Physics of Nanoscale Devices

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ECE

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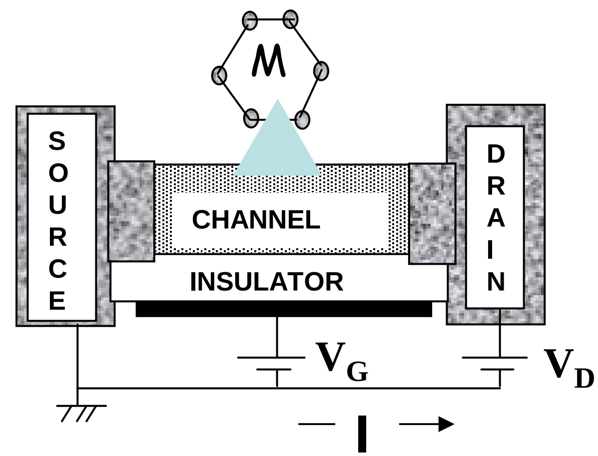
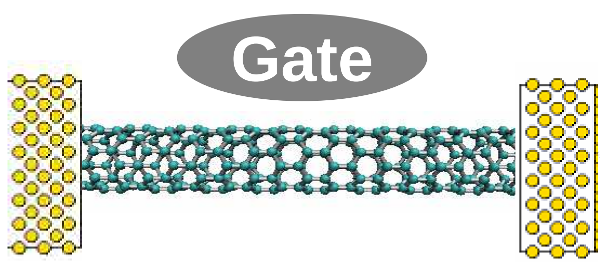
F. Tseng, Y. Yang, B. Muralidharan, L. Siddiqui
S. Datta, M. Lundstrom

(DARPA, SRC, ARO-DURINT, NCN, INAC)

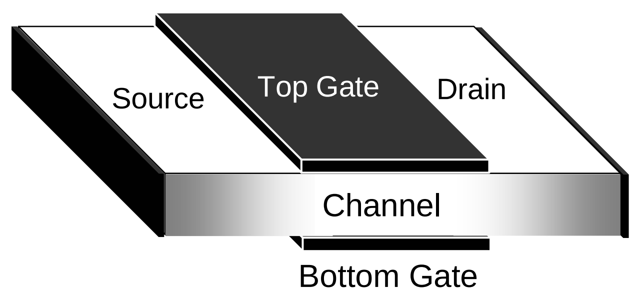
Molecular Sensor



CNT Interconnects

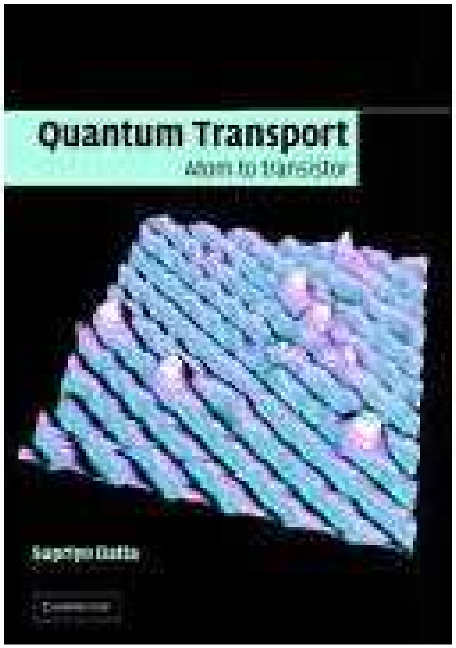


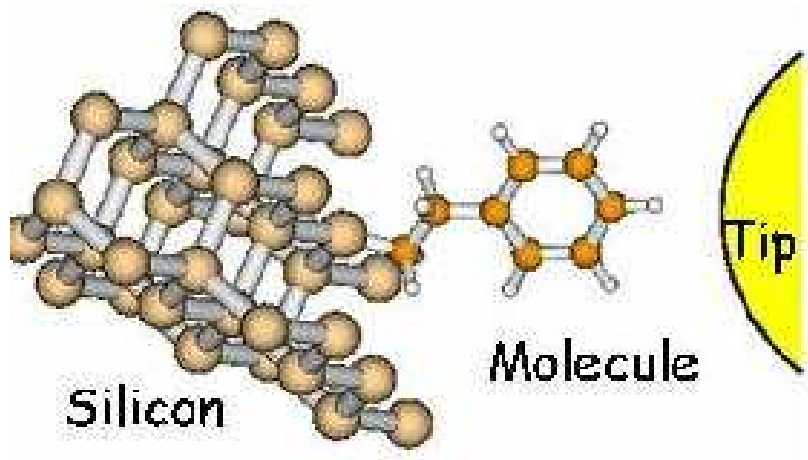
Si/Ge transistors



Overview

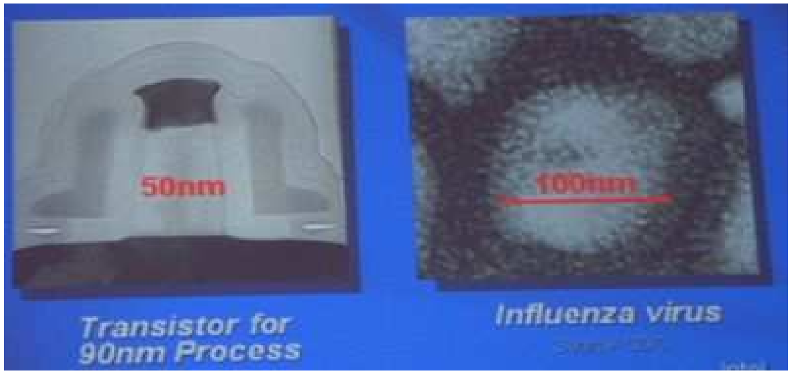
- Basic Physics of current flow
- Incorporating explicit details: bandstructure, chemistry, electrostatics
- Correlation Effects
- Future?



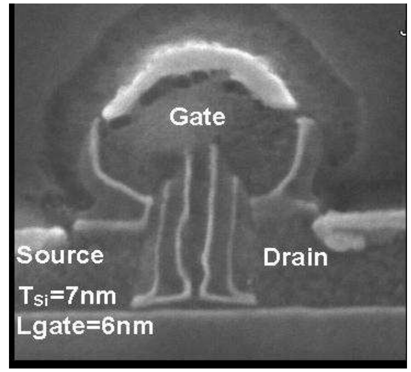


ECE 687
(Fundamentals of Nanoelectronics)

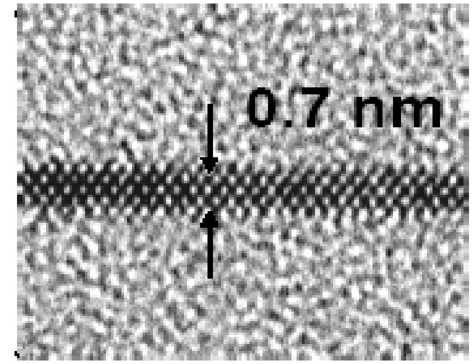
The incredible Shrinking Transistor



Intel's 2003 transistor
(Nanoelectronics in action !)



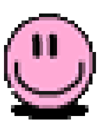
6 nm MOSFET
Bruce Doris, IBM



0.7 nm thick MOSFET
Uchida, IEDM 2003

"Small is Different" – quantum and atomistic effects

- Confinement, Leakage, atomistic bandstructure effects, quantum tunneling, surface scattering

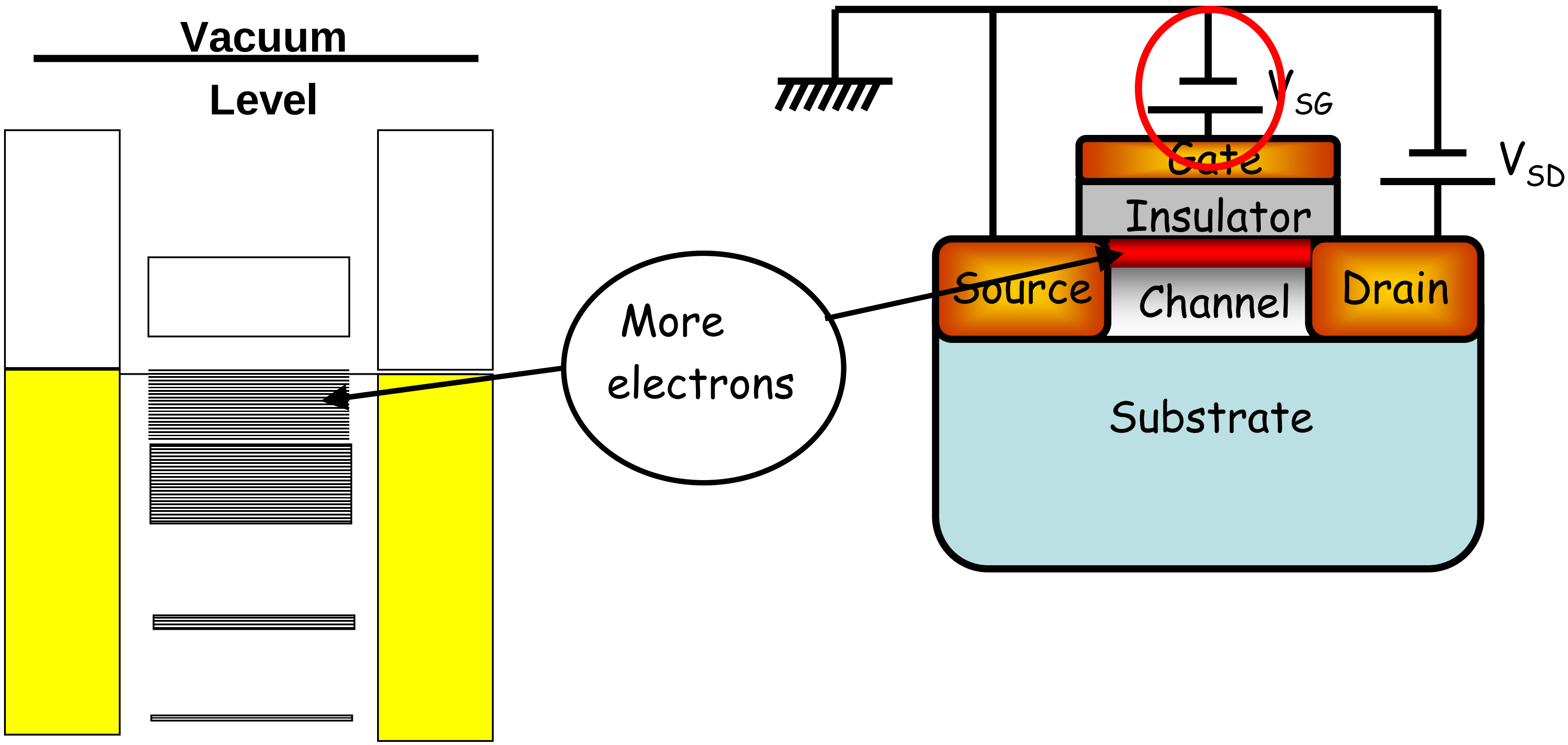


- Novel sensors, designer materials, ultradense memories, high speed computers, molecular relays

Operation of a transistor

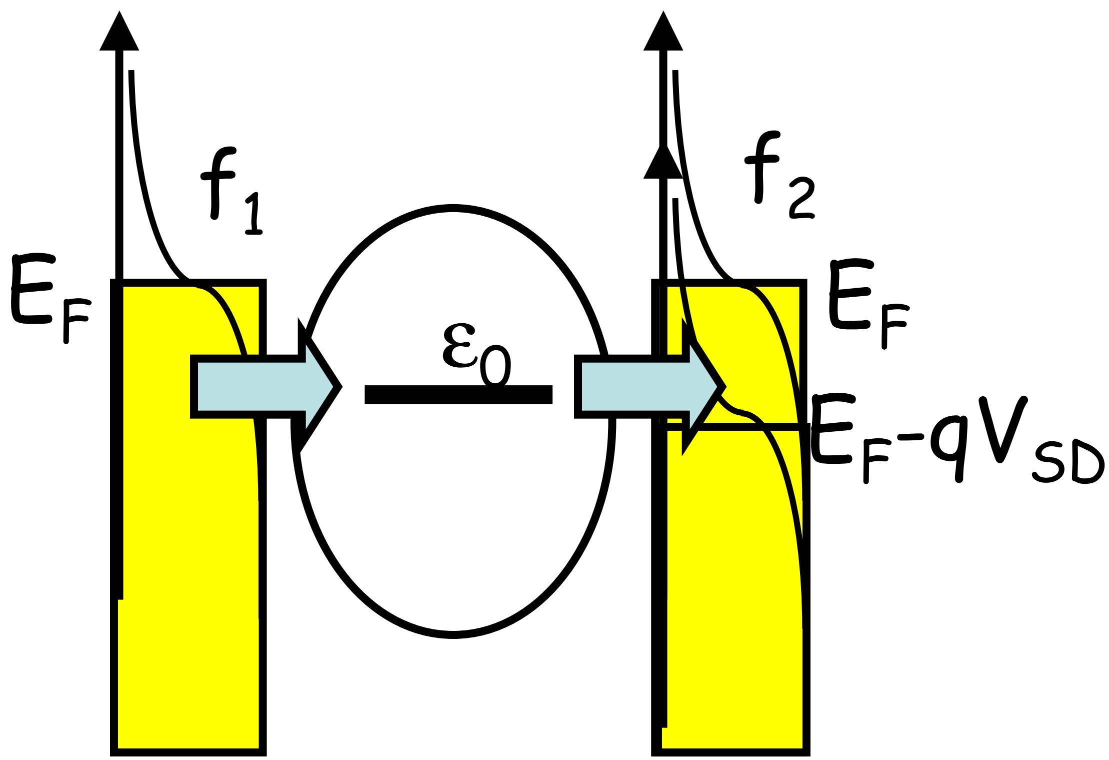
$V_{SG} > 0$

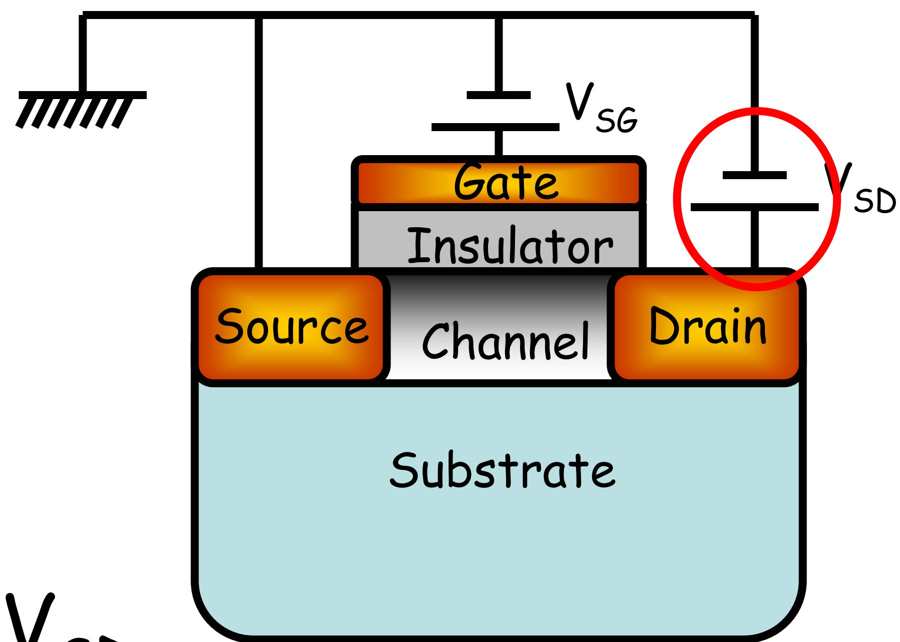
n type operation



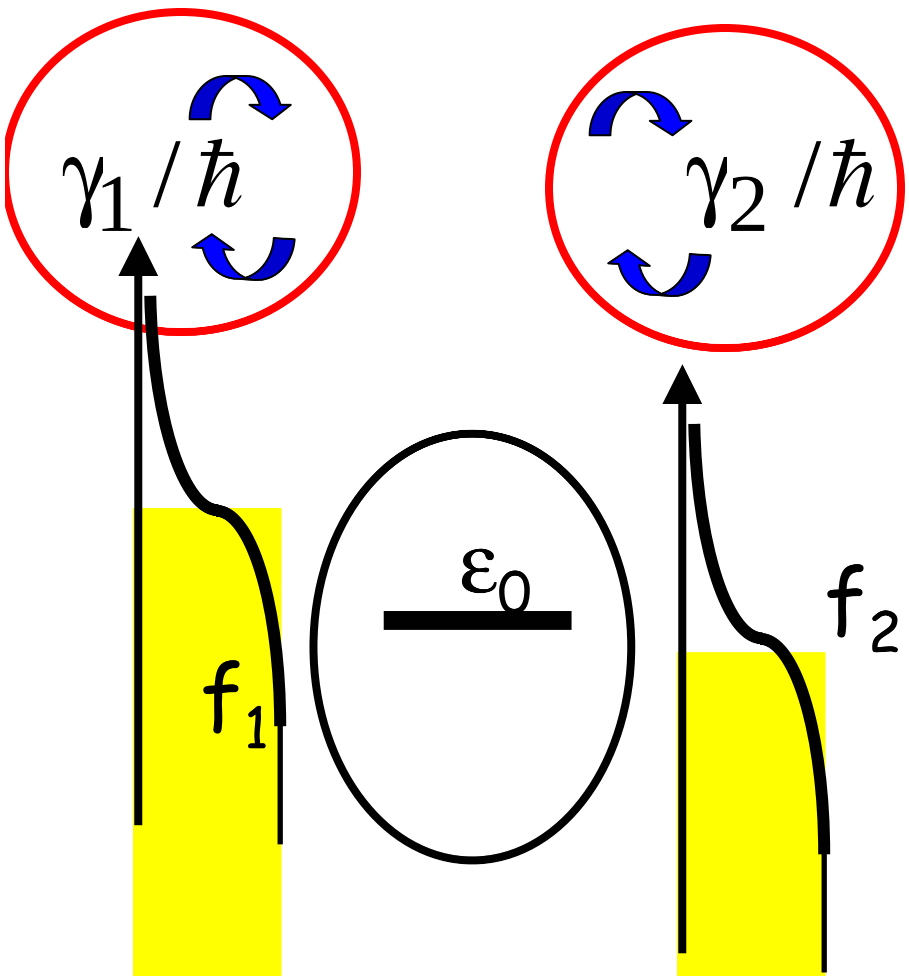
- Positive gate bias attracts electrons into channel
- Channel now becomes more conductive

Current flow through 1 level





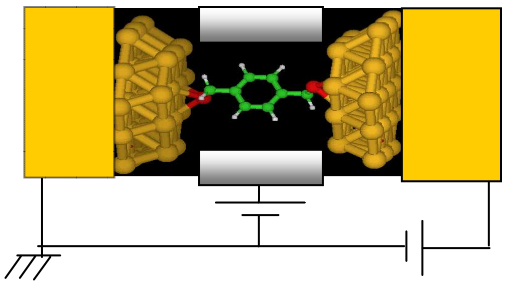
Escape time



γ: strength of bond between contact and channel

~ escape rate into leads

Toy Model : Current



$$I_1 = q\frac{\gamma_1}{\hbar}[f_1 - N]$$

$$I_2 = q\frac{\gamma_2}{\hbar}[N - f_2]$$

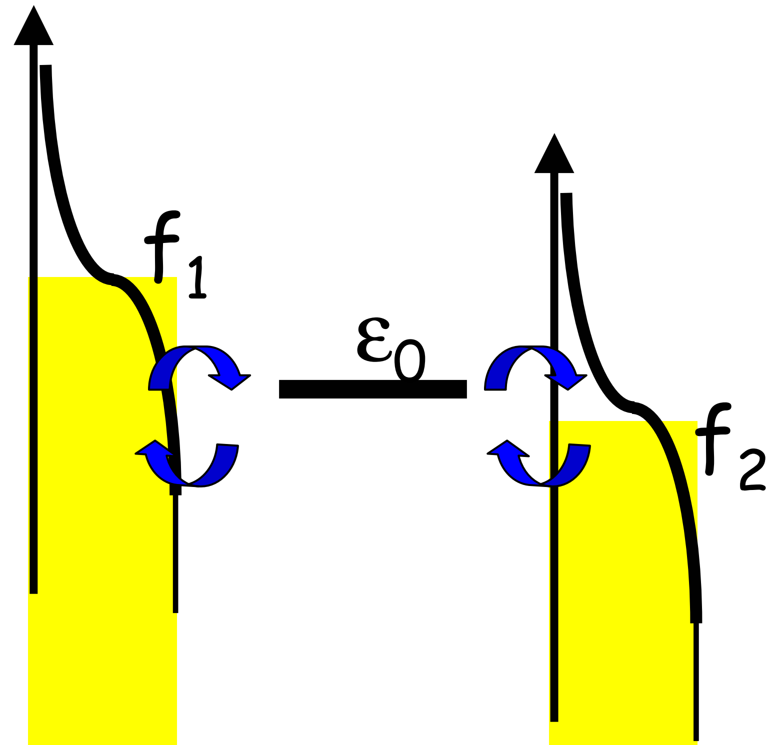
$$N = \left[\frac{\gamma_1 f_1 + \gamma_2 f_2}{\gamma_1 + \gamma_2}\right]$$

(weighted average of $f_{1,2}$)

$$I = \frac{q}{\hbar}\frac{\gamma_1\gamma_2}{\gamma_1 + \gamma_2}[f_1 - f_2]$$

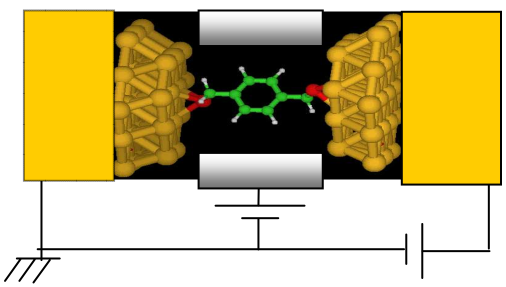
(Only levels near E_F conduct)

(Net escape time $1/\gamma = 1/\gamma_1 + 1/\gamma_2$)



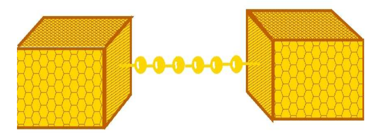
Must include Broadening

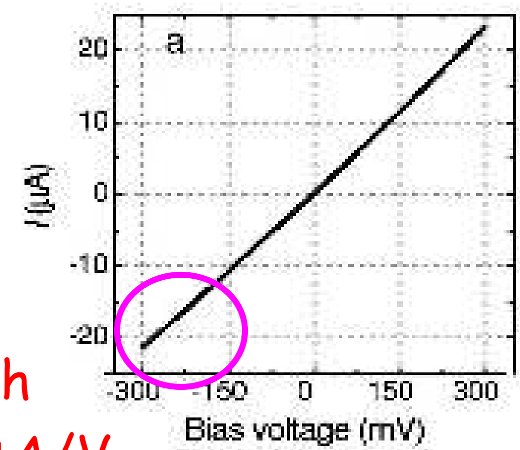
Keeps conductance
in check



$$N = \int dE\; D(E) \left[\frac{\gamma_1 f_1 + \gamma_2 f_2}{\gamma_1 + \gamma_2} \right]$$

$$I = \frac{q}{\hbar} \int dE\; D(E)\; \frac{\gamma_1 \gamma_2}{\gamma_1 + \gamma_2} [f_1 - f_2]$$

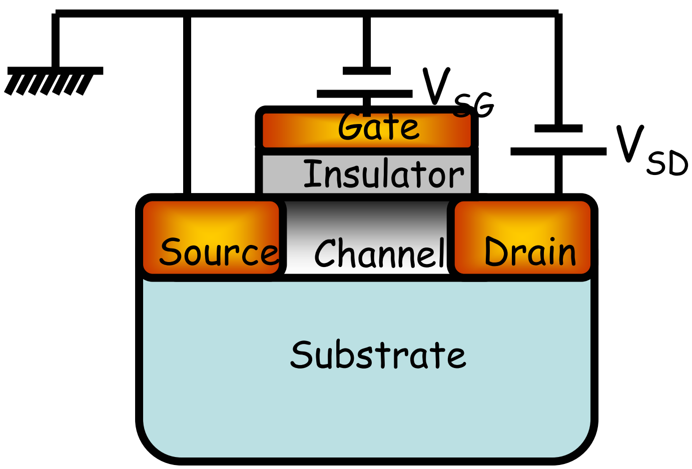


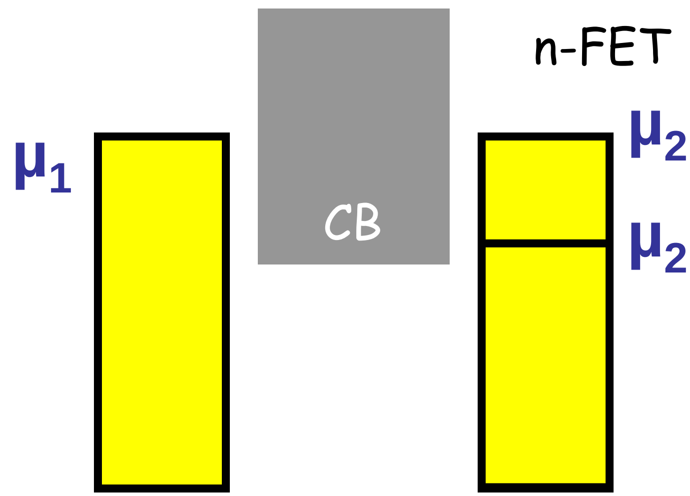


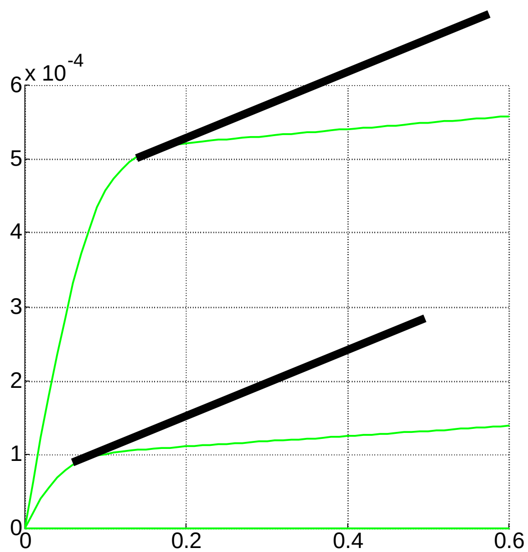
G_0
$= 2q^2/h$
$= 77\ \mu A/V$

EXPT Halbritter (PRB '04)

Must include local potential



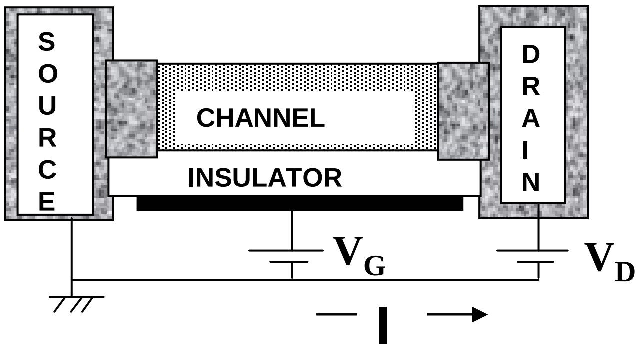




Saturation occurs if channel DOS is closed

Current is compromised once band-edge slips due to local potential U

Minimal Model for Transport



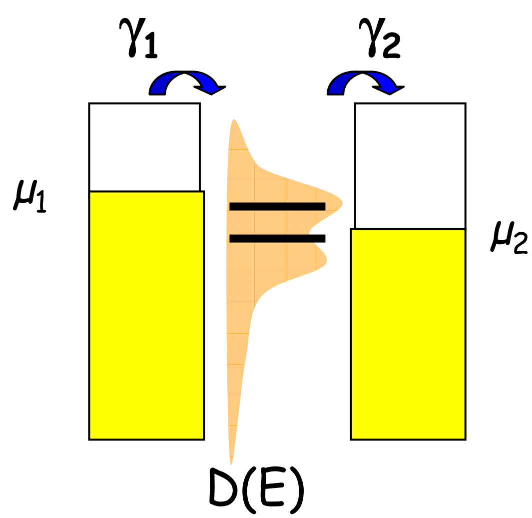
$$N = \int dE\ D(E-U)\left[\frac{\gamma_1 f_1 + \gamma_2 f_2}{\gamma_1 + \gamma_2}\right]$$

$$I_1 = \int dE\ D(E-U)\frac{2q}{\hbar}\frac{\gamma_1\gamma_2}{\gamma_1 + \gamma_2}[f_1 - f_2]$$

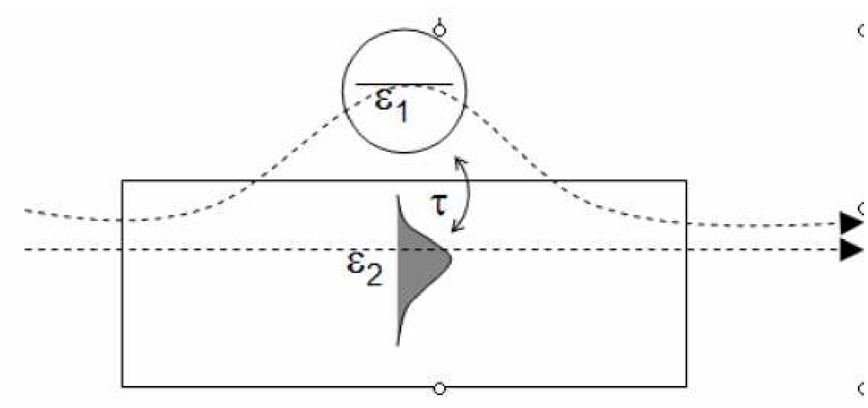
Poisson: $U = U_L + U_0(N-N_0)$

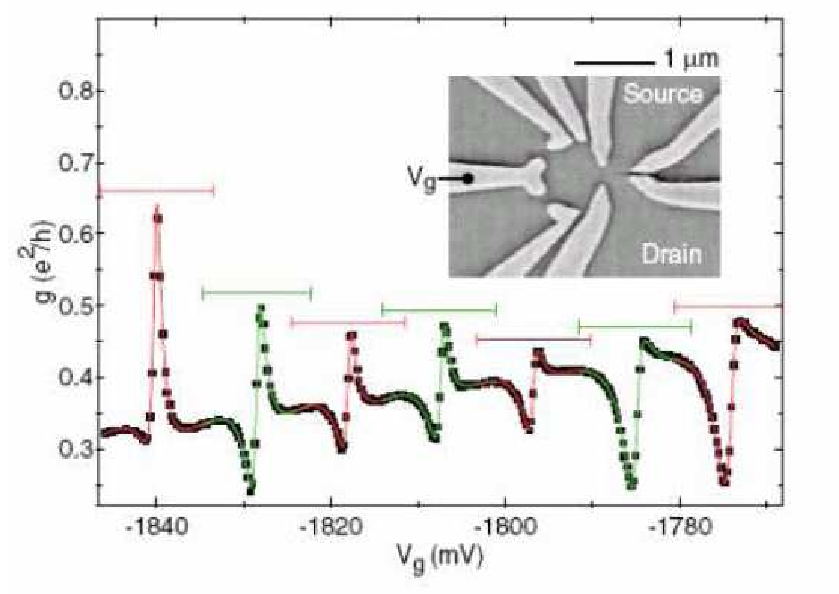
	Rate equation	$\gamma_{1,2}$, $f_{1,2}$
+	Broadening	D(E)
+	Electrostatics (Self-consistent Field)	U

Silicon / Nanotubes / Molecules



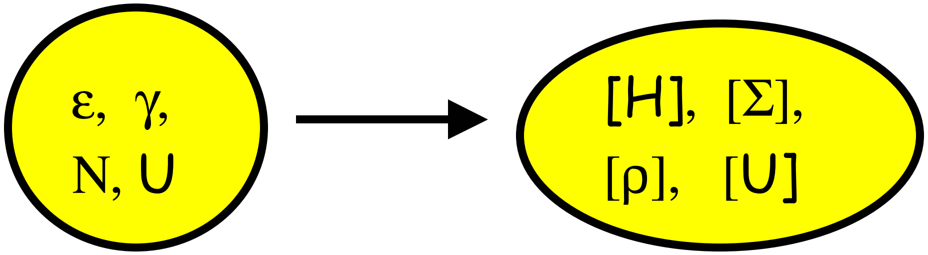
Beyond independent levels: Interference





Fano interference

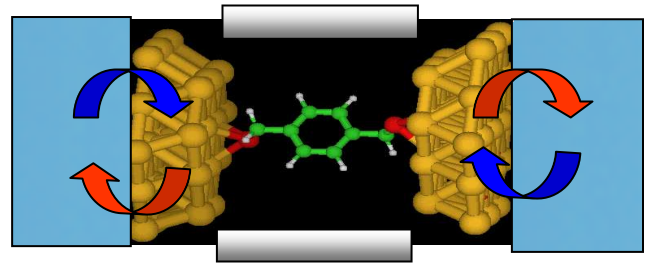
Beyond the independent level model

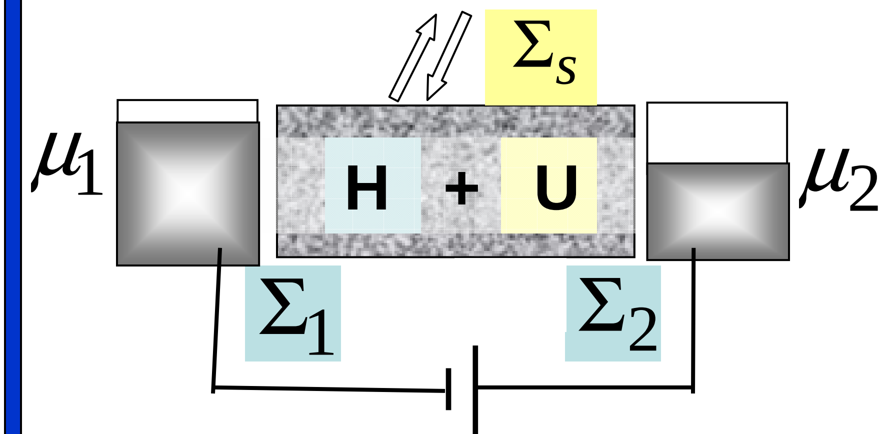


$$I_1 = \frac{\gamma_1}{\hbar}\left[f_1 - N\right]$$

$$\frac{1}{\hbar}\,\text{Trace}\,\left[\Gamma_1 A\right] f_1$$

$$\frac{1}{\hbar}\,\text{Trace}\left[\Gamma_1 G^n\right]$$

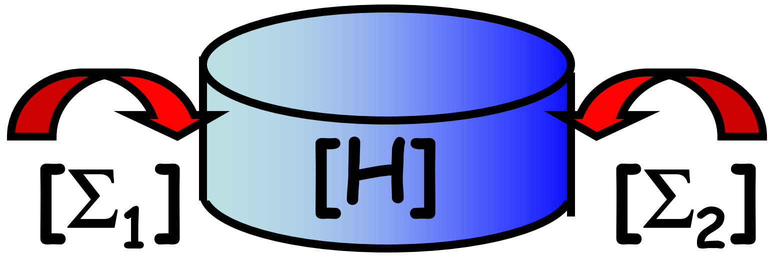




Unified approach

Non-Equilibrium Green's Function formalism (NEGF)

Classical vs Quantum Transport



Classical

Newton's Law

↓ Statistics

Langevin Equation

$mdv/dt - F + \gamma v = N(t)$

↓ Collective

Boltzmann Transport Eqn
Distribution function f

Quantum

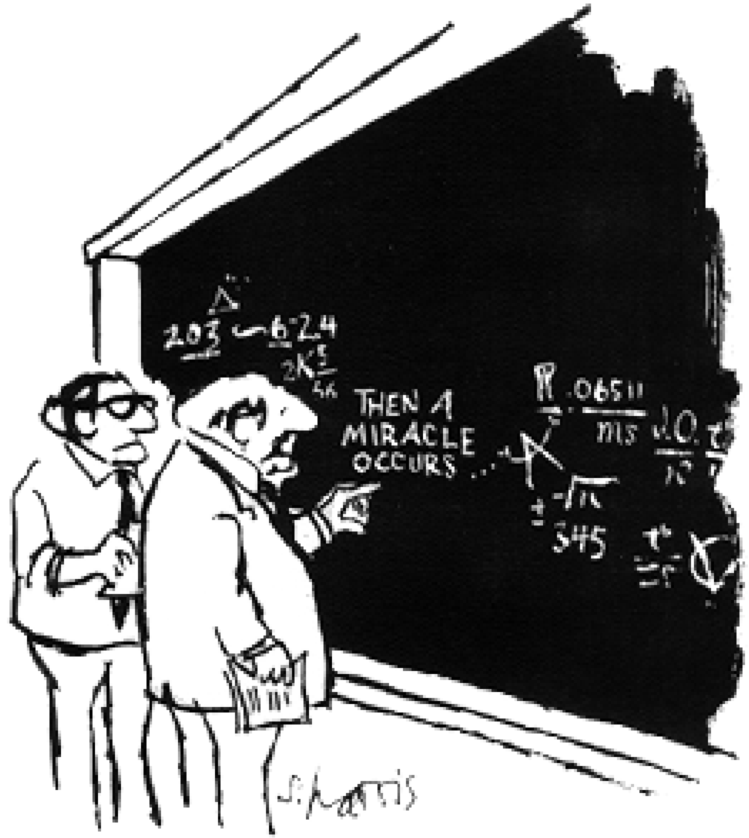
Schrödinger Equation

↓ Statistics

$i\hbar\partial\psi/\partial t - H\psi - \Sigma\psi = S(t)$

↓ Collective

NEGF
Correlation $G^< \sim \langle\psi\psi^+\rangle$



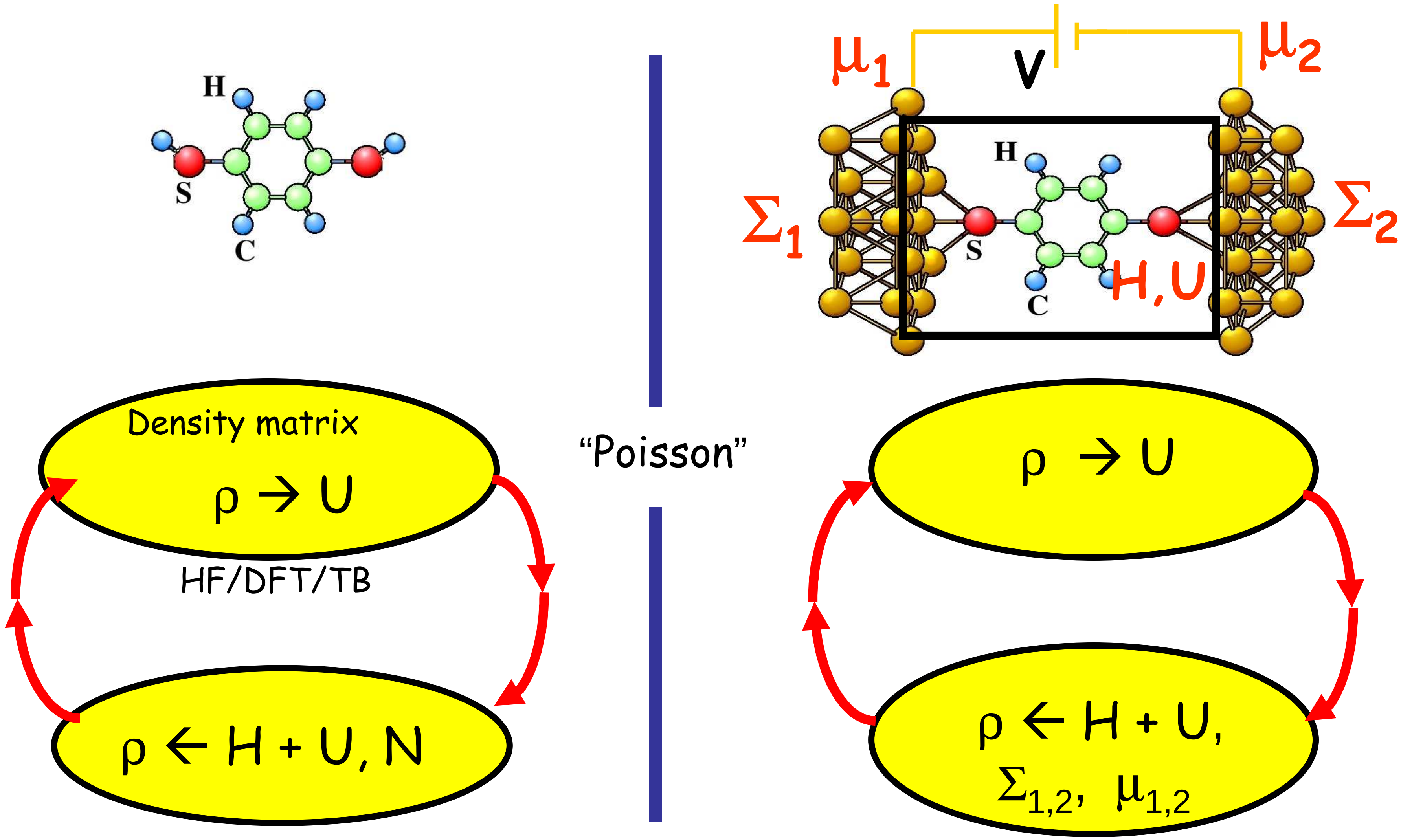
"I think you should be more explicit here in step two."

Details are important!

Computational chemistry to device simulation

Computational Chemistry
(closed systems in equilibrium)

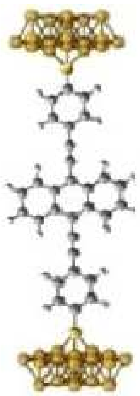
Computational Electronics
(open systems under bias)

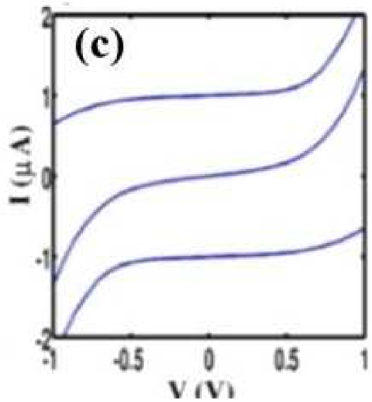


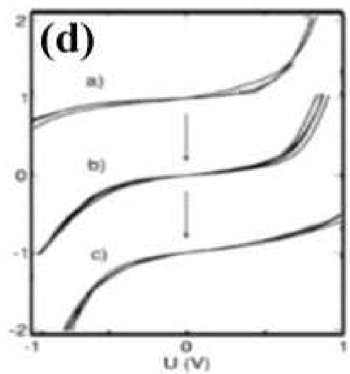
fill N eigenstates

transport (NEGF)

Molecular I-Vs



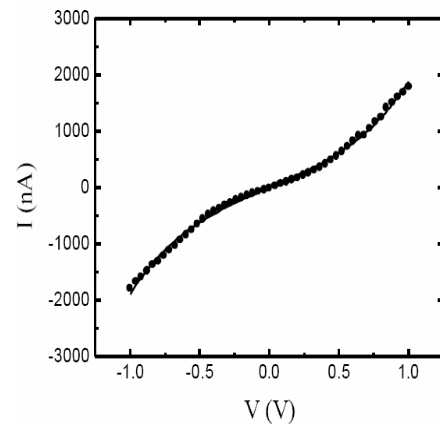


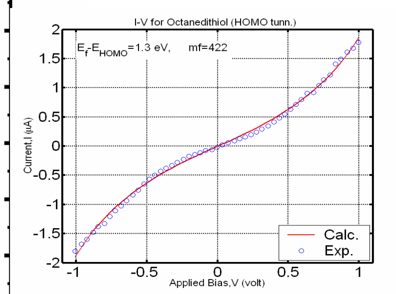


THEORY:
PRB 2004

EXPT:
Weber Group
PRL

Rectification in porphyrin





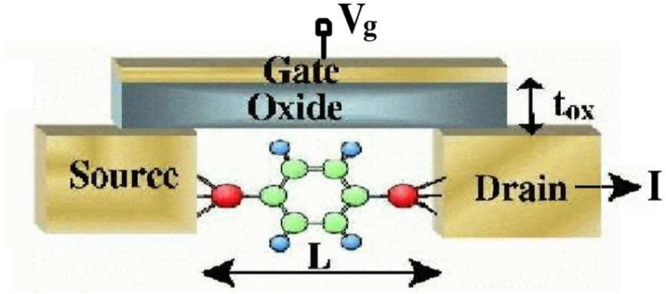
EXPT:
Reed Group
Nano Lett.

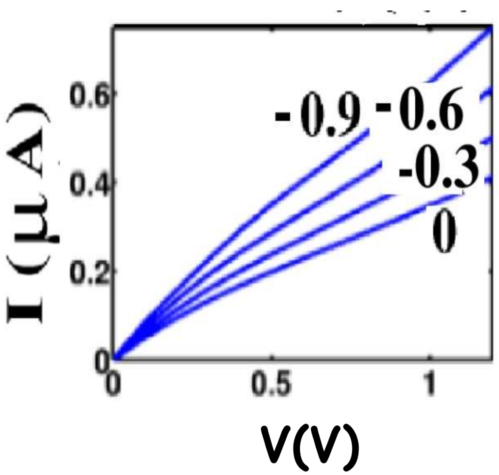
THEORY:
PRB '05

Tunneling in alkanethiols

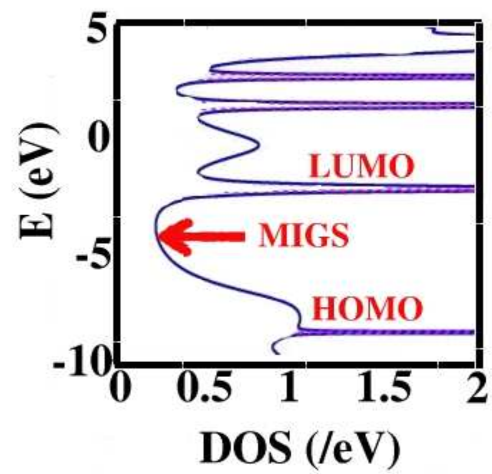
Interconnects
Strained Si/SiGe MOSFETs
Si nanowire FETs
Carbon nanotube/Graphene FETs

Molecular Transistors?





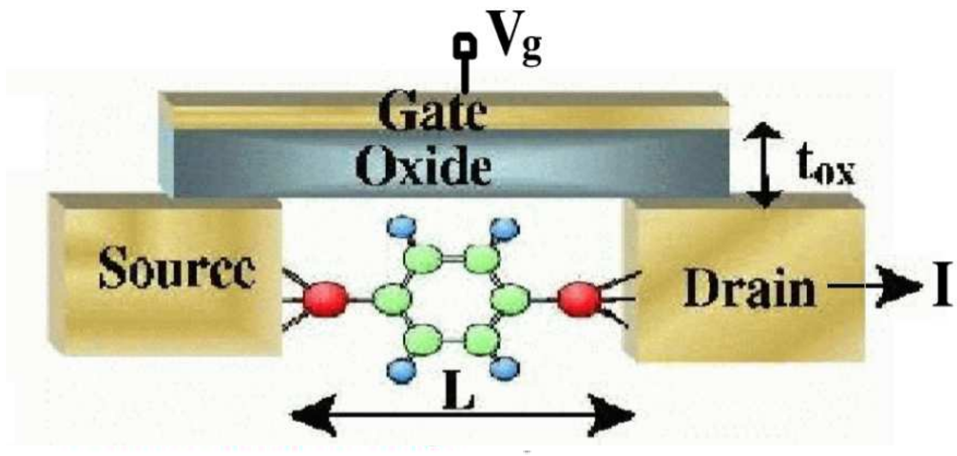
Electrostatic control hard to get



Lot of Metal states near Fermi energy
→ hard to turn off the transistor

(Damle/Rakshit/Paulsson/Datta, IEEE-NANO '02;
Liang/Ghosh/Paulsson/Datta PRB '04)

Conformational Transistors (MEMS)?

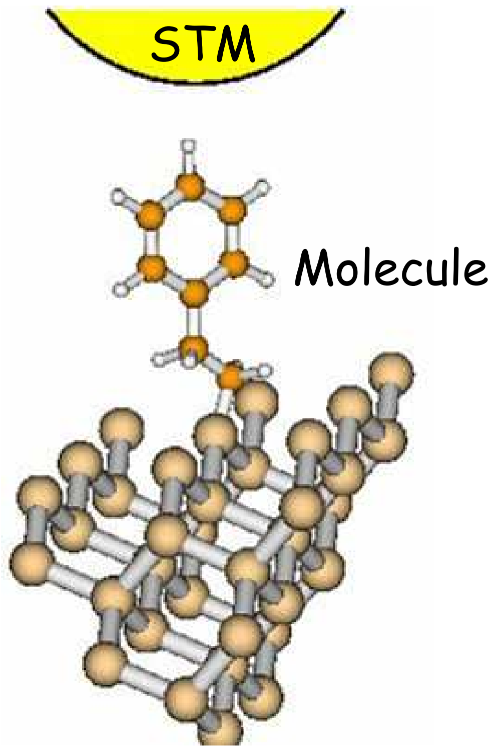


Electrostatic gating: need at least 60 mV gate voltage to change current by factor of 10

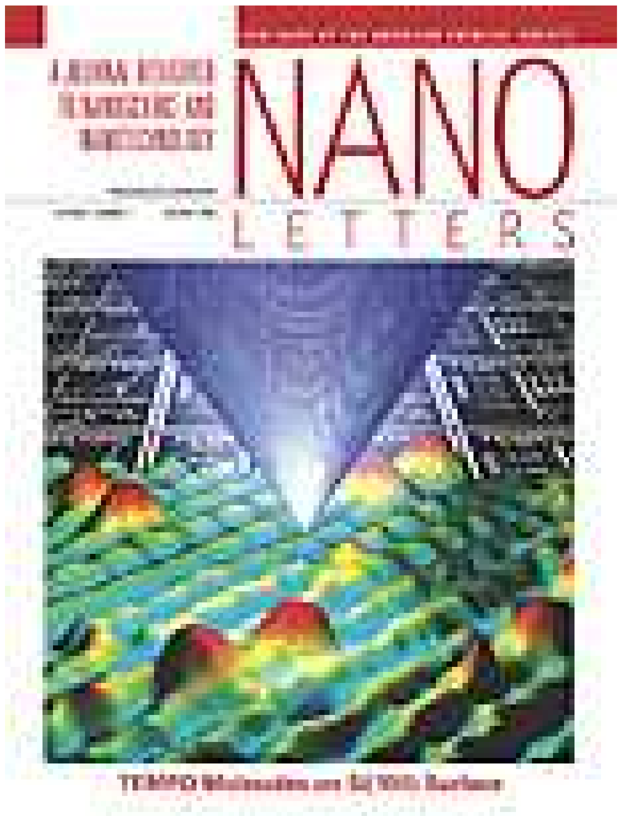
Conformational gating: can beat this textbook limit by engineering a large dipole !

Ghosh, Rakshit, Datta
(Nanoletters, 2004)

Hybrid molecule-silicon devices ?

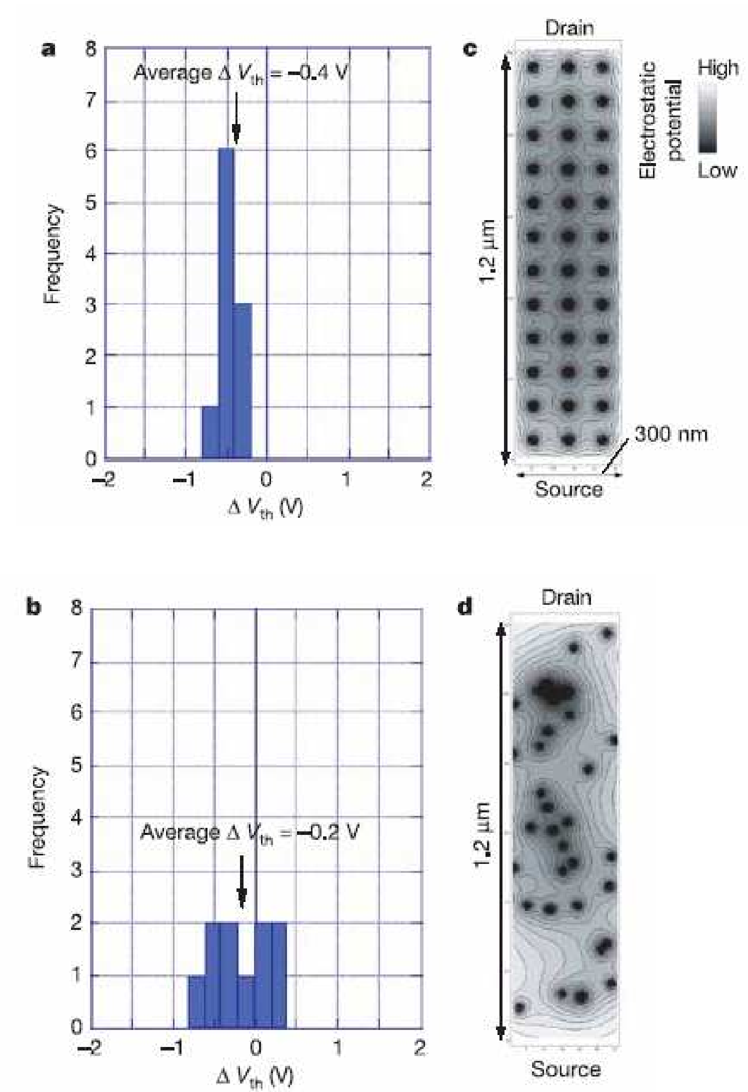


Si(100)

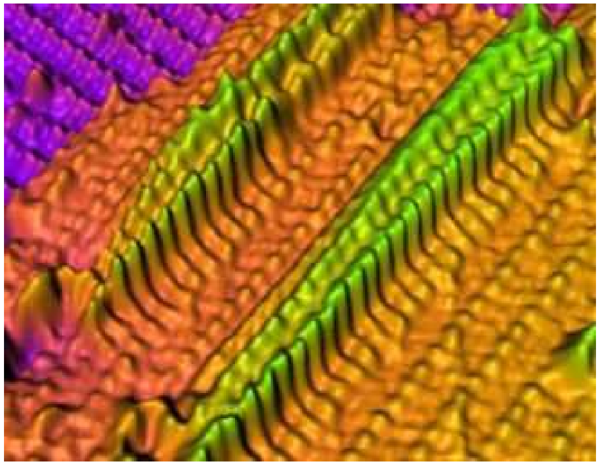


Nano Letters cover story
Jan '04

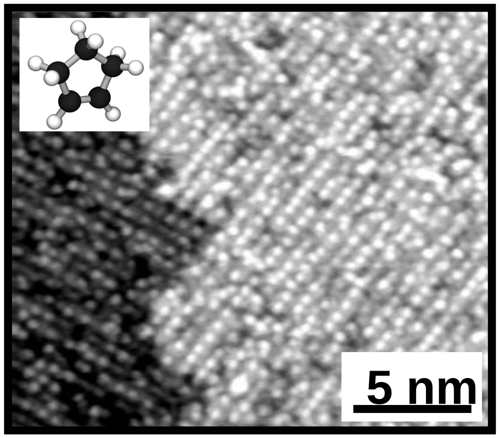
Within CMOS: Better dopants?



Shinada et al, Nature '05

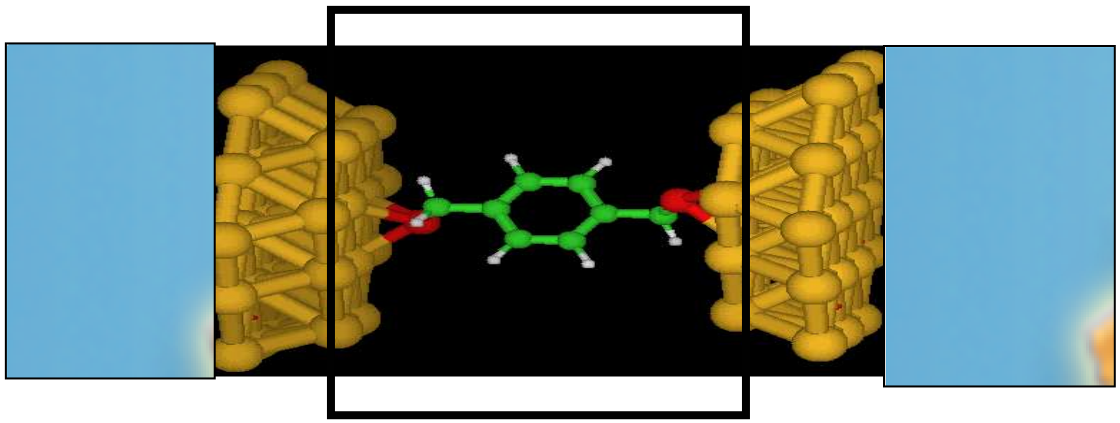


Hersam et al
Multi-step Feedback controlled Litho



Cyclopentene monolayer
Hersam group, Nanotechnology 2004

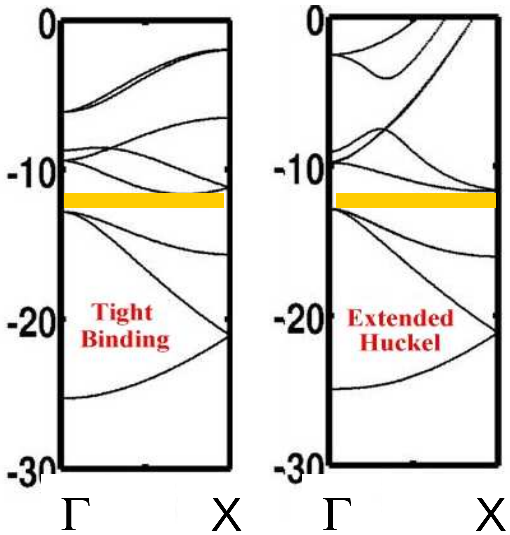
Bridging Disciplines



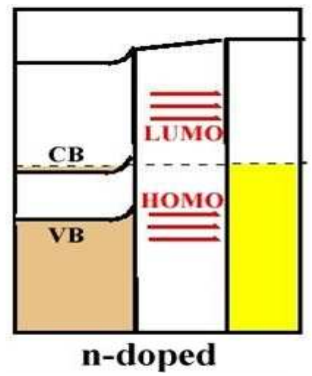
$$[\Sigma_1] \quad [H] \quad [\Sigma_2]$$

Atomistic Silicon modeling → challenging !!

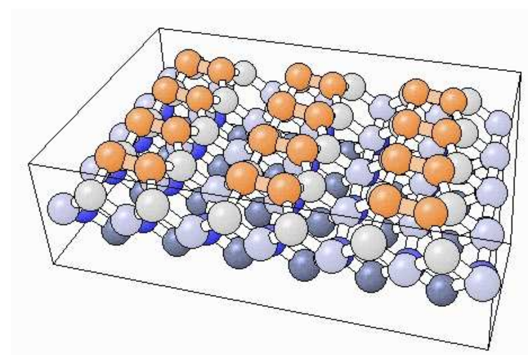
Bulk Silicon



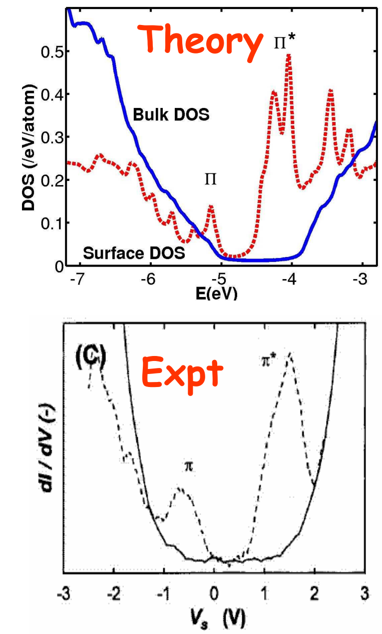
Band-gap, Effective masses, Strain



Doping and Band-bending



Reconstruction



Surface States

Electronic Structure theories for molecules and silicon different

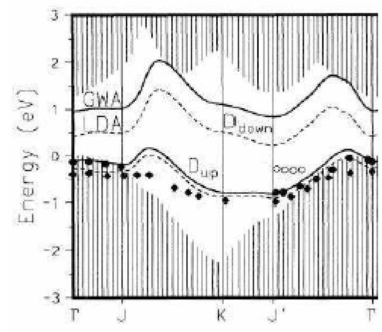
Solve Boundary value problem to combine engineers' and chemists' worlds

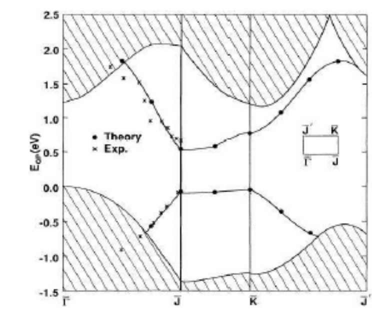
Silicon modeling

Combining chemistry and bandstructure for transport

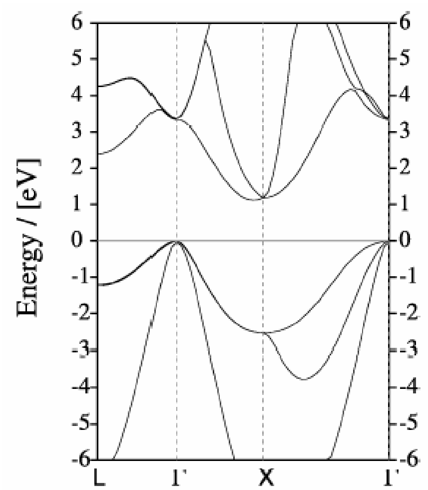
DFT underestimates bandgap, tight-binding gets wrong chemistry

Expt/GW

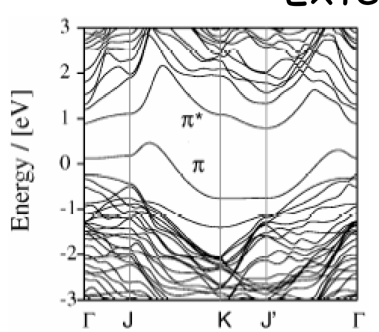


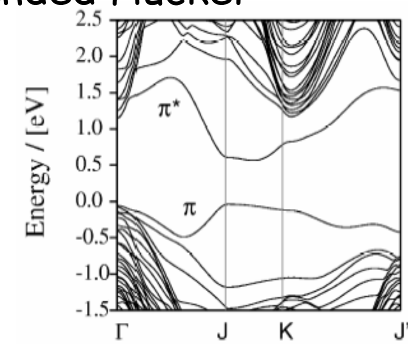


Extended Huckel



Bulk Si

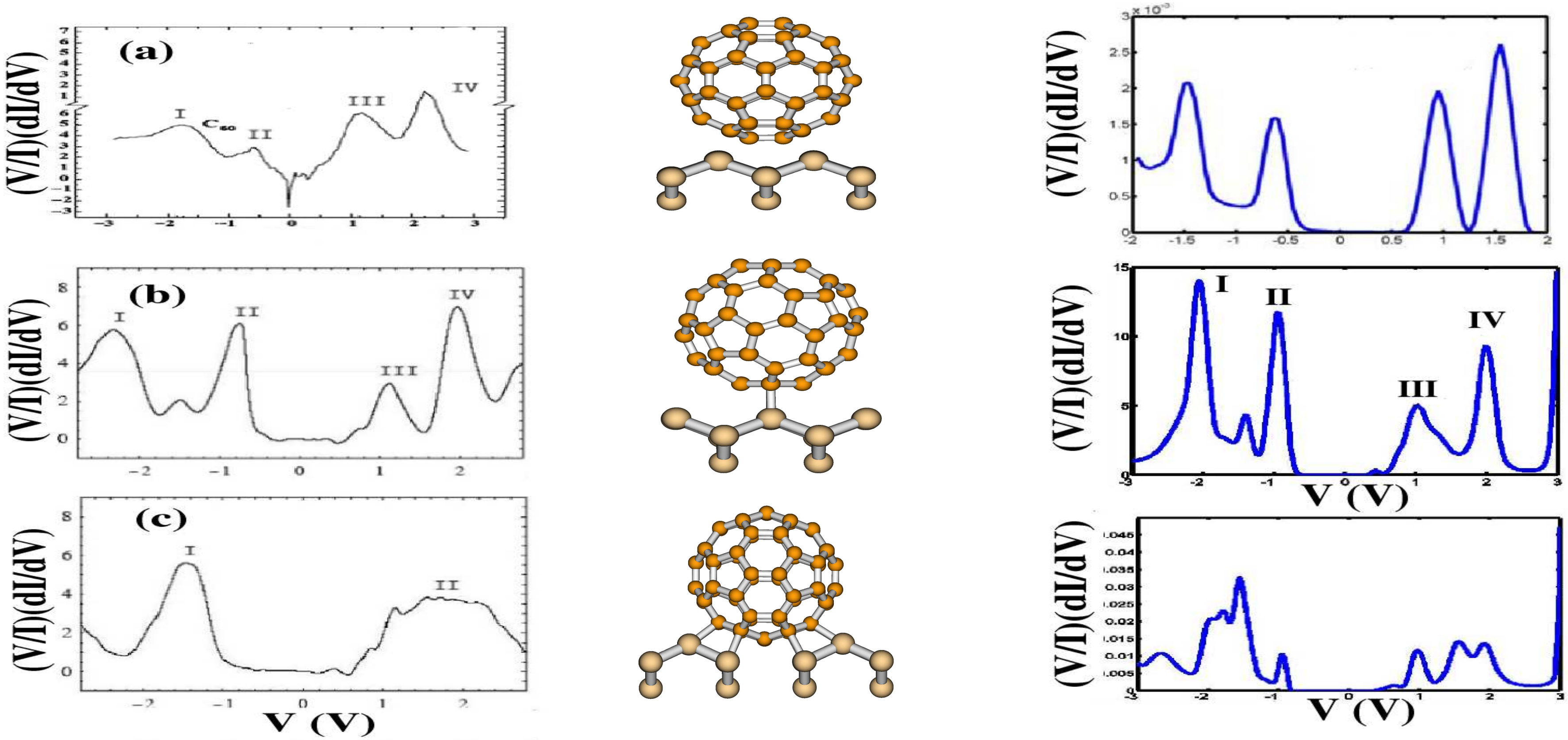




Si(100) 2x1 Si(111) 2x1

Kienle, Bevan, Siddiqui, Liang, Ghosh, Cerda

C60 transport spectra on Si(100)



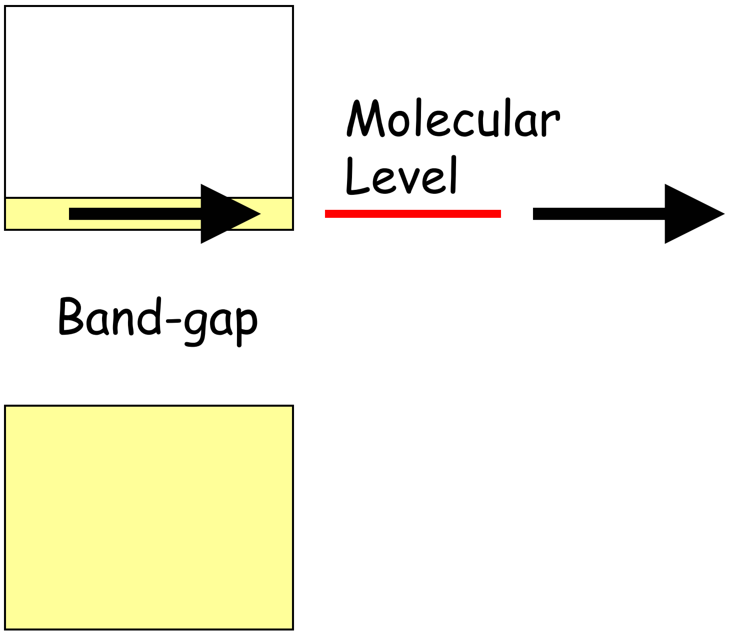
STS measurements:
(a) Dekker, et al., surface science '02.
(b) Yao et al, surface science '96
(c) Yao, et al, surface science '96

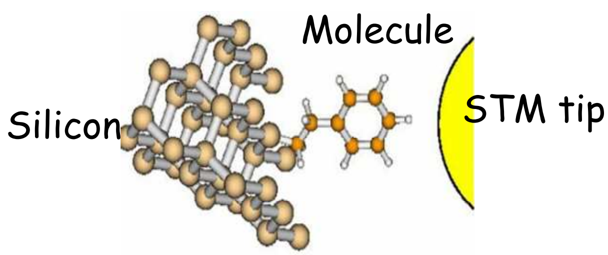
Theory:
Liang, Ghosh
PRL '05

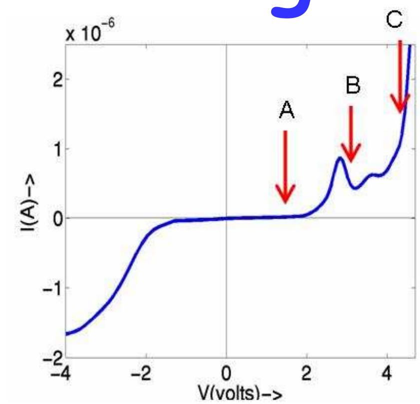
Deconstruct role of contacts in molecular I-V

Silicon – not just an 'interesting' contact

Can we drive molecular levels past a silicon band-edge?

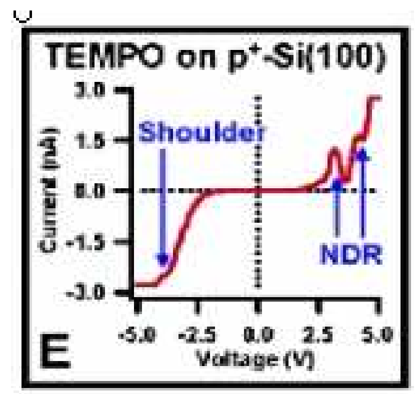






Theoretical Prediction

Rakshit, Liang, Ghosh, Datta, NanoLett. 4, 1803, 2004

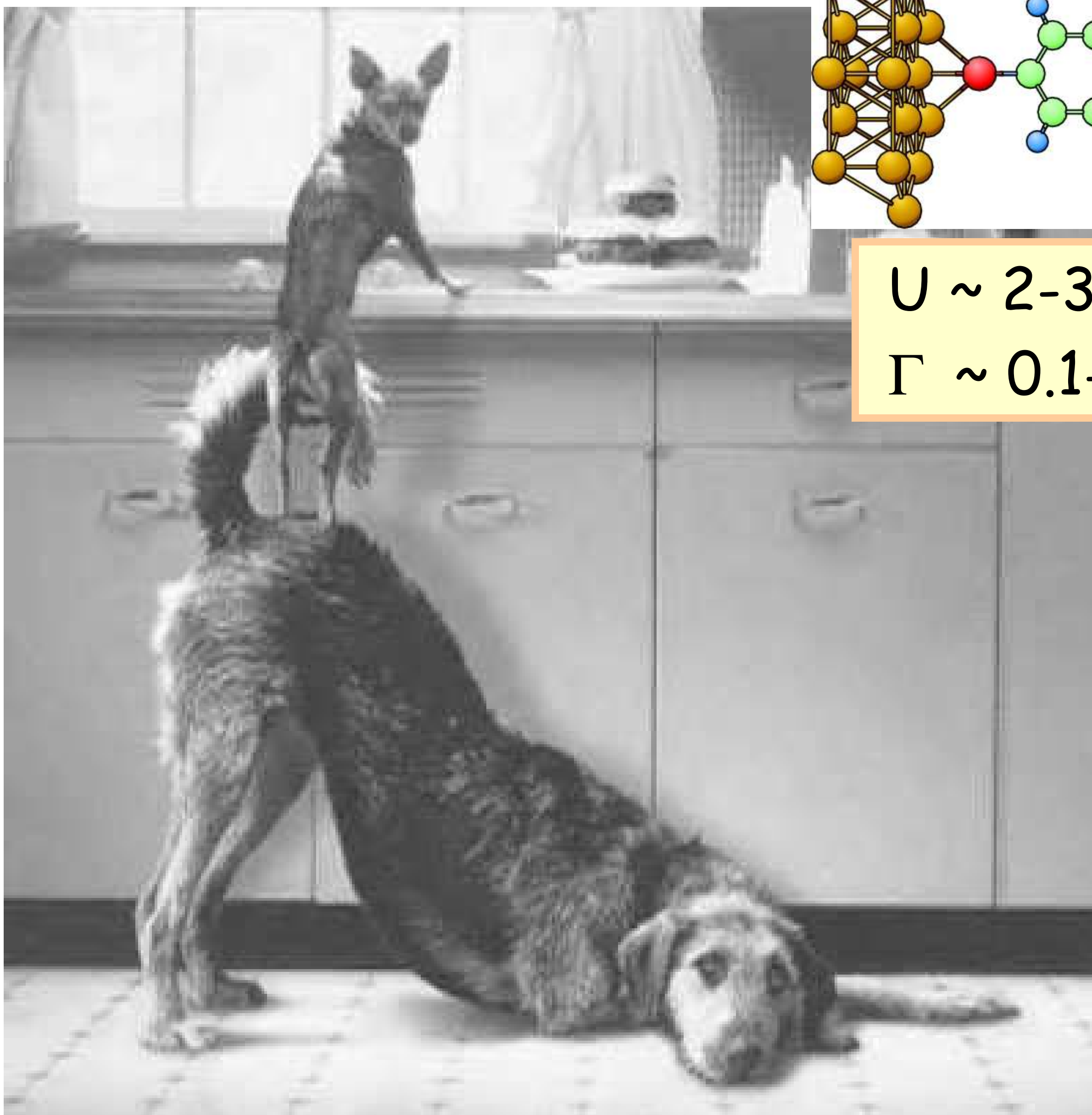


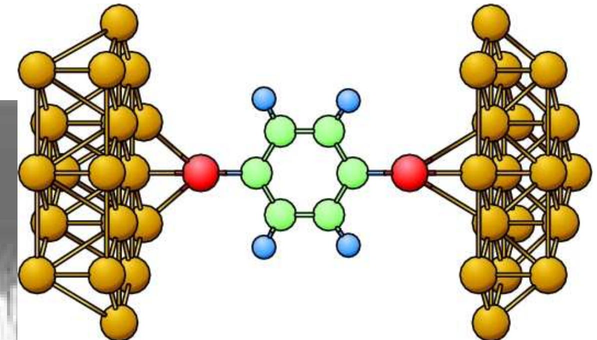
Possible experimental verification?
Unresolved issues, lots of activity

Hersam group, Nano Lett 4, 55, 2004

We seem to have qualitative and quantitative understanding, even on complex substrates

What's missing?





U ~ 2-3 eV

Γ ~ 0.1-0.2 eV

One-electron Transport

$$i\hbar \partial\psi/\partial t - H\psi - \Sigma\psi = S(t)$$

Outflow   Inflow

'Noise' statistics in contacts drives current flow

1-electron Correlation

$G^{<}(t,t') \sim \langle \psi(t)\psi^{+}(t') \rangle$

Many-body Transport

$$i\hbar\partial c/\partial t - Hc - \Sigma c = S(t)$$

Outflow Inflow

$$\{c(t),c^+(t')\} = \delta(t-t')$$

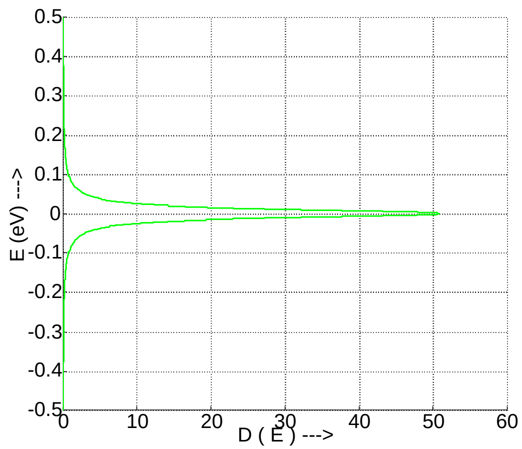
Second quantization

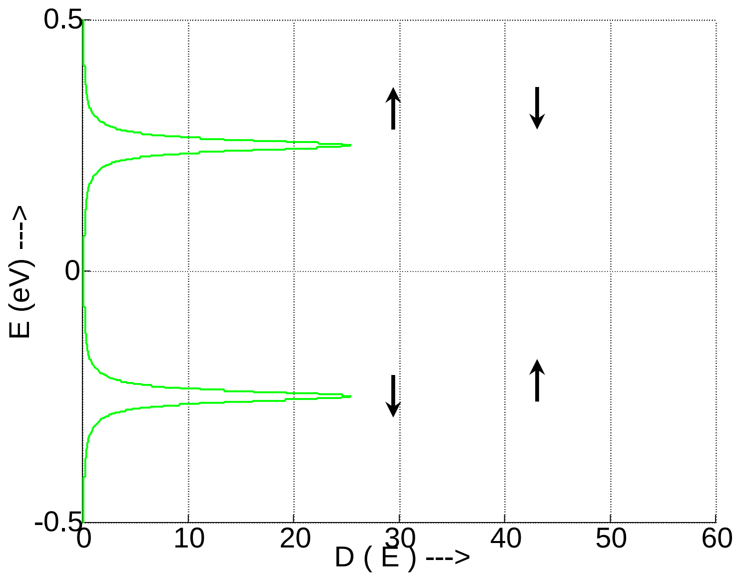
Correlation
$$G^<(t,t') \sim \langle c(t)c^+(t')\rangle$$

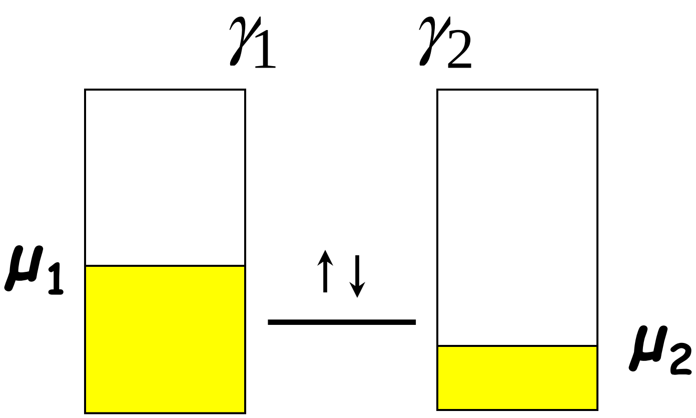
Interactions renormalize $\Sigma(E)$ for evolution of c, 'dressed particle'

Modifies DOS through, Coul. Blockade, Kondo & polaronic fingerprints

Electron-electron correlation: Coulomb Blockade



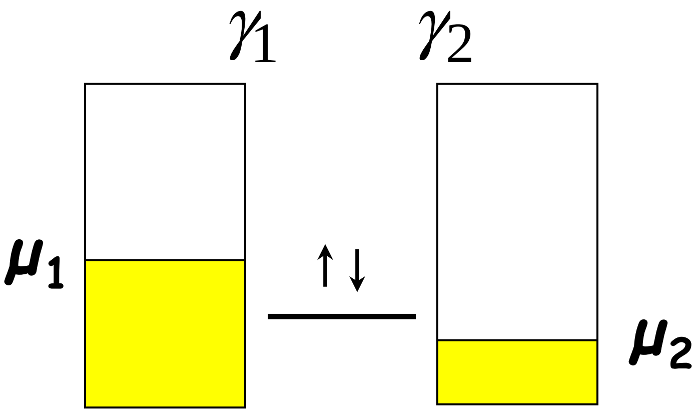




Levels split for large U_0 due to self-interaction correction
(Metal-insulator transition)

$$Bad\ Contacts: \quad \gamma << U_0$$

Getting CB approximately

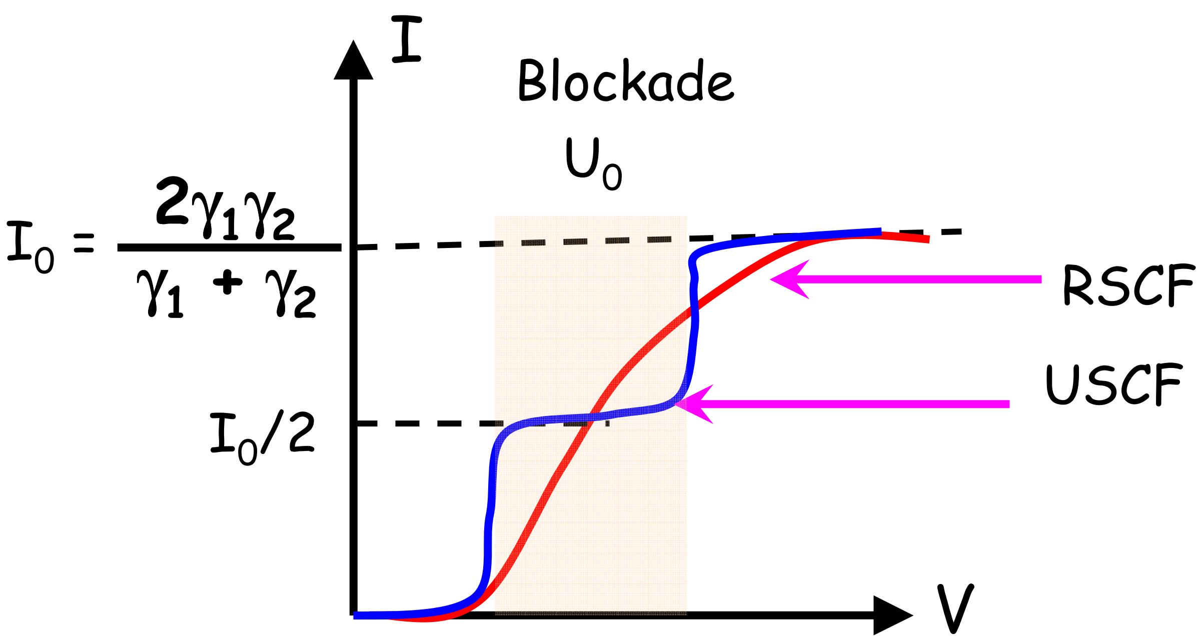


$$I_1 = q\frac{\gamma_1}{\hbar}[f_1 - N]$$

$$I_2 = q\frac{\gamma_2}{\hbar}[N - f_2]$$

$$U_\uparrow = U_L + U_0(N_\downarrow - N_0/2)$$

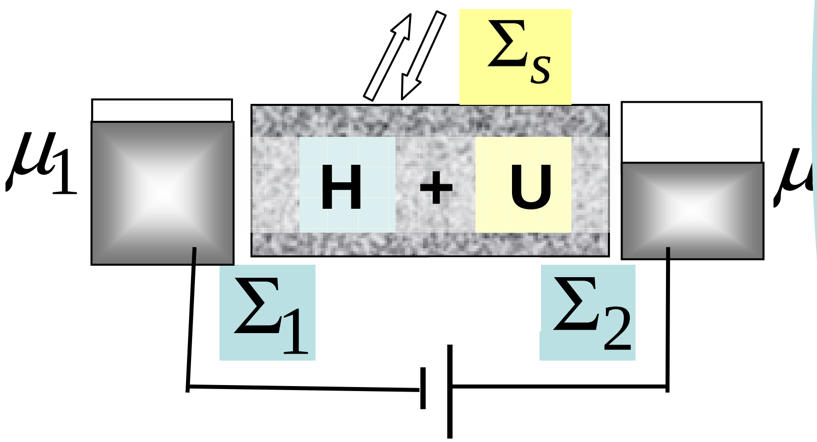
$$U_\downarrow = U_L + U_0(N_\uparrow - N_0/2)$$



Details incorrect!

Hilbert space to Fock space

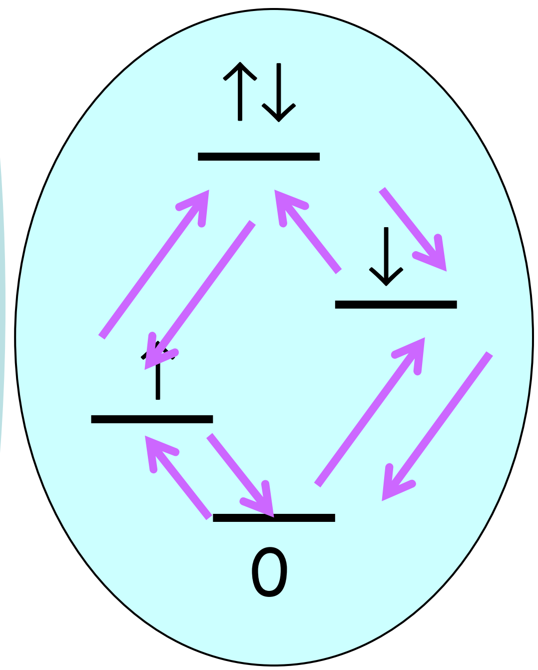
N one-electron levels



Works for $\Gamma \geq U$

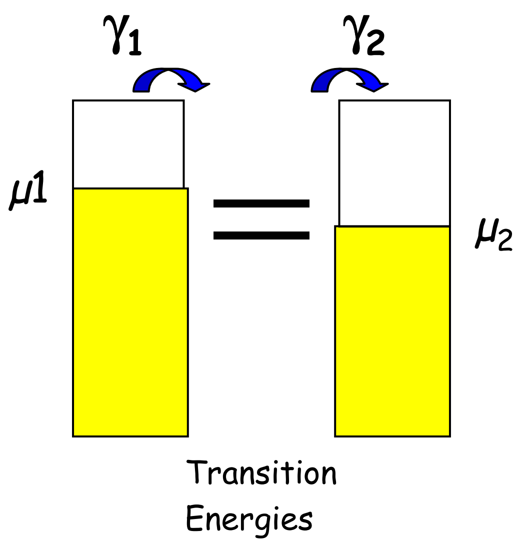
Fine str
constant
e^2/hv
$= U/\Gamma$
~ 1

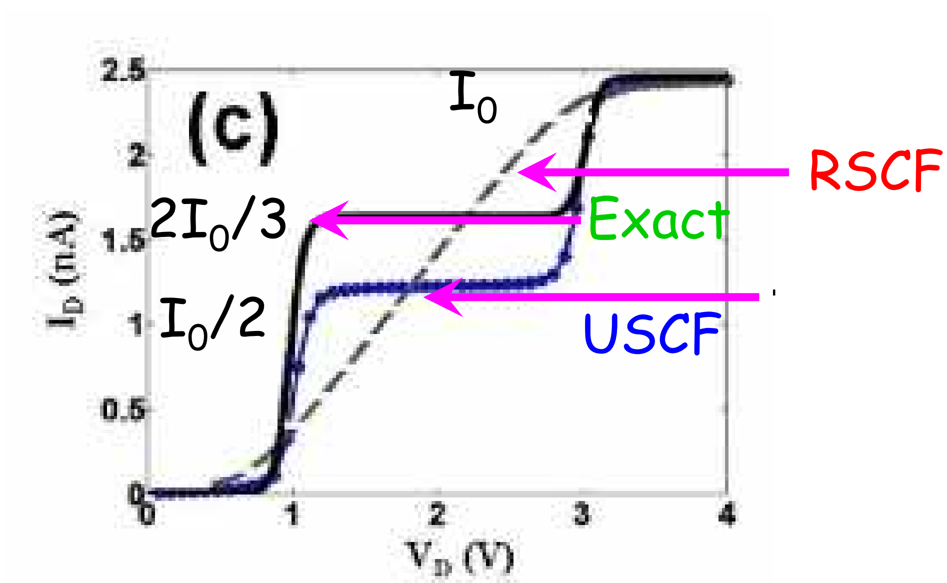
N many electron levels

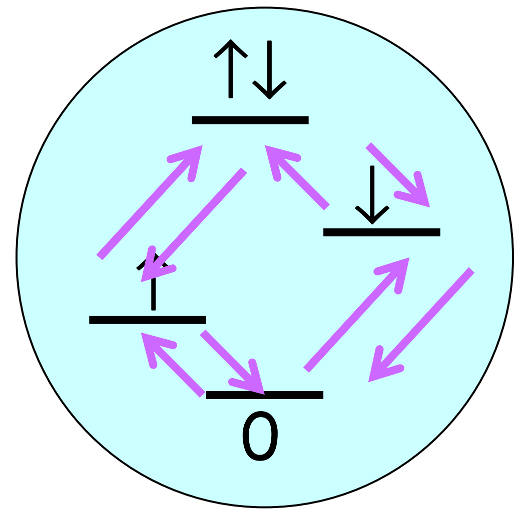


Works for $\Gamma << U$

Exact Result



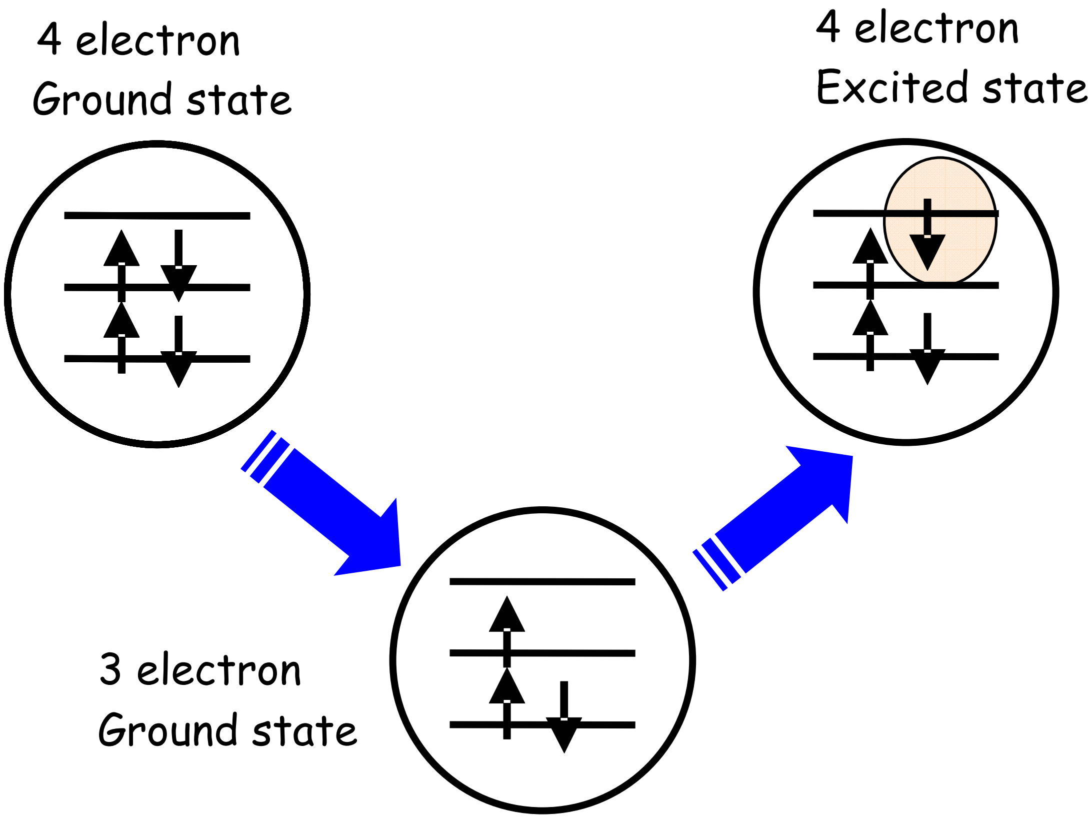




Muralidharan, Ