View from Computational Nanoelectronics

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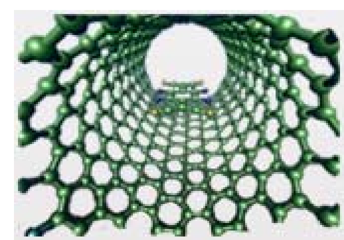


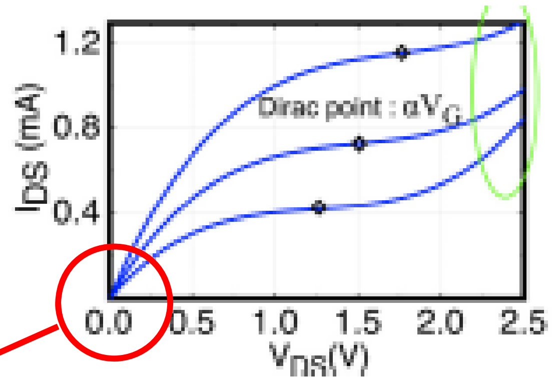
$$: NSF CAREER, NSF-NIRT, NRI, DARPA, SRC, NanoStar

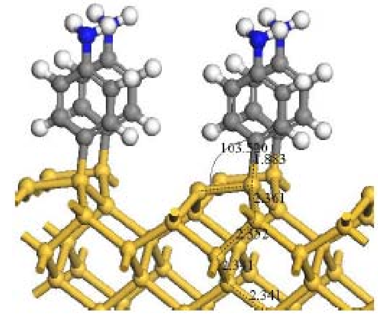
Past affiliation with NASA-INAC at Purdue

VIrginia **N**an**O**Computing **(VINO)**

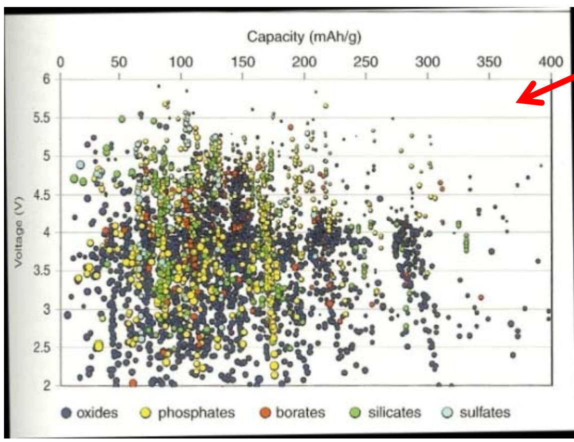
http://www.ece.virginia.edu/vino

NanoMaterials: Near-eqlm properties





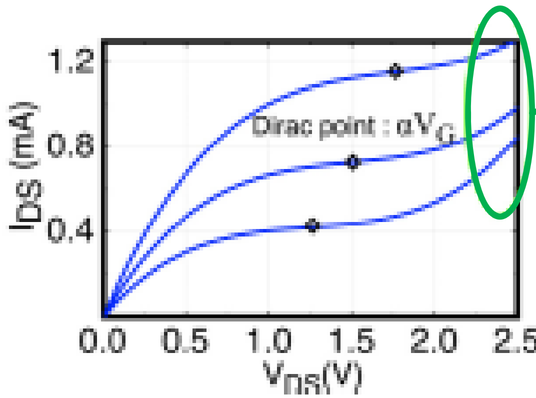
Geometries

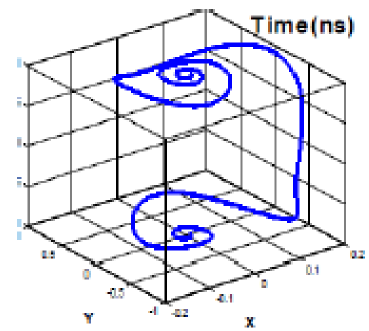


Battery activity
(Materials Genome Project)
Ceder, MRS Bulletin'10

- **Formalism understood**
  TB/DFT/GW + Kubo
- **Know how to multiscale (from atom to ckt)**
- **Bandstructure effort primarily European**
  (Spain, Germany, UK/Ireland, Austria)

NanoElectronics: NonEqlm properties



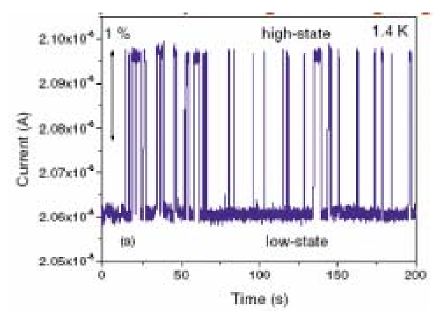


Spin torque driven switching
(STTRAM – ultimate memory?)

- **Weak el-el interactions understood**
- **Strong nonequilibrium interactions (QDs)?**
  Potentially insoluble!

(Transport in a QD with modest hybridization with leads)
PRB '06, '08, '09; J Phys '08; IEEE Nano '07; Elsevier'11

- **No efforts on multiscaling (G, G<)**

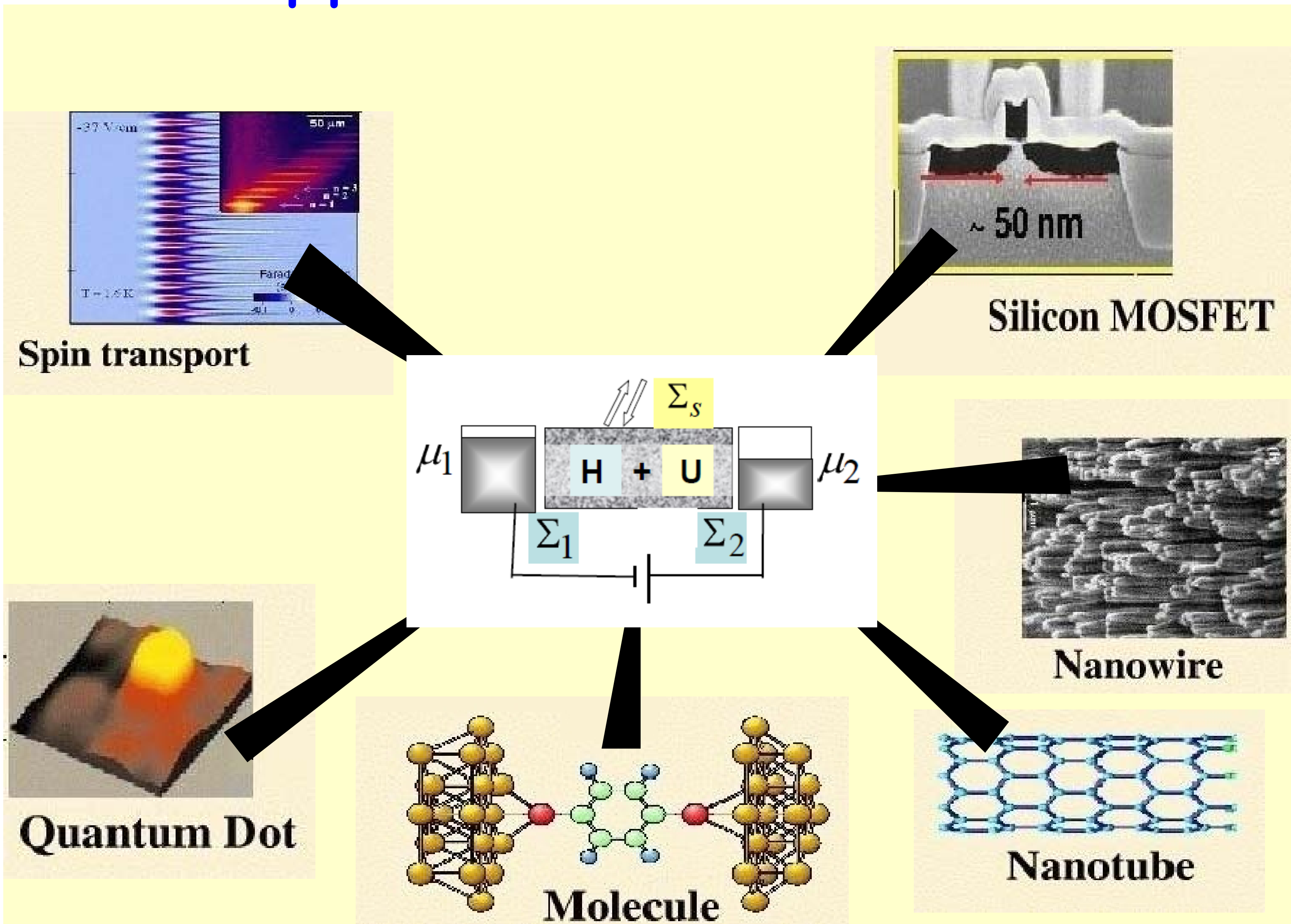


Current Noise around switching point
(UCLA data; Models Vasudevan/Ghosh '08,'09)

What works for equilibrium may not work for non-equilibrium…

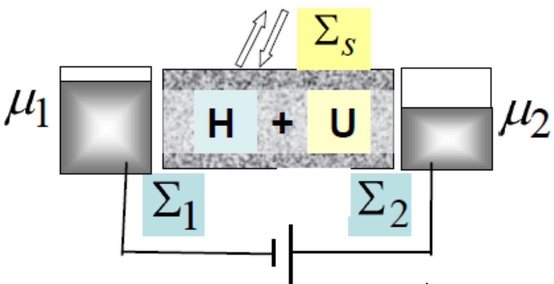
…and there are experimental evidences to prove that !

Unified approach to nanoscale devices

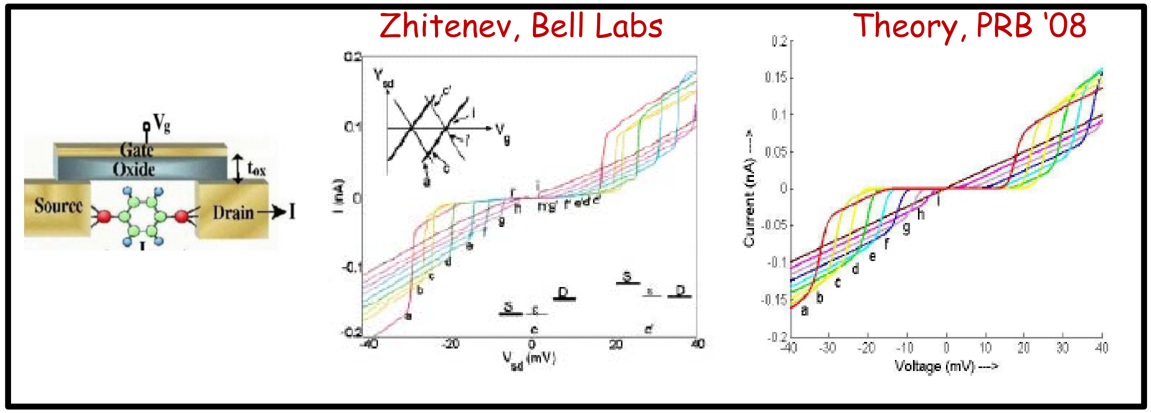


Interfaces, Interactions, Stochasticity, Correlations, …

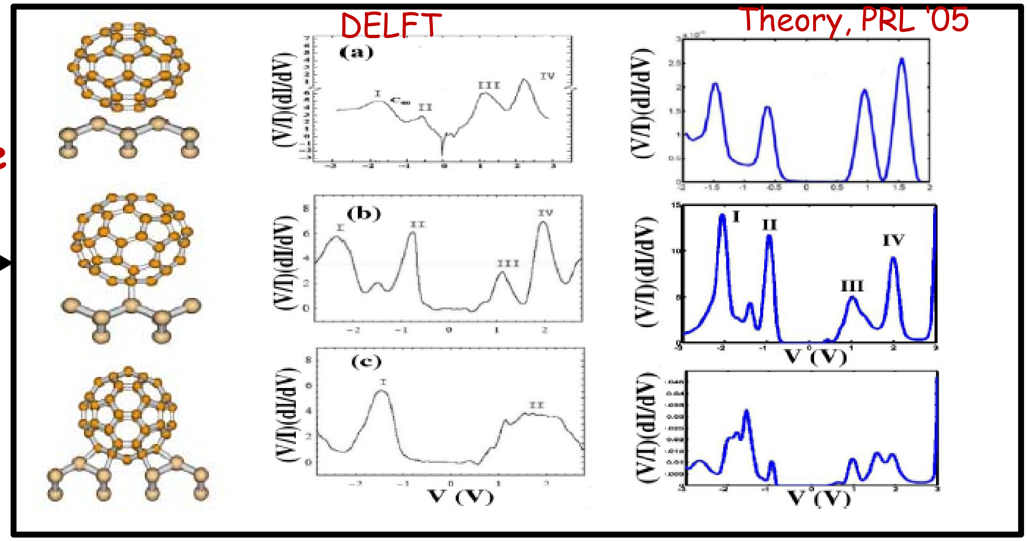
Modest Successes…



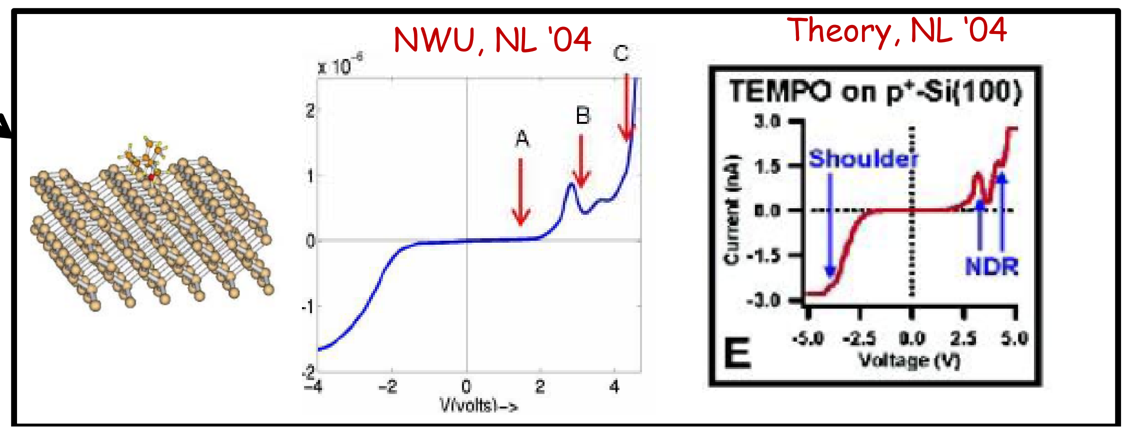
Qualitative



Quantitative ('Ab-initio')



Predictive?



15 classes of expts in moletronics modeled and summarized in "Electronics with Molecules", A. W. Ghosh, Elsevier 2011

… So what are some of the outstanding challenges in nano-electronics?

1. Can we reinvent the transistor?

Clear shift in focus – **E**lectrostatics to **E**nergetics

~10^5 kT in isolation, ~10^7 kT in ckts (Bandyopadhyay)

$$V = (\alpha NkT/q)\ln(1/p)$$

Ferroel Trans^n
~40 mV
Domains?

Nanomagnetics
~60mV for ALL spins
But overheads too expensive !

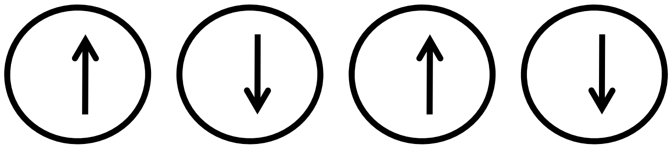
Tunneling FETs/
Graphene pn
~40mV/charge
But low currents

NEMFETs
~0.1 mV/device
But hysteresis

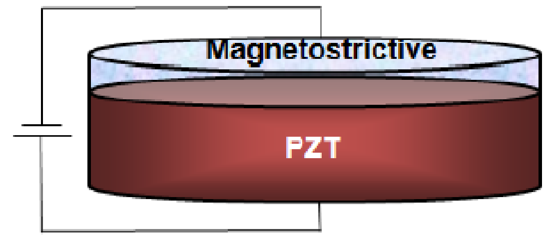
Ratchets
~40mV
But dynamic dissipation
Speed compatibility…

How to design a mV switch?

1.1. A few promising candidates…



Spintronics: Nanomagnetic logic



- Rotating 10^4 spins costs about the same as 1 spin ! (Datta et al)

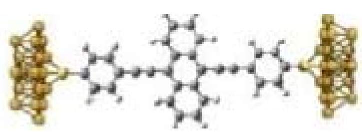
- BUT: How do we rotate spins in an energy-efficient way?

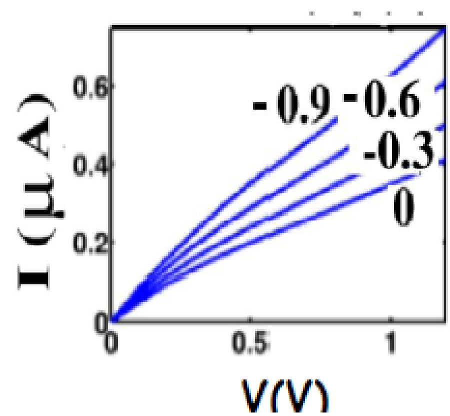
Magnetic fields (MRAM) – "kiss of death"
Spin torque (STTRAM) – better, but energy, WER too high! (DARPA)
Straintronics in multiferroics – looks great … so far

Operate at 200 kT/bit at 1 GHz, CMOS at 10^5-10^7 kT
(Bandyopadhyay/Jayasimha, VCU)

Experiments non-existent, much more research needed…

2. New materials: What are the killer apps?



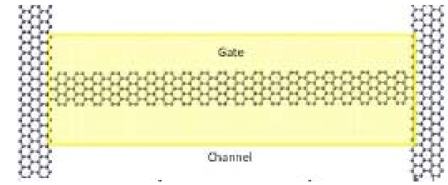


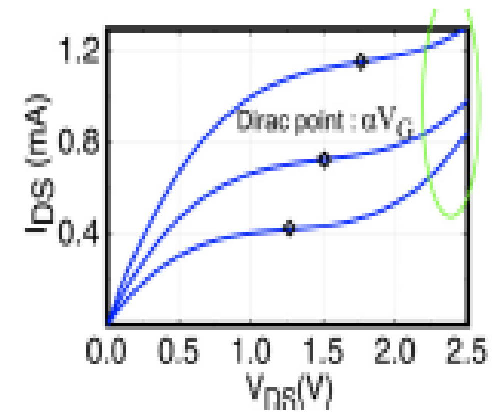
Review:
Ghosh, Elsevier'11
Ed. P. Bhattacharya

Fundamental reasons behind:

- Poor saturation, gateability
- Poor mobility/RC constants

(Ghosh/Rakshit, NL 2004)





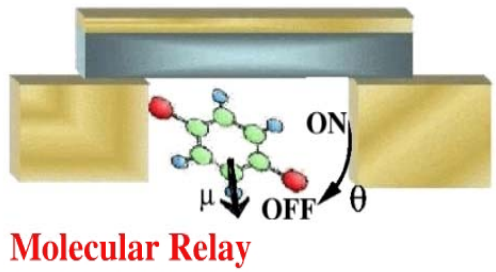
Reviews:
Ghosh et al, Springer1 Ed. H. Raza
Springer2 Ed. R. Murali

Fundamental reasons behind:

- Poor ON-OFF, saturation
- Increasing ON-OFF kills mobility due to bandstructure alone!

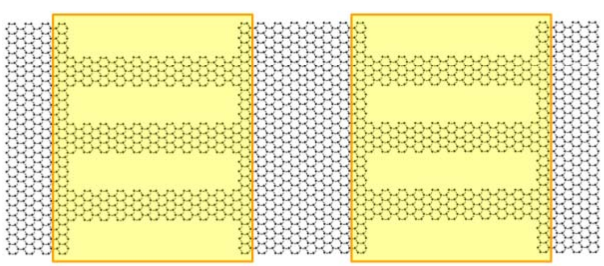
(Tseng/Ghosh, cond-mat '10)

2.1 Using materials for what they do best…



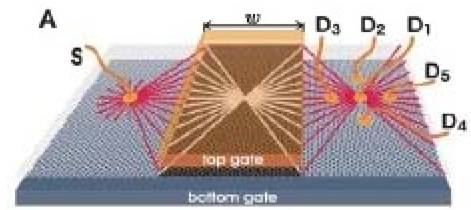
Molecular "NEMFETs"
(Use **mechanical flexibility**)

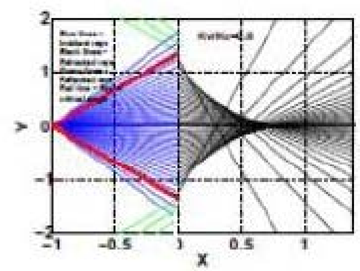
Ghosh/Rakshit, NL '04

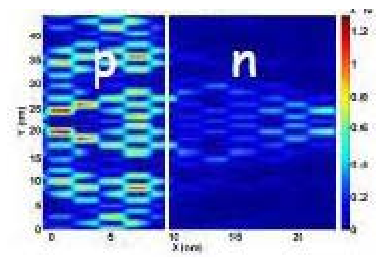


Wide-Narrow-Wide all graphene devices:
Better **electrostats**, contacts,
2D patterning possibilities
Also, RF applications

Unluer/Tseng/Stan/Ghosh, IEEE Nano '10;
2 review articles in Elsevier upcoming







Total Internal Reflection (TIR)

Electron 'optics' and waveguiding in graphene and bilayer graphene PNJs

Cheianov et al, Science '07

Creating transmission windows:

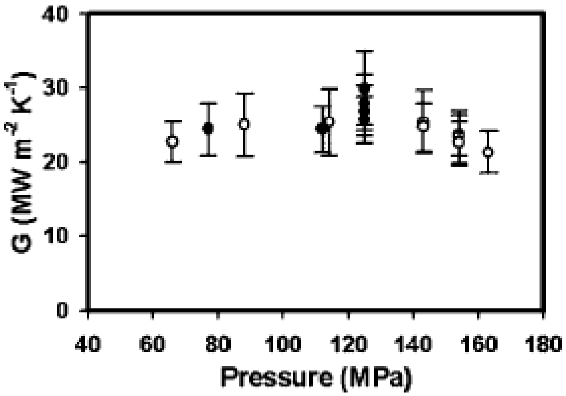
Sajjad/Ghosh, '11

We need to creative in exploiting the specific strengths of these emerging materials.

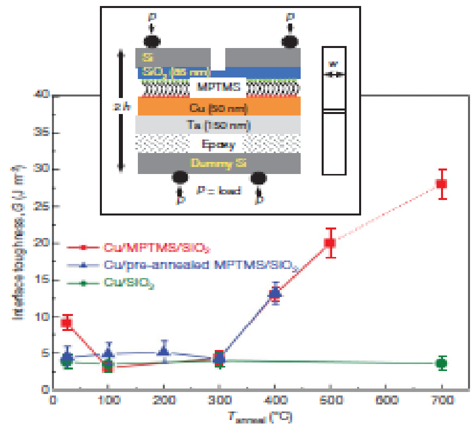
Not everything can be (or needs to be) a good switch !!

3. Nanoscale Energy Flow

Electrical Conductivity can be tuned by 20 orders of magnitude!
Thermal Conductivity is seen to vary only over 4 orders.... (Majumdar et al)



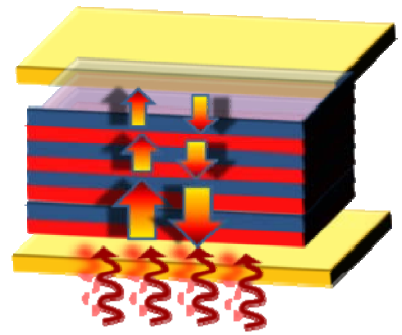
Phonon filtering
(Reddy et al)

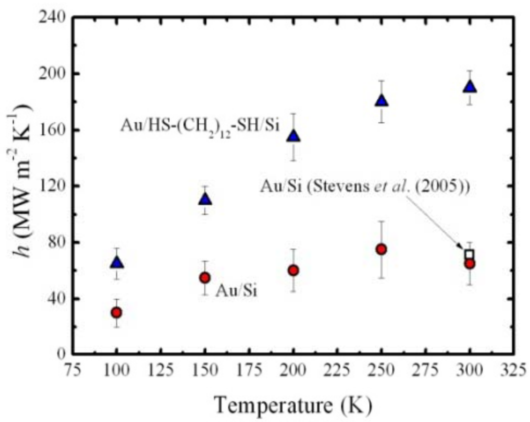


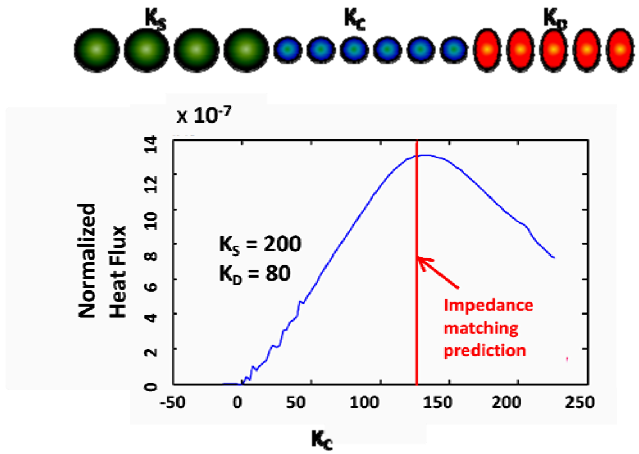
Superior tethering at high T
by molecules → Nano "Glue"
(Gandhi et al, Nature '07)

Why this discrepancy, and what can we do about it?

3.1. "Engineering" Thermal Transport?







Down-to-earth:

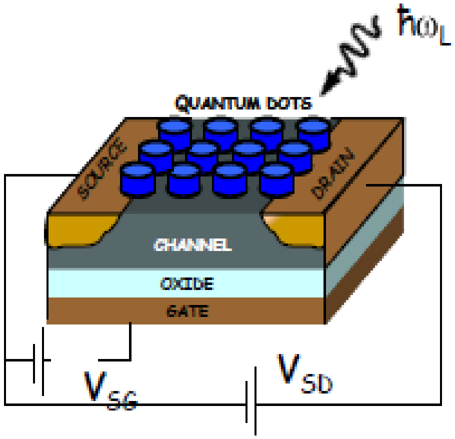
- Molecular SAMs at interfaces
- Match between crystal phonons and molecular vibrons
- Upconversion of phonons by alkanes (Hopkins et al)

Pie-in-the-sky:

- Phononic "Phase engineering" ?

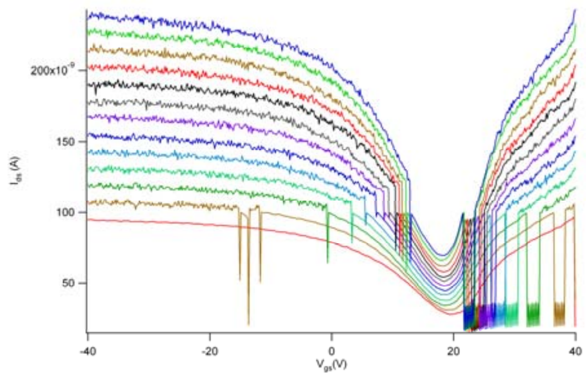
Wave-guiding, matched filters, Sub-wavelength 'gratings' etc..

4: Can we detect a single 'trap' ?



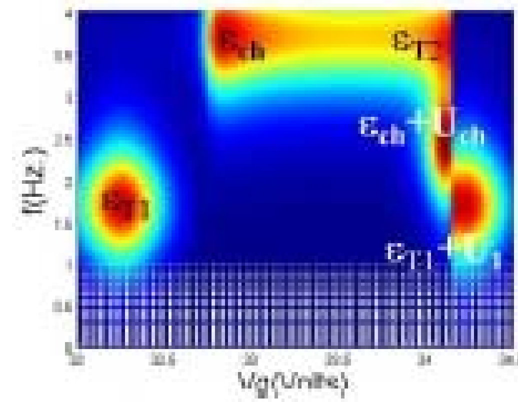
Nano-Micro
(NSF-CAREER)

- Phase coupling
(PRB '10)
- Charge scattering
(PRB '09; IEEE Sens '08)
- Potential scattering
(JAP '09)
- Phononic scattering



Nanotube Data
Williams group, UVA (PRB'09)

80% current modulation,
Room temperature!
High resolution:1D CNT electrostatics

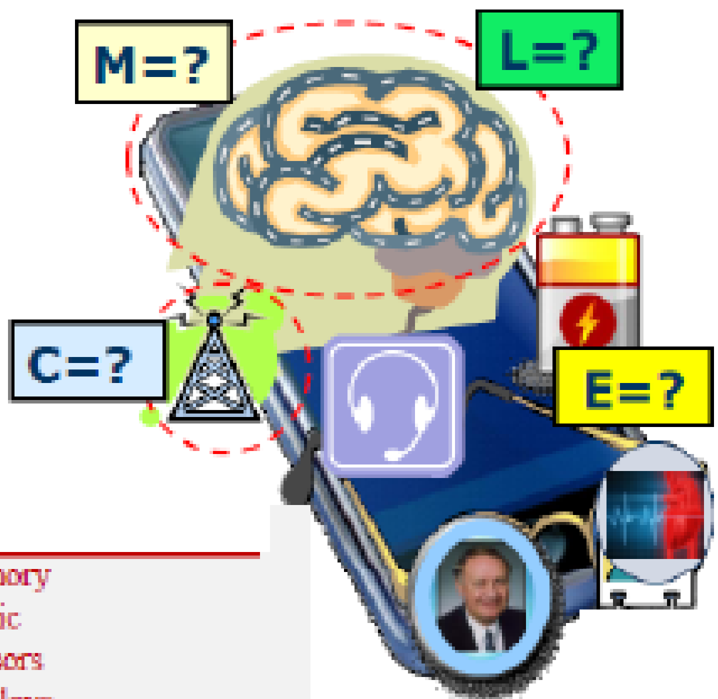


Snapshot of trap dynamics
(Vasudevan, PRB '09)

Molecule specific signatures
(**Need experiments !!**)

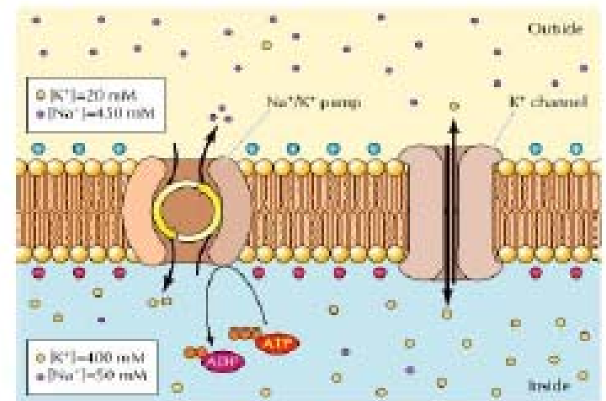
"SurFETs" vs "ChemFETs"
Molecular "Barcode" from Room-T Current Noise!
Molecule-specific, no false positives
Utilizes naturally occurring noise at low-D

5. What can biology teach us?
Si-Computers vs C-"Computers"



M - Memory
L - Logic
S - Sensors
D - Displays
C - Communication
E - Energy

Zhirnov/Cavin, SRC



Ionic flow in neural axons

Levy/Ghosh,
Nanostar Seed Grant

Information encoded as pulse **amplitudes** for small 'interconnects',
Changes to **pulse position modulation** for long ones, with periodic 'repeaters'

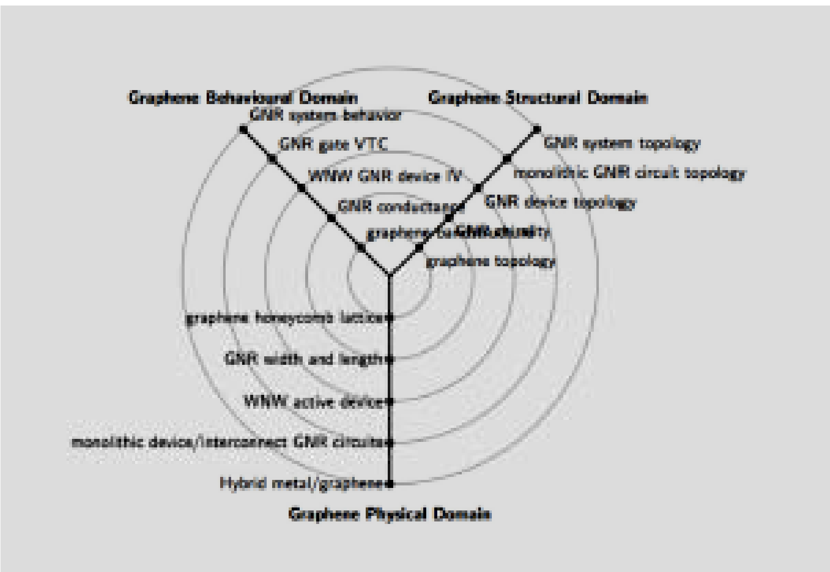
Language barriers vs unifying principles

Wholistic understanding needed !

Nano-electronics "by design": Targetted research coupling fundamental physics with computational materials science towards novel devices/circuits

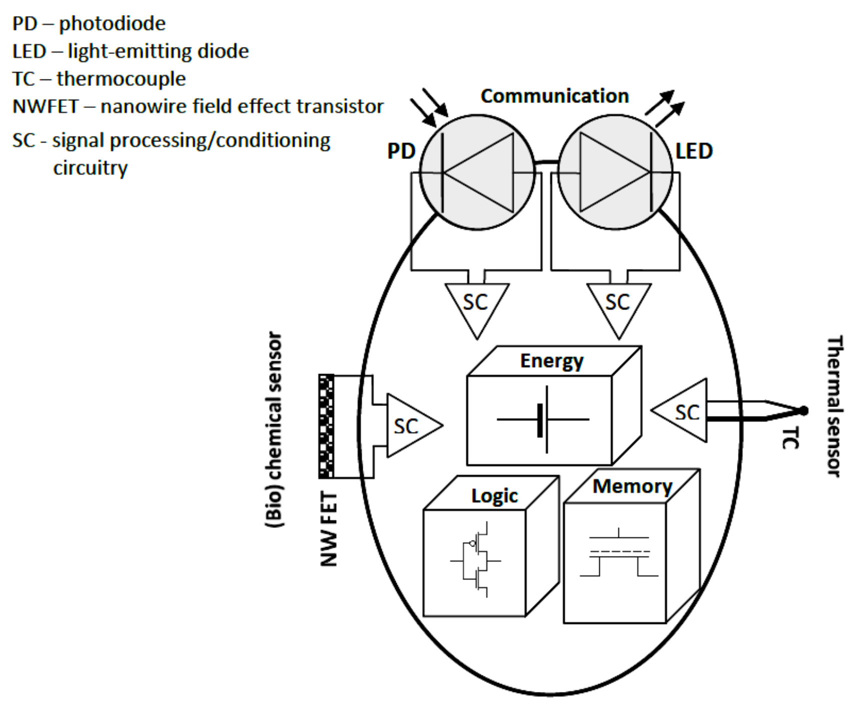
Computation ≠ Insights !!

HIERARCHICAL DESIGN



Y-chart, Gajsky-Kuhn

FUNCTIONAL DESIGN



Nanomorphic cell, Zhirnov/Cavin

Challenge: Seeing the forest for the trees…