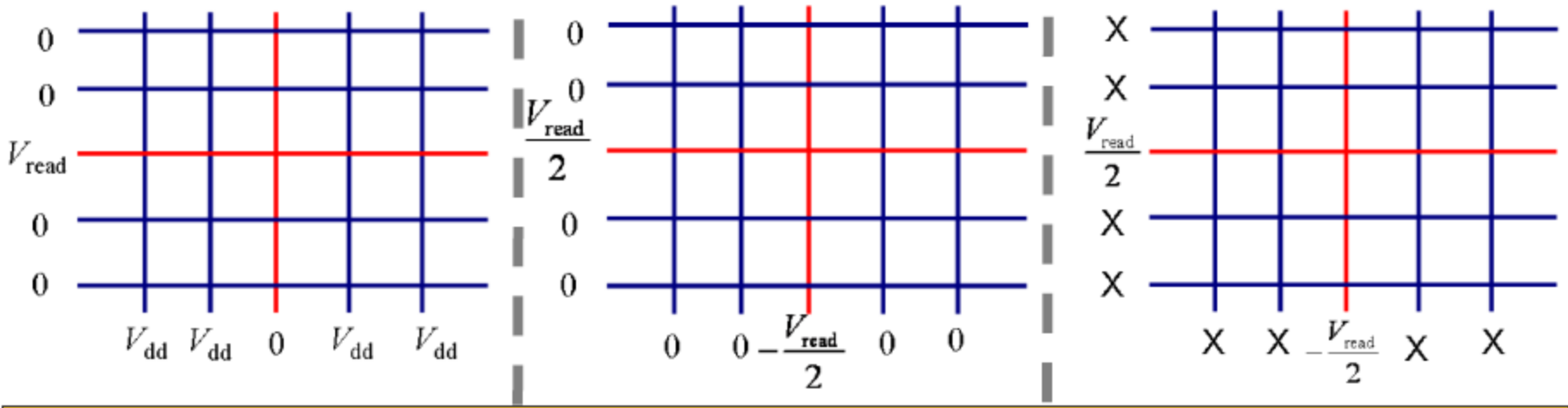


b)



c)

Cross-bar architecture: read out scheme



Scheme I

- Overall leakage can be high
- Parasitic currents does not change the read-current significantly
- Figure of merit for diode: I_{on}/I_{off}

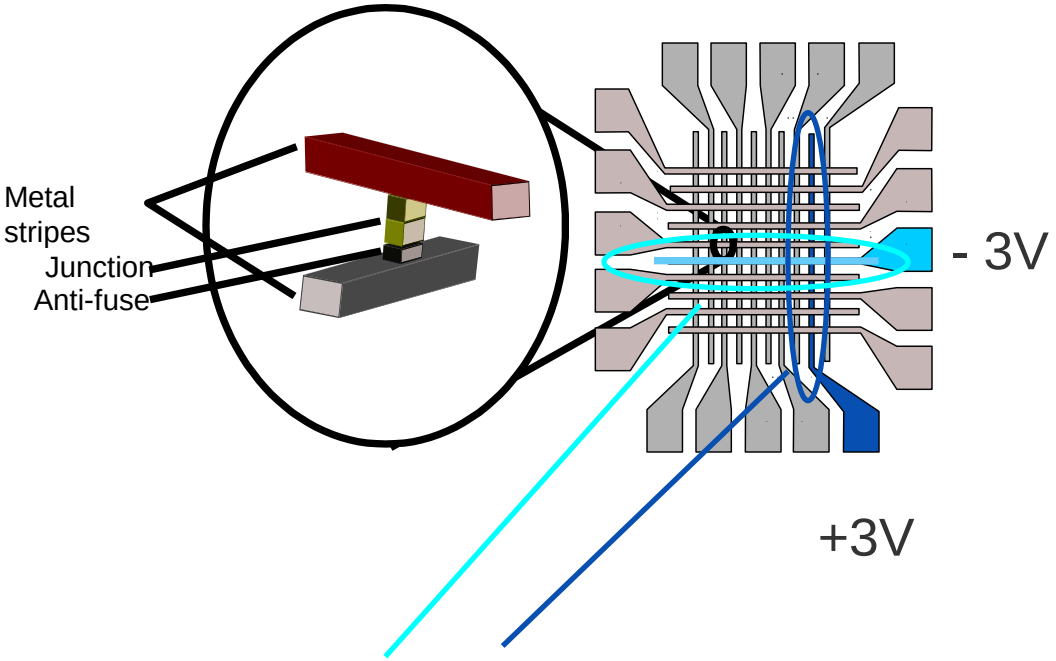
Scheme II

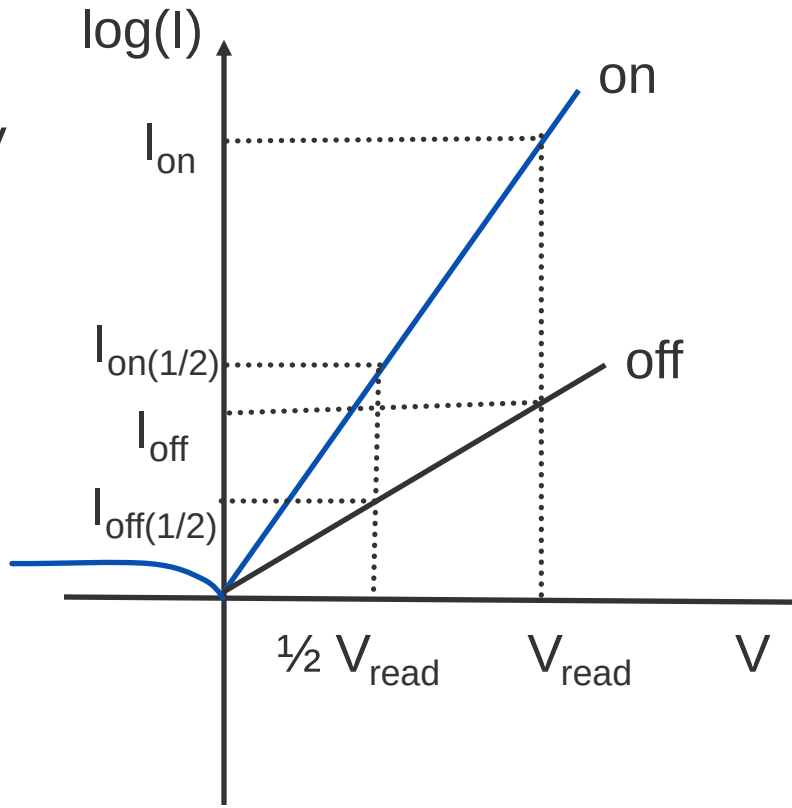
- Overall leakage is very low
- Parasitic currents limit scalability
- Figure of merit for diode: $I_{on}/I_{on/2}$

Scheme III

- Overall leakage is very low
- Parasitic currents have little effect
- Capacitive effects may play an important role

Requirements



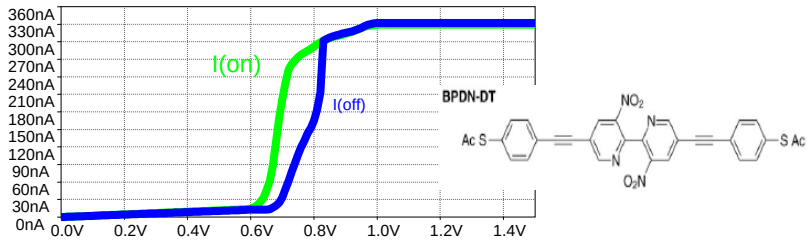


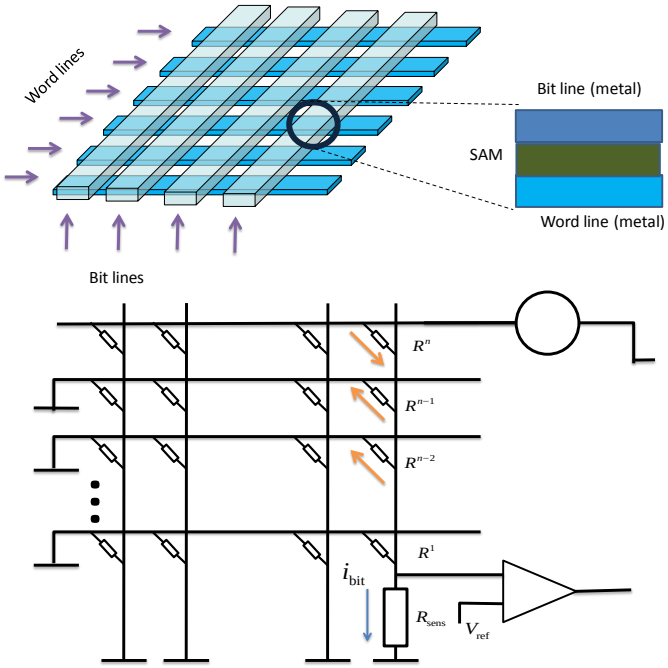
Each junction "sees" a voltage of $I_{1/2}$ => The parasitic current depends on $I_{on}/I_{on1/2}$

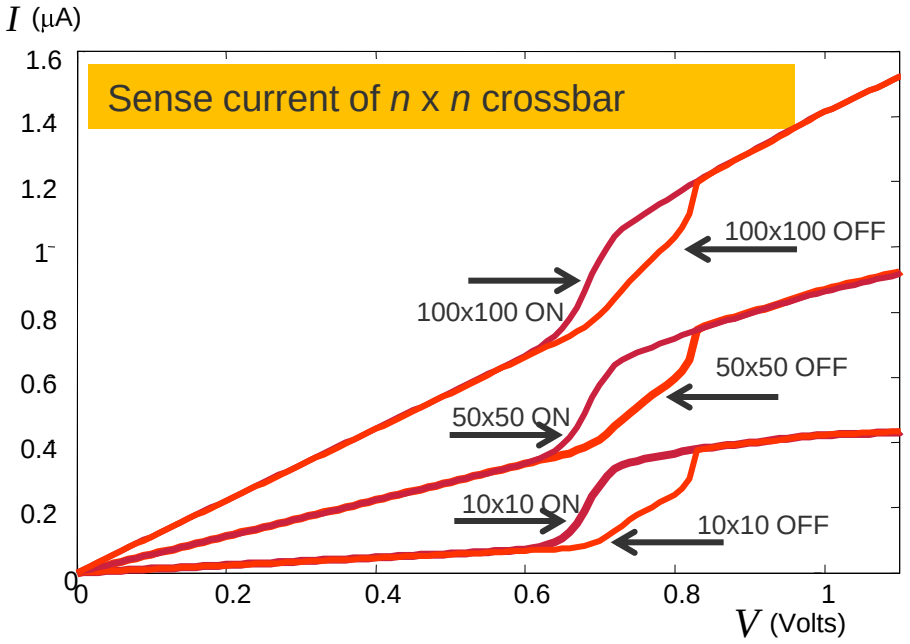
- **The $I_{on}/I_{on(1/2)}$ should be 10^4**
- **The junction should deliver high currents at low voltage, ideally below 6 V.**
- **Stability with time (10 years) and to electrical cycling (10^{6-8} for reading, 10^4 for writing)**

Cross-point arrays with nonlinear junctions

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)







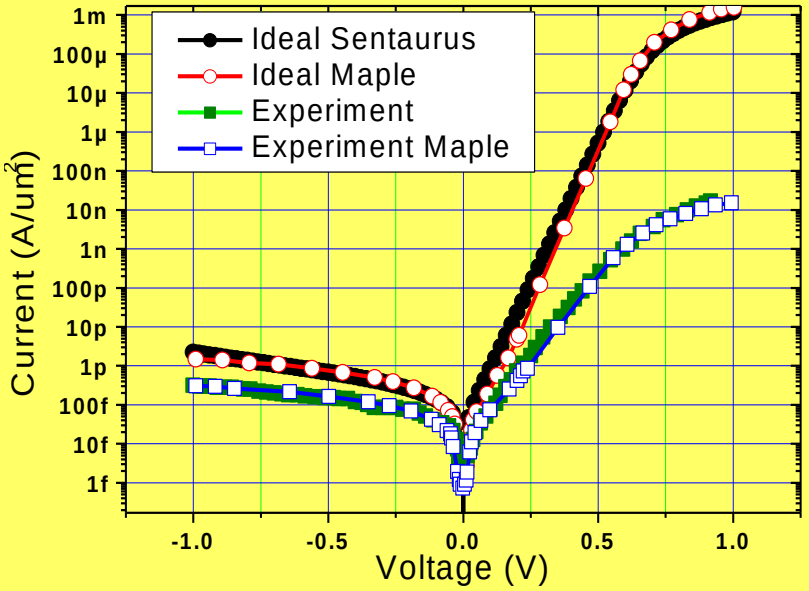
- Nonlinearity of the molecule IV characteristics enhances read-out margin
- Coupling molecular layer with solid-state diodes enables large-scale circuits

Cross-bar architecture with ZnO diodes

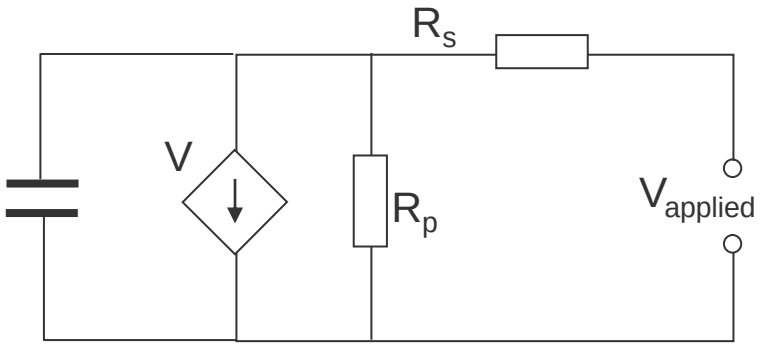
With all the information gathered it is possible to optimized the diode and know what are the characteristics that it must have.

- Low contact resistance (<10^{-5} Ωcm^2)*
- Carrier concentration < 10^{17}cm^{-3}).
- High Schottky barrier (ZnO/Ag → 0.9 eV).

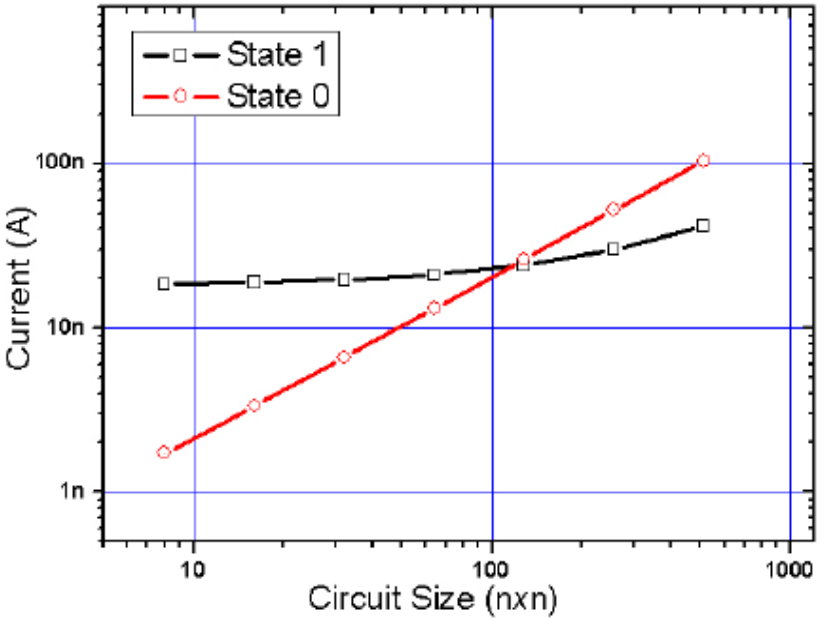
*Carrier concentration dependence of Ti/Al/Pt/Au contact resistance on n-type ZnO K. Ip, Y. Heo, K. Baik, D. P. Norton, S. J. Pearton, and F. Ren, Appl. Phys. Lett. **84**, 2004.

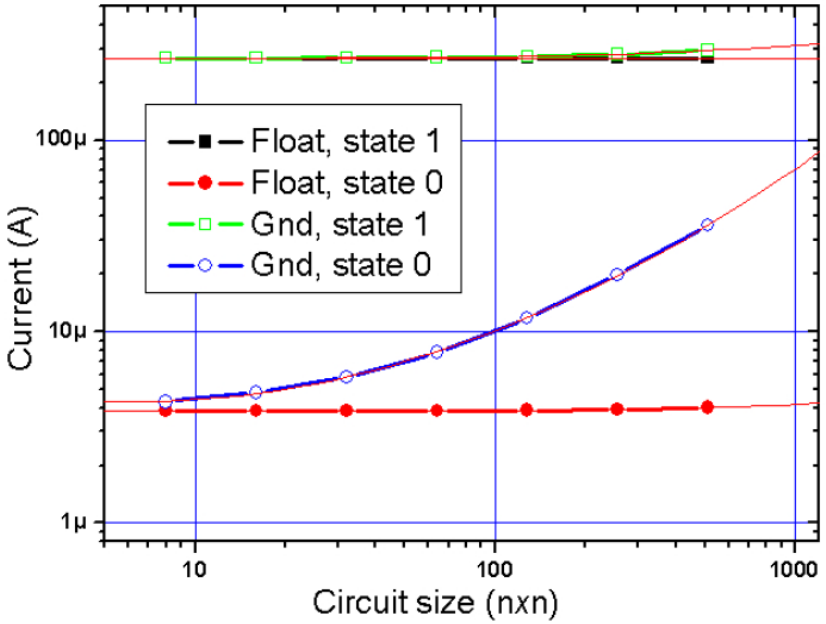


We implemented a Matlab-script, which is able to generate circuits up to a million nodes (junctions). Behavior of large crossbar arrays can be analyzed this way.



Crossbar Performance with ZnO Diodes



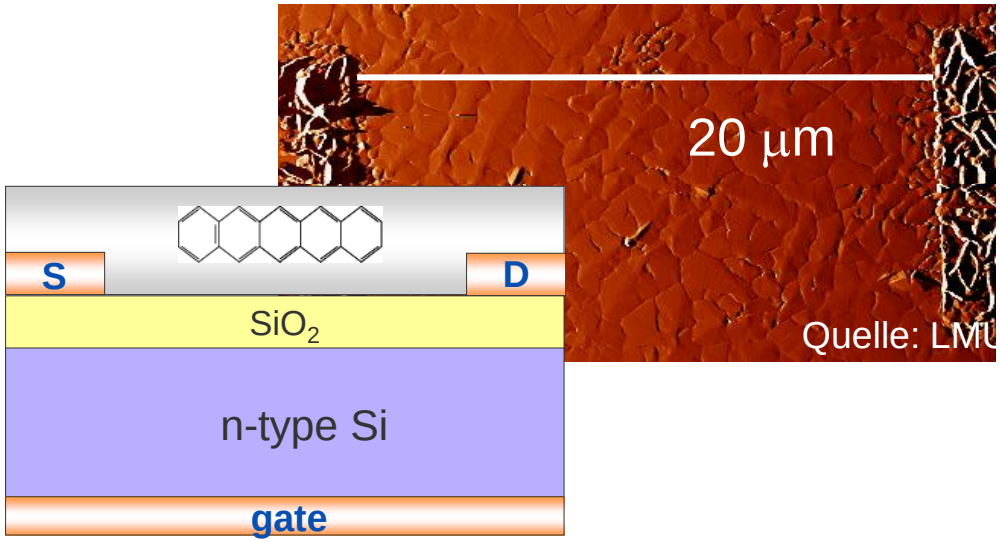


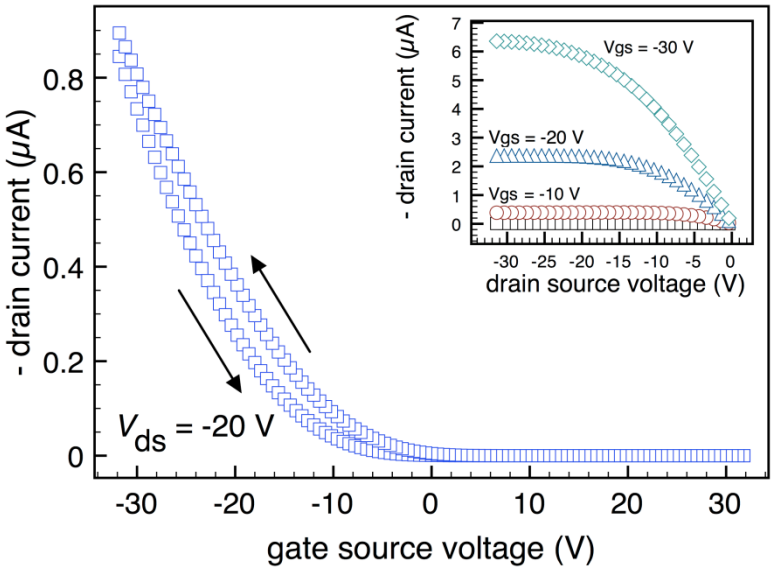
For circuits larger than ca. 100 x 100 junctions, the difference between 0 and 1 written bit value disappears – in a worst-case scenario, parasitic currents overwhelm the current to be sensed.

For **optimized** diodes, a 1 Mbit array seems plausible with any bias scheme

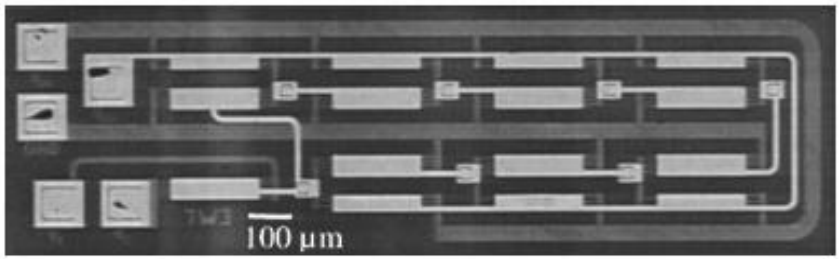
OFET transistor and inverter

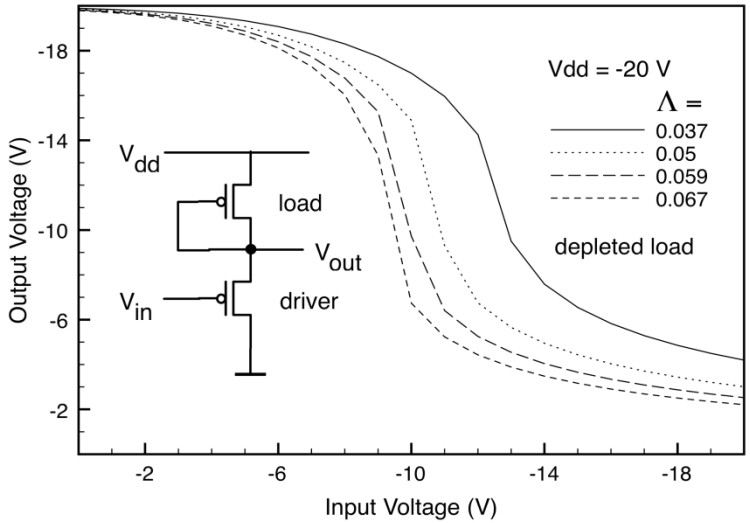
Organic Field Effect transistor are usually p-type, it is hard to obtain n-type devices





Inverters with depleted load can be built using only p-type OFETs



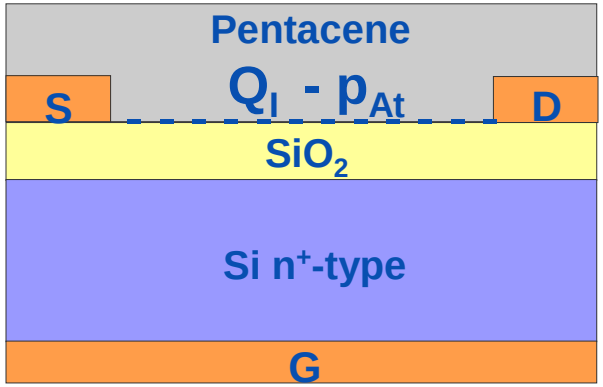


Fix et al., Fast polymer integrated circuits, APL 81(9), 1735 (2002).

The simulation employs a modified *drift-diffusion model* implemented in the industry tool CENTAURUS (former ISETCAD).

Input parameters are

- **device geometry,**
- **electronic levels in Pentacene, and**
- **properties of the material interfaces.**



SiO_2/Pentacene interface

Q_I fixed interface charges

$p_{At} = N_{At} f_n$ acceptor-type traps, i.e. negative if filled, neutral if empty

The Drift-Diffusion Approach

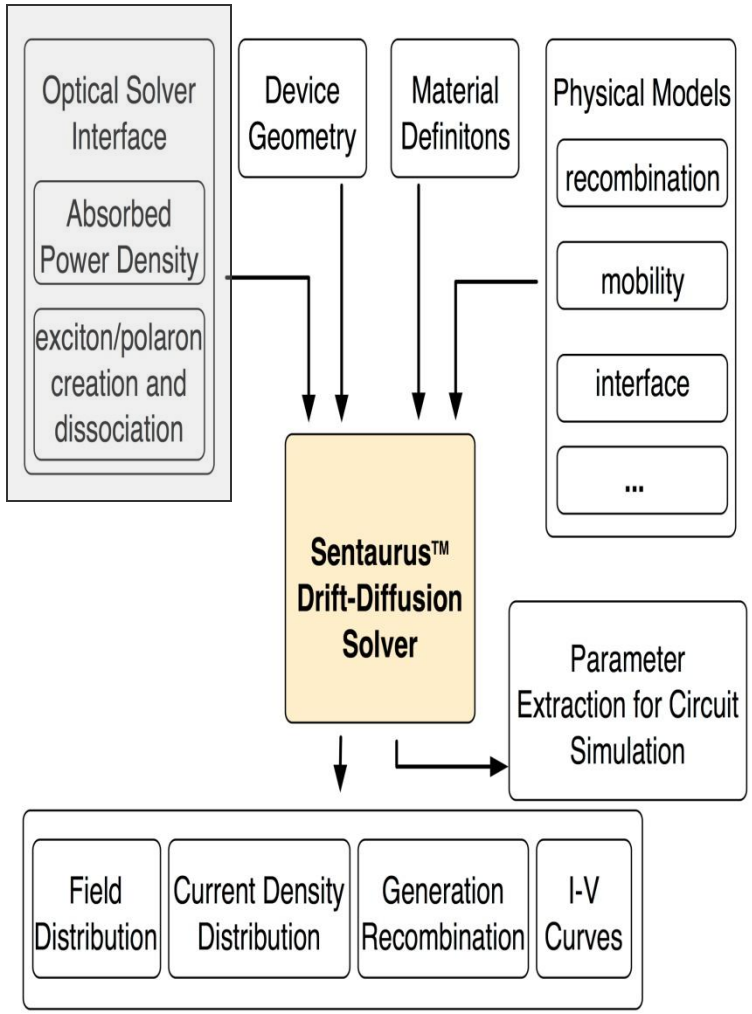
$$J_n = -q\mu_n \nabla V + qD_n \nabla n$$

$$J_p = -q\mu_p \nabla V - qD_p \nabla p$$

$$\Delta \varepsilon_0 \varepsilon_r V = -q(p - n - p_{At} + Q_I)$$

$$\nabla \cdot J_n = q(R - G)$$

$$\nabla \cdot J_p = -q(R - G)$$



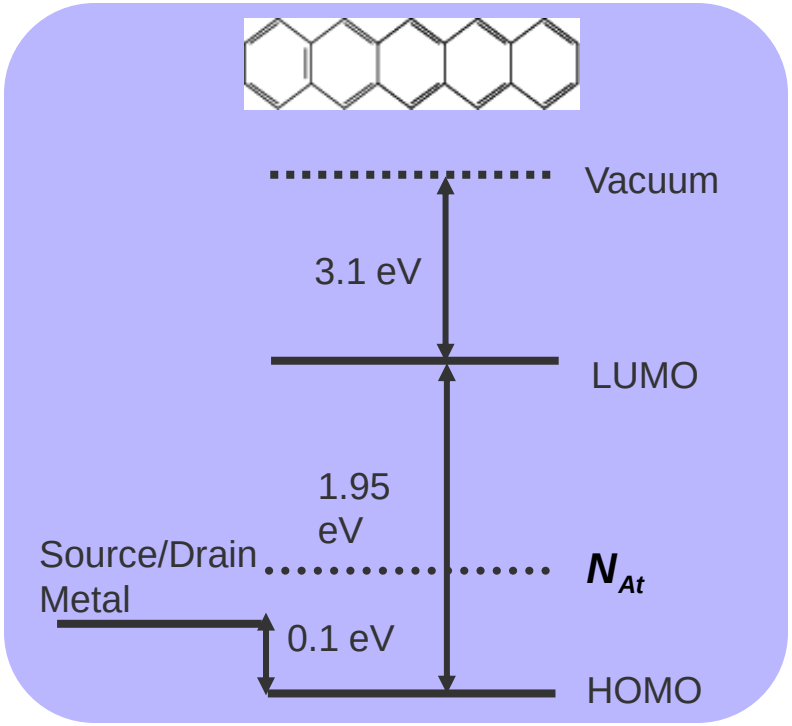
The self-consistent simulator scheme numerically solves the coupled equations on a spatial grid which models the device geometry

A. Bolognesi, et al. J. Comp. Elec. 2, 297 (2003)

C. Erlen, et al. J. Comp. Elec. 5, 345 (2006)

P. Lugli, et al. Appl. Phys. A, Vol. 87, No. 3., 2007

Material and Mobility Model (e.g. Pentacene)



Field-dependent mobility has been implemented according to

$$\mu = \mu_0 \cdot e^{\sqrt{\frac{E}{E_{critical}}}}$$

The low-field mobility μ_0 is a transistor property and has to be extracted via simulations.

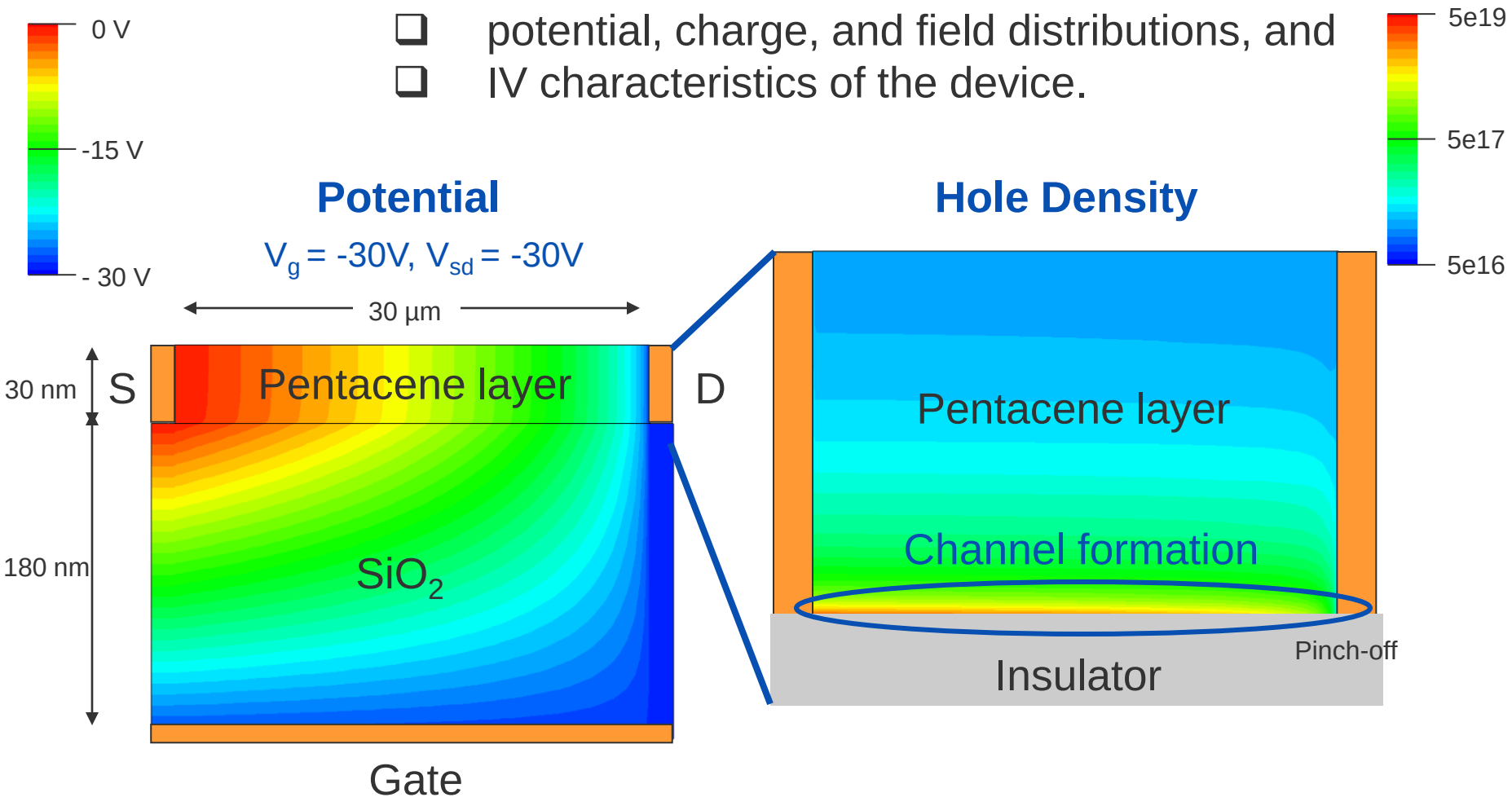
Effective DOS = 1e21 cm^{-3}
Contact Barrier = 0.1 eV

Lee et al. APL 84(10):1701, 2004

Bolognesi et al. IEEE Trans. El. Dev., 51(12):1997, 2004

Simulation Output

- The simulator returns
  - potential, charge, and field distributions, and
  - IV characteristics of the device.



- Multiscale approaches for nanostructures
  - Simulation of nanostructures
  - Cross Bar Architectures
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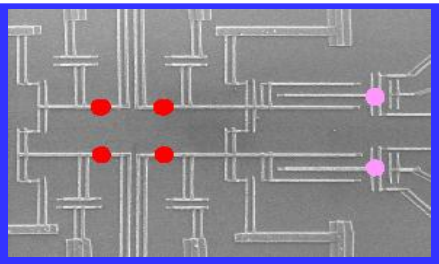
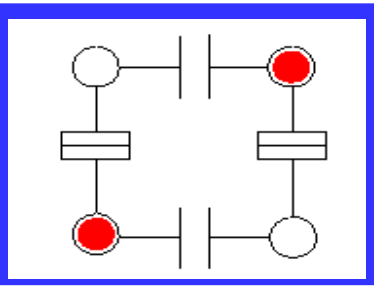
Field coupled architectures

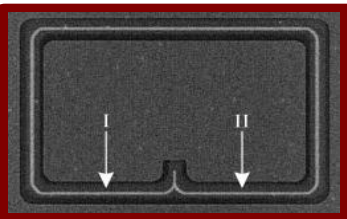


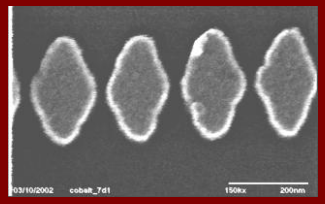
Snider et. al. Science

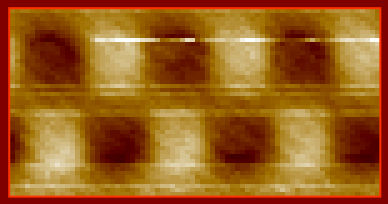


Single electron transistors

Experimental demonstration for reduced complexity → it works only at sub-kryogenic temperatures



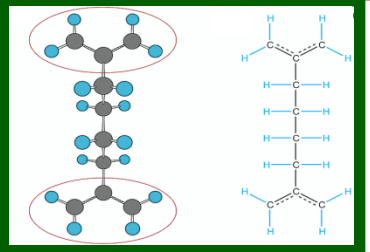


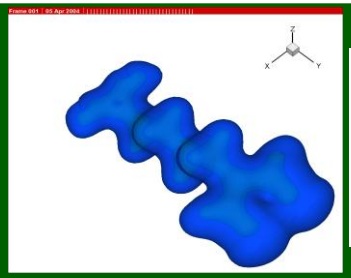


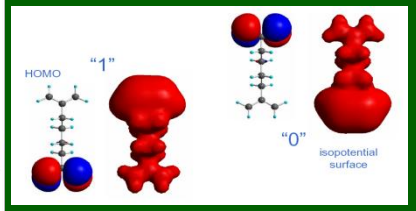
Cowburn et. al, Science

Coupled nanoscale magnets

Very promising, experimentally demonstrated at room temperature → slow





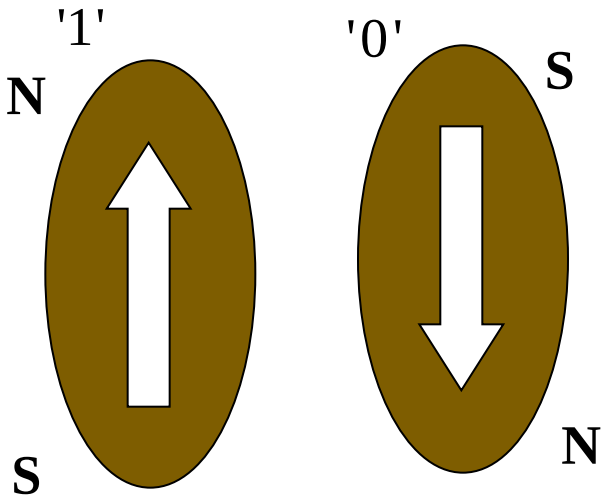


Lent et. al. JACS

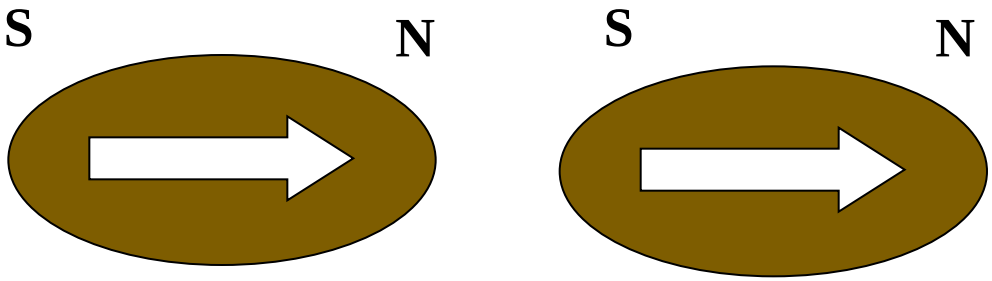
Coulomb-coupled molecules

Not yet demonstrated

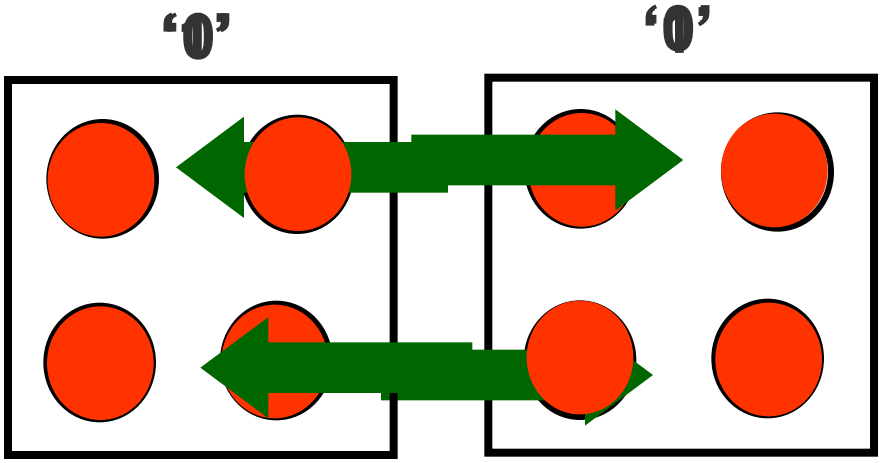
Idea of field-coupling



‘Antiferromagnetic‘coupling

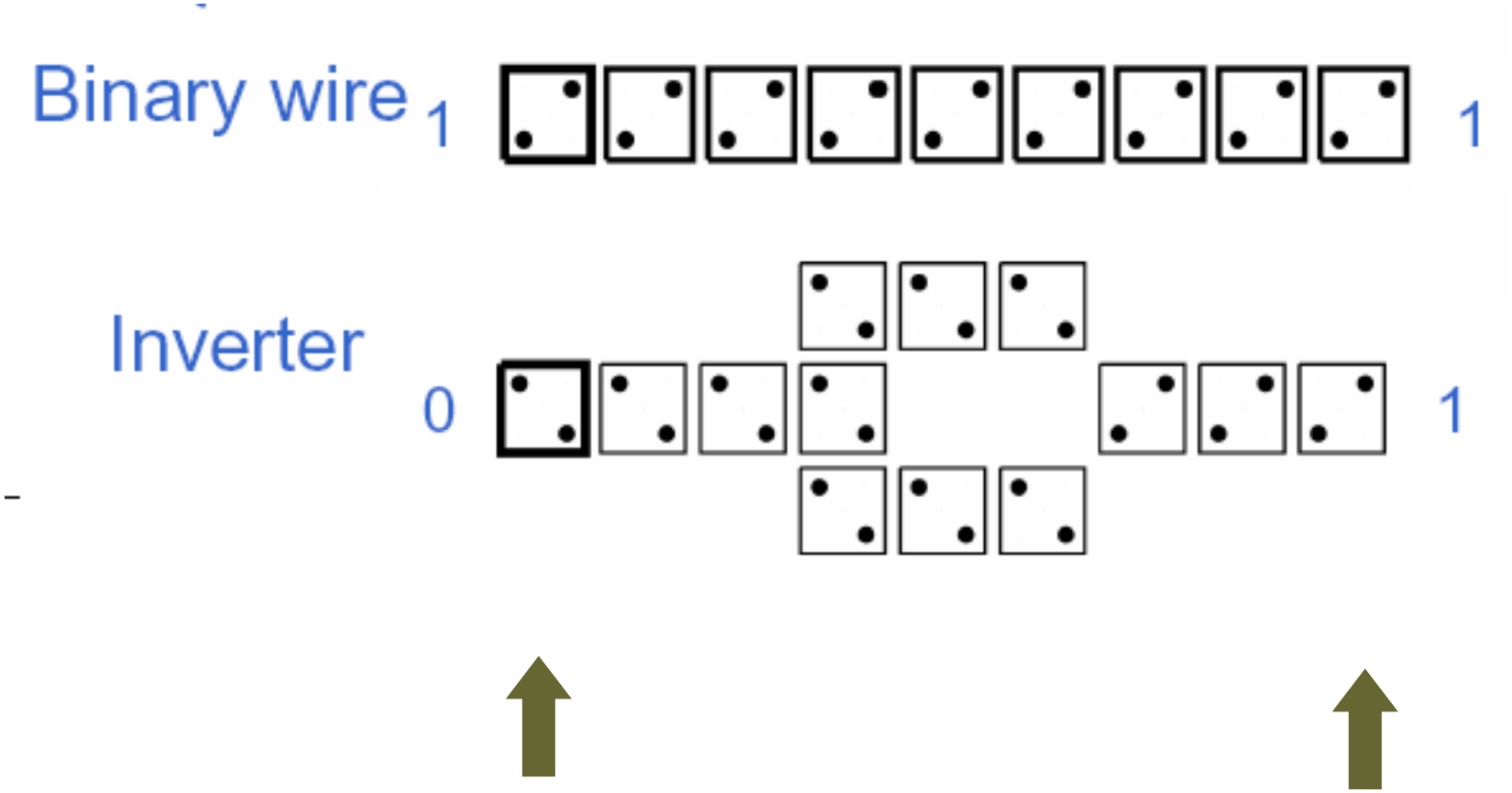


‘Ferromagnetic‘coupling

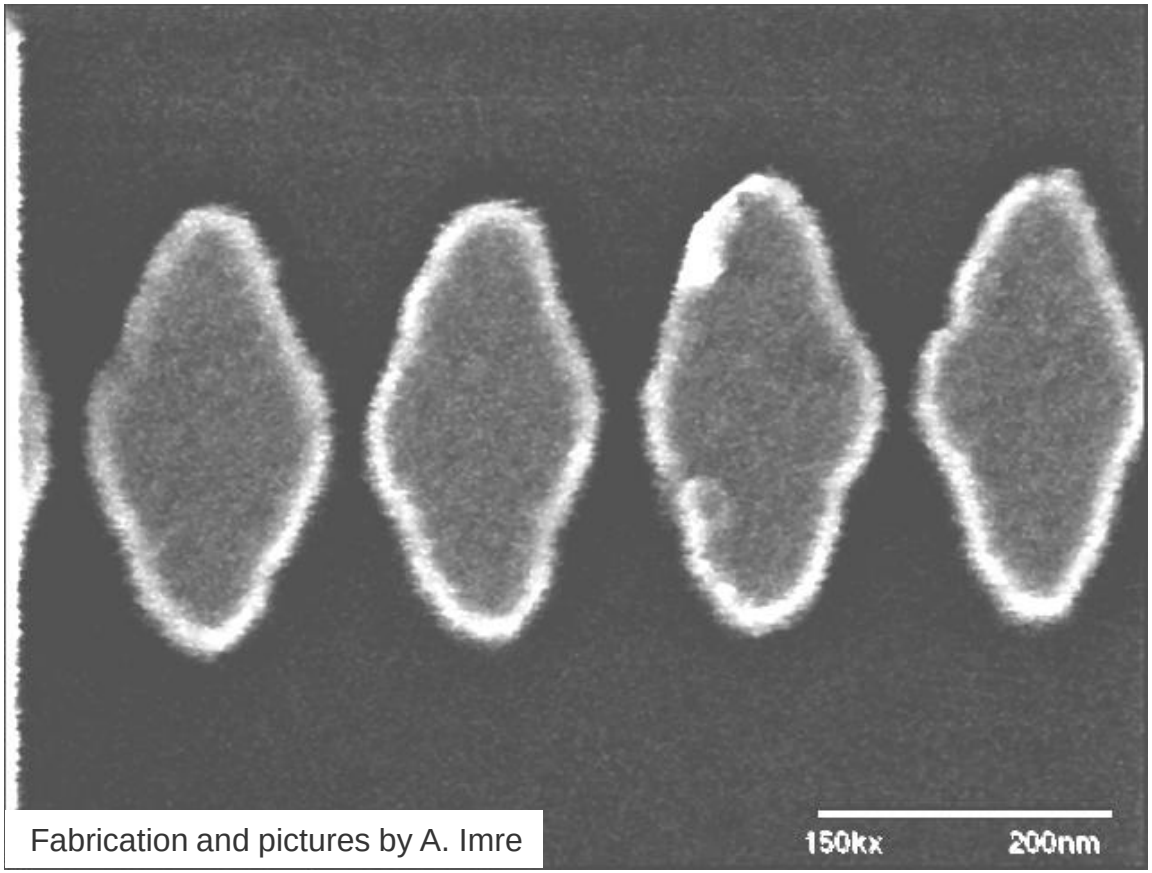


← Original proposal (1990s) Coulomb-repulsion of electrons in a quantum dot system

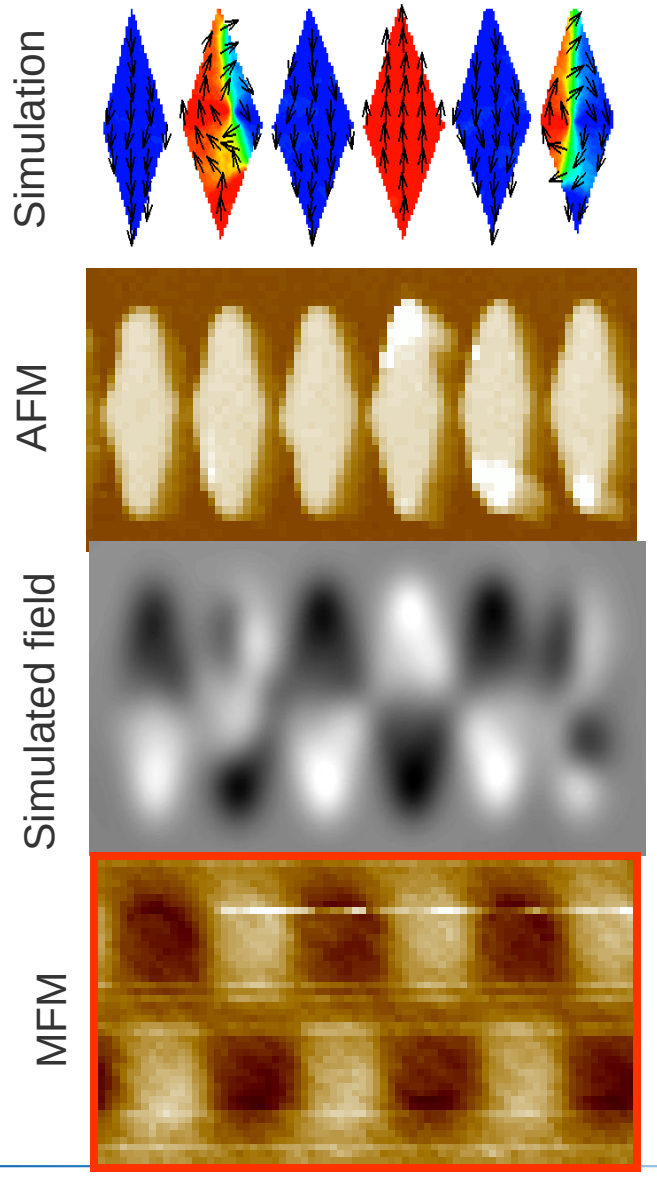
Wire and Inverter



Coupled nanomagnets



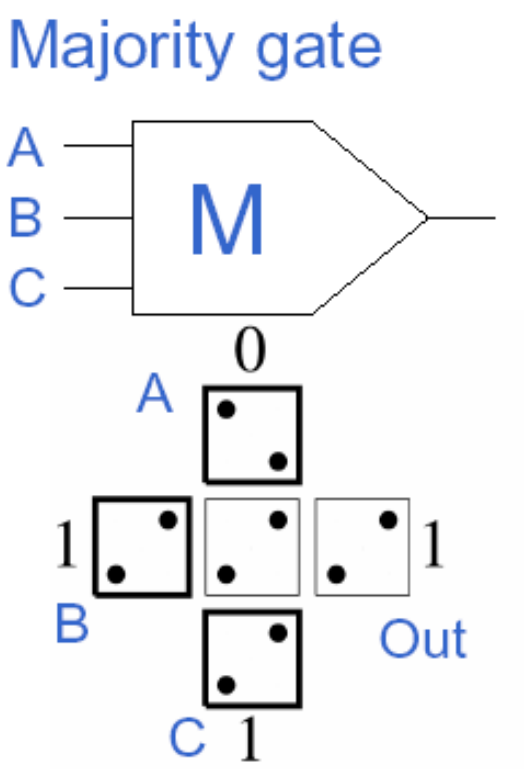
Fabrication and pictures by A. Imre



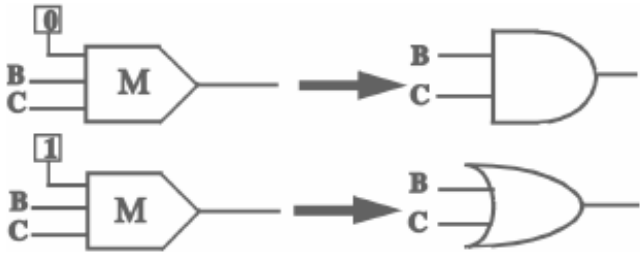
Investigations of permalloy nanomagnets (thermally evaporated and patterned by electron beam lithography) confirm the simulation results

Courtesy of W. Porod, Notre Dame University

Majority Gate: the Universal Logic Gate



	A	B	C	Output
AND gate	0	0	0	0
	0	0	1	0
	0	1	1	1
	0	1	0	0
OR gate	1	1	0	1
	1	1	1	1
	1	0	1	1
	1	0	0	0



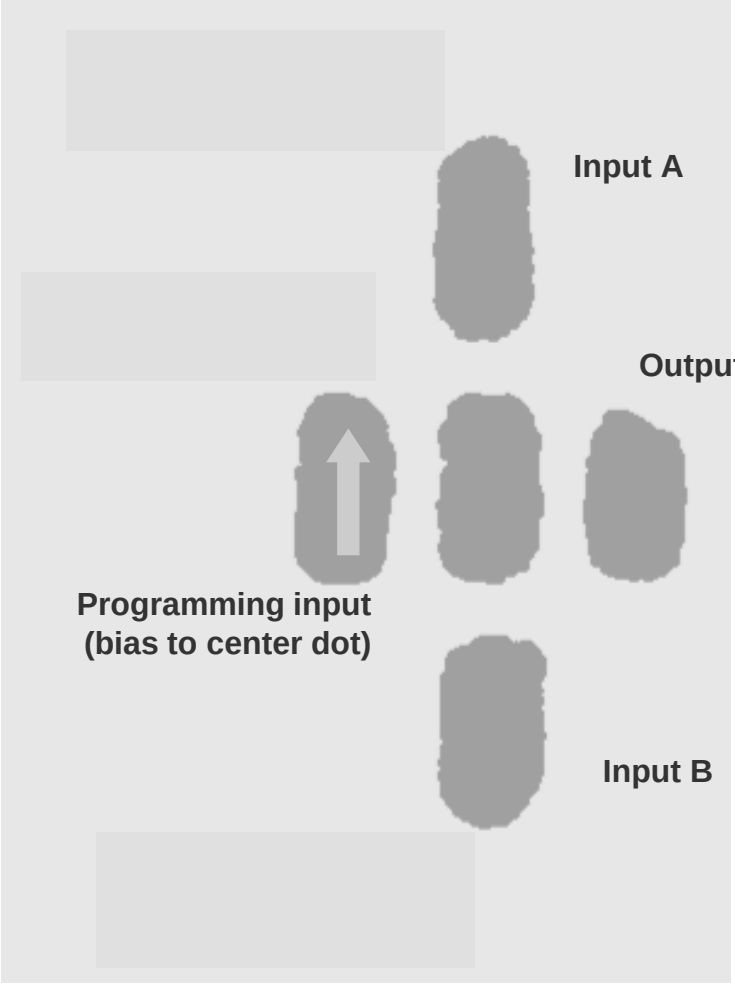
Programmable 2-input AND or OR gate.

With the majority gate, all Boolean logic functions could be realized

Benefits of QCA architecture:

- No static dissipation
- No Interconnection problem
- Potentially simple fabrication and scalability to molecular level

Logic gates by magnetic interaction

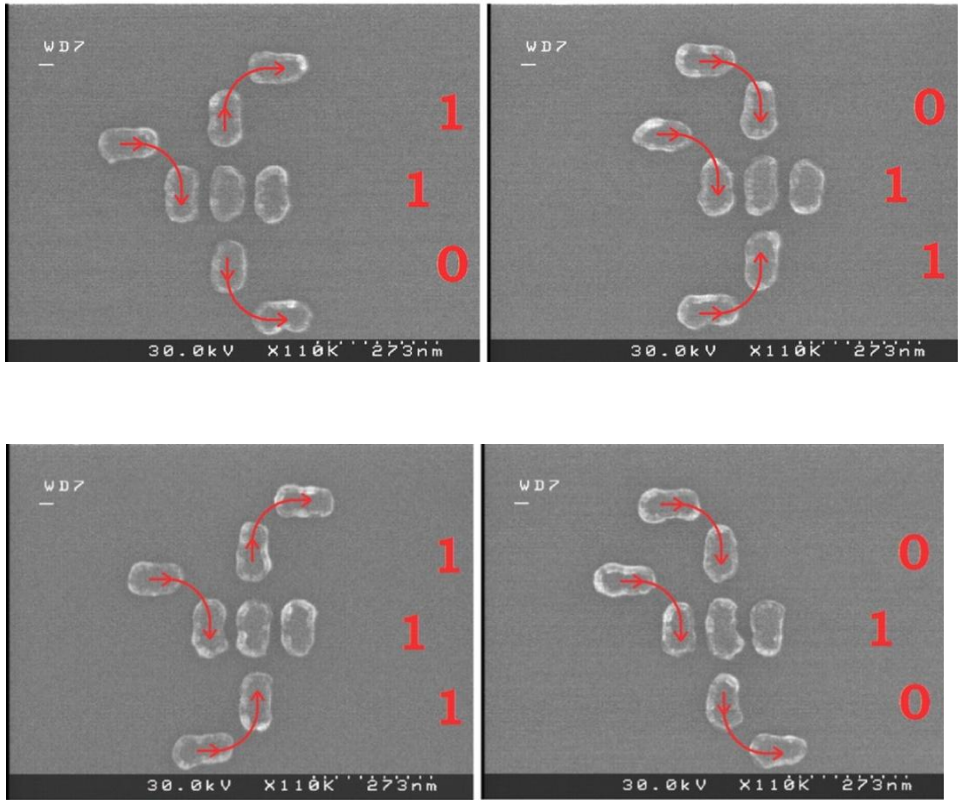


Output points down only if both inputs are pointing up → NAND gate.

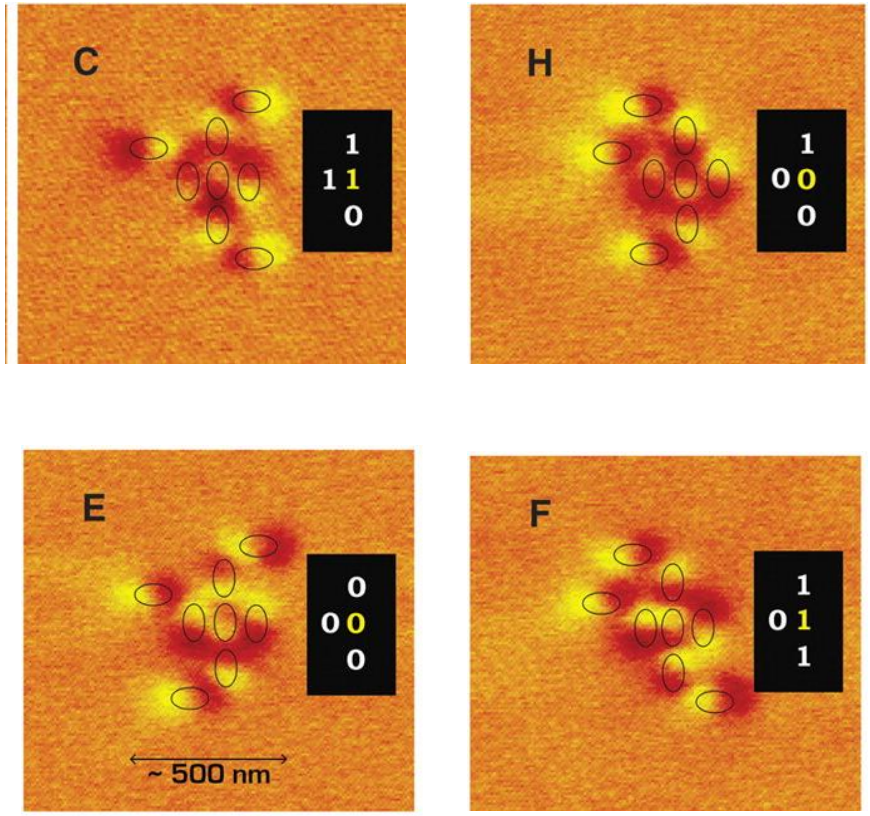
- Difficult to design – ferro- and antiferromagnetic couplings to the central dot should be equally strong
- Electrical inputs are difficult to fabricate – horizontally lying dots provide a hard-wired input. No output, we just imaged it with the MFM
- Design is based on Parish and Forshaw: Magnetic Cellular Automate Systems IEE Proc.-Circuits Devices Syst., Vol. 151, No. 5, October 2004

Imre et. al. *Science* 2006

Working majority gate with nanomagnets



SEM images



MFM images

Imre et. al. *Science* 2006

Two vector fields: $\mathbf{M}(\mathbf{r},t)$ $\mathbf{H}_{\text{eff}}(\mathbf{r},t)$

$$\frac{\partial \mathbf{M}(\mathbf{r},t)}{\partial t} = -\gamma \mathbf{M}(\mathbf{r},t) \times \mathbf{H}_{\text{eff}}(\mathbf{r},t) - \frac{\alpha\gamma}{M_s}\left[\mathbf{M}(\mathbf{r},t) \times \mathbf{M}(\mathbf{r},t) \times \mathbf{H}_{\text{eff}}(\mathbf{r},t)\right]$$

Landau – Lifshitz equation: how the magnetization distribution changes under the influence of an effective field $\mathbf{H}_{\text{eff}}(\mathbf{r},t)$

The effective field:

$$\mathbf{H}_{\text{eff}}(\mathbf{r},t) = \mathbf{H}(\mathbf{r},t) + \mathbf{H}_{\text{exch}}(\mathbf{r},t)$$

Maxwell equations
"Real" magnetic field

$$\mathbf{H}(\mathbf{r},t) = \frac{\mathbf{B}(\mathbf{r},t)}{\mu_0} - \mathbf{M}(\mathbf{r},t)$$

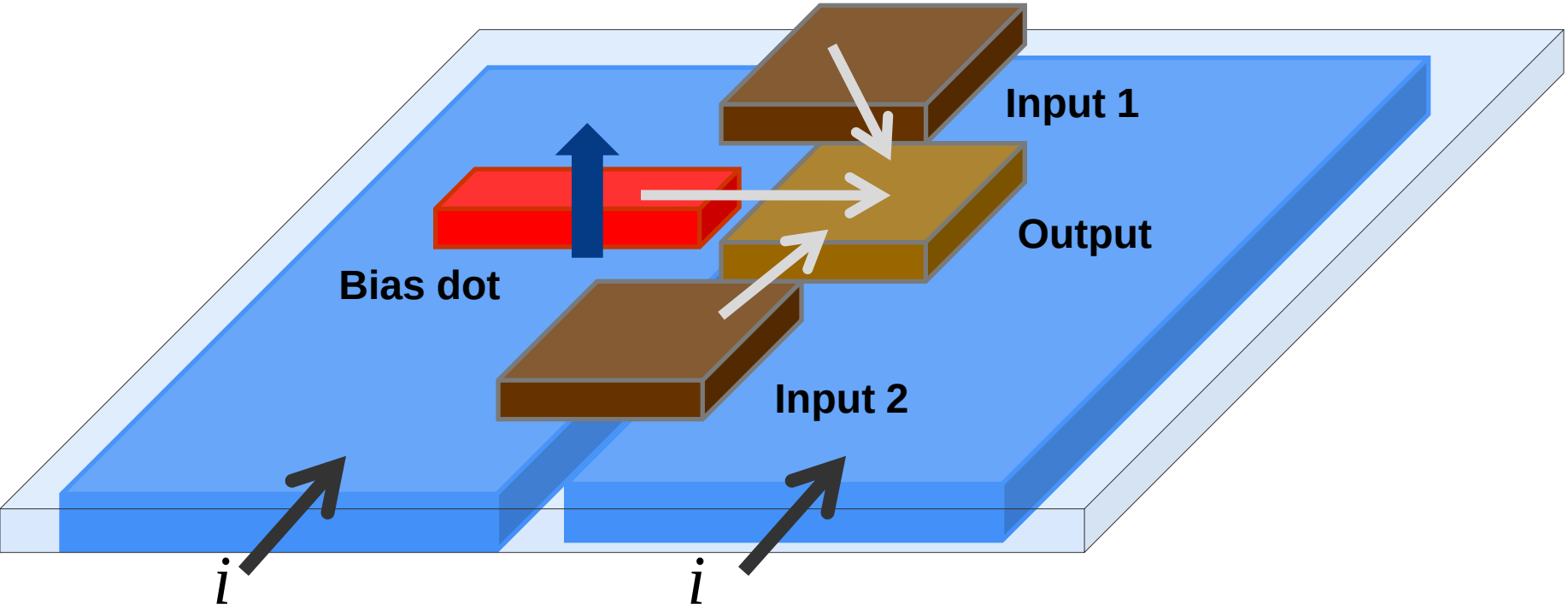
$$\operatorname{div}\mathbf{B}(\mathbf{r},t) = 0$$

$$\mathbf{H}_{\text{exch}}(\mathbf{r},\mathbf{t}) = \frac{2A_x \Delta \mathbf{M}(\mathbf{r},t)}{\mu_0 M_s^2}$$

Exchange field: a quasi – classical inclusion of quantum – mechanical interactions

→ Magnetic domain theory

NOR gate construction

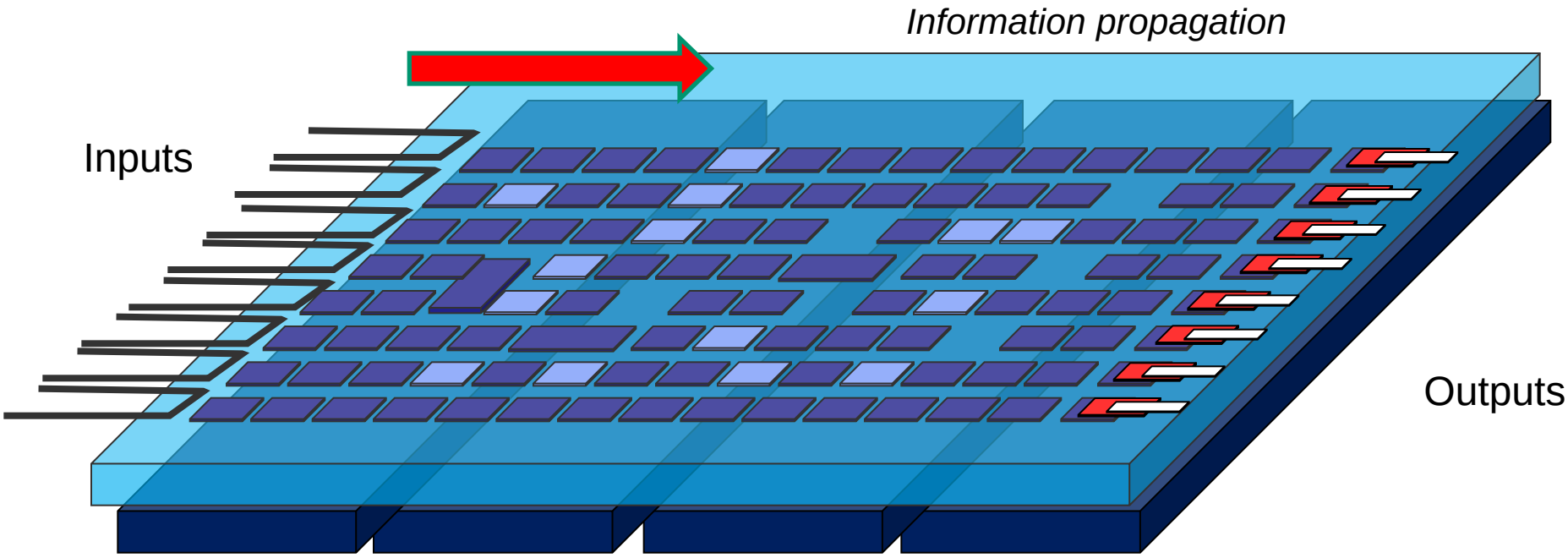


Output points up (1) only if both inputs are down (0).

Design rules:

- Biasing dot is smaller than inputs
- Output is of the gate is shifted to the left → switches later

A computing system concept



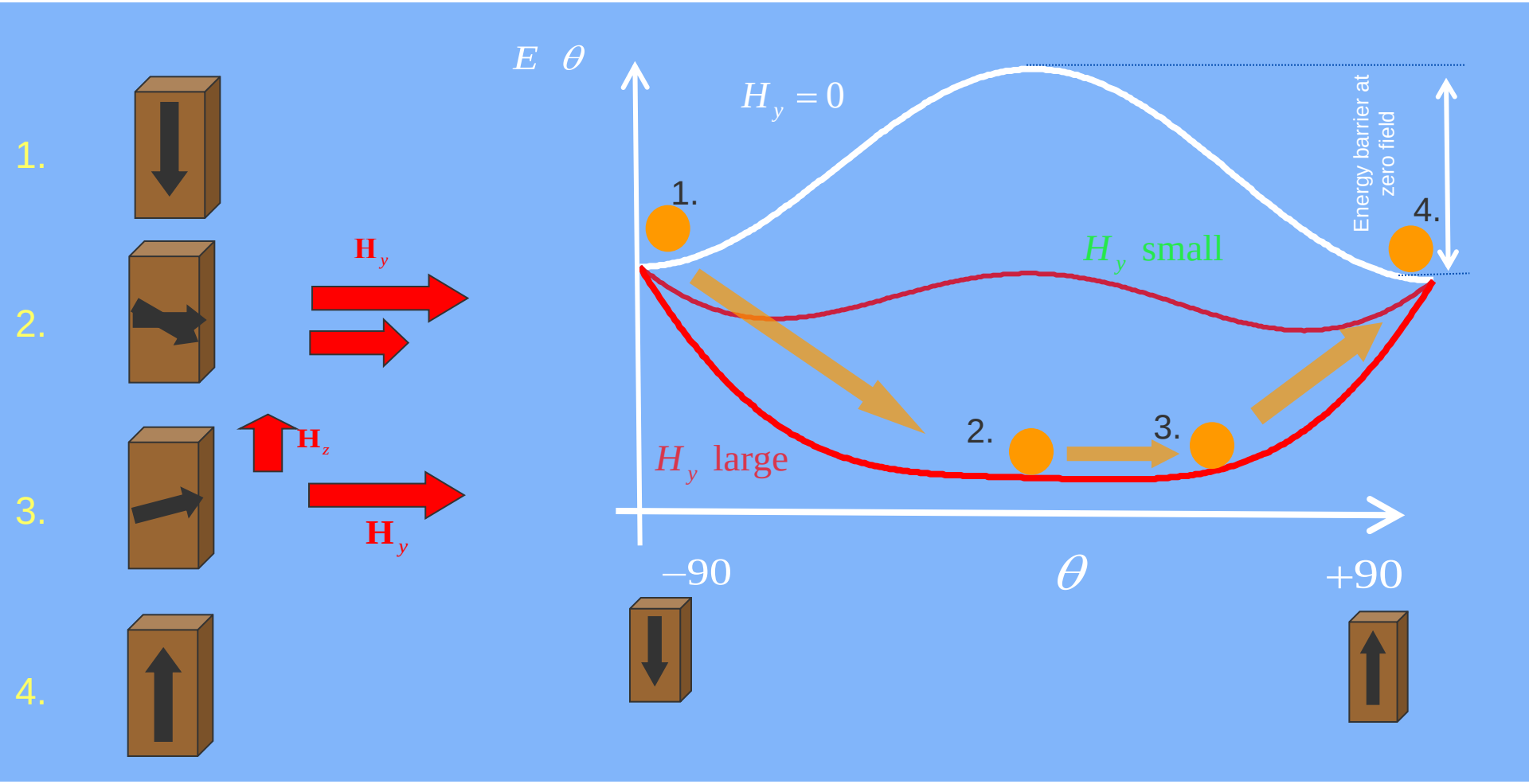
The challenges:

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

Adiabatic Switching

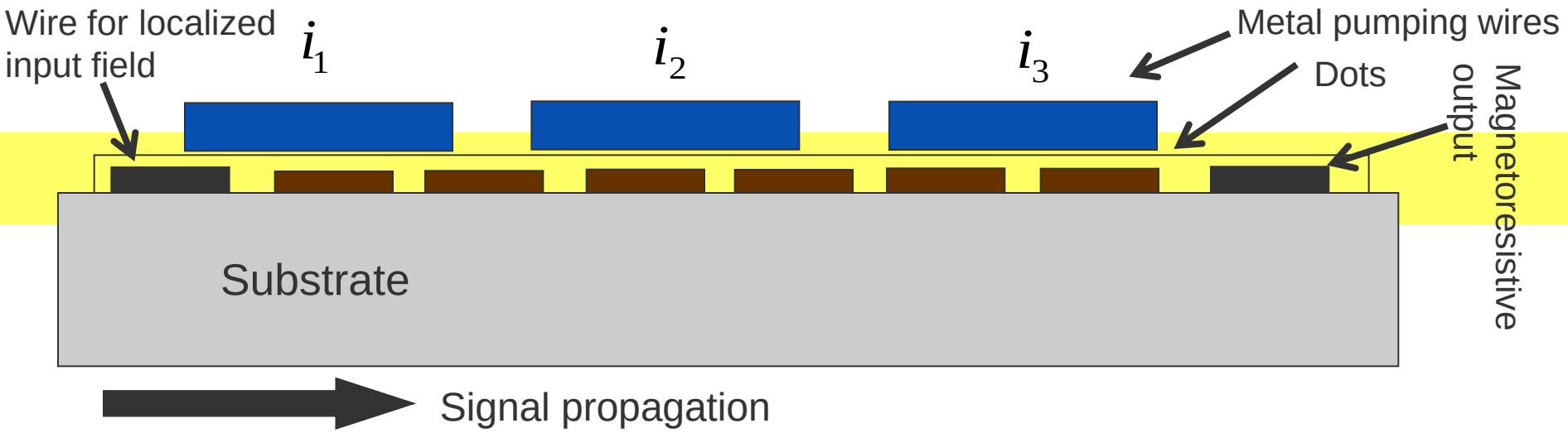
Rapidly moving domain walls are the main source of dissipation in magnetic materials

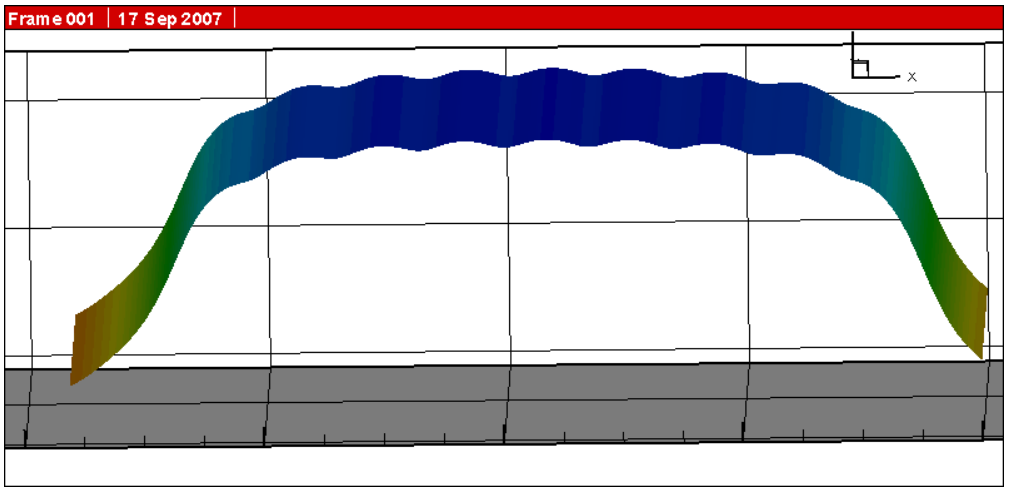
- Make the magnets sufficiently small (submicron size magnets has no internal domain walls)
- Switch them slowly (use adiabatic pumping)



Integrated Clocking System

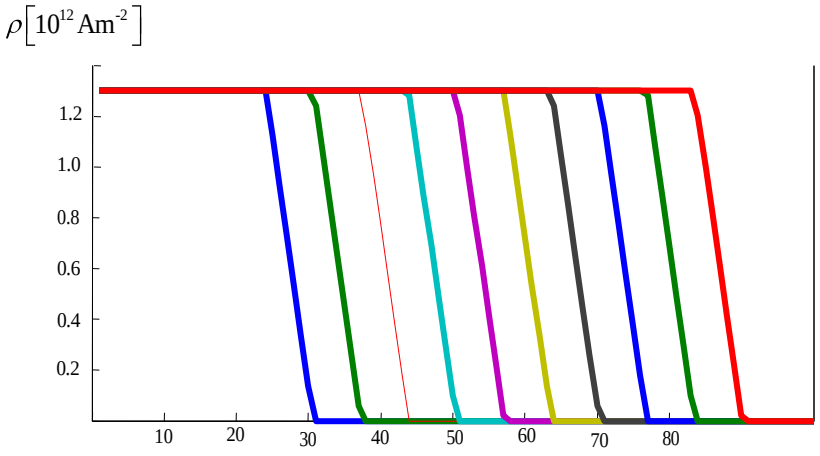
Architecture: Layer of pumping wires above the dots:

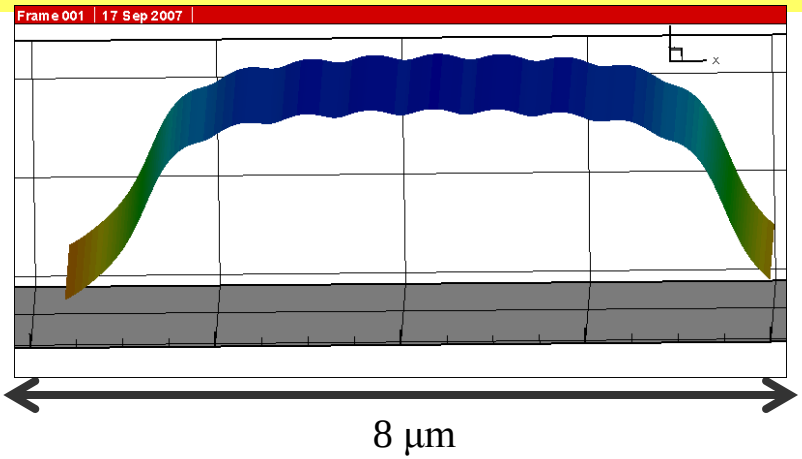




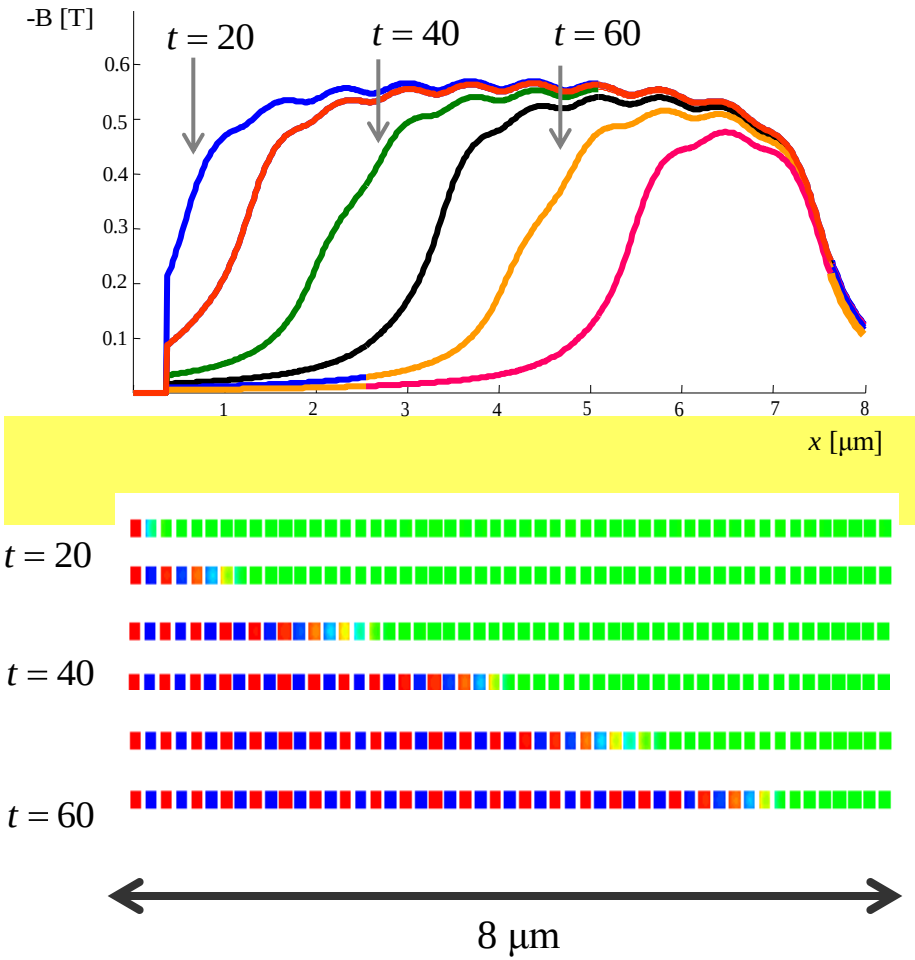
Wires placed above / below the dots can provide a wave-like propagating magnetic field, which switches the magnets one after the other.
This simulation shows the horizontal magnetic field distribution above the wires.

Propagation of the Ordering Wave





Switching off the current of the wires on after the other creates a magnetic field 'wave' in the plane of the magnets.



At the wavefront magnets are switching to their up / down state – even a long wire becomes perfectly ordered.

Conclusions

- A variety of nano devices can be reliably fabricated from various materials
- Novel circuits and architectures are going to be needed for a full exploitation of nanocomponents
- Several open questions still exist concerning the mode of operation of such devices
- Modeling and simulation can provide important answers
- A multiscale approach is needed in order to describe realistic systems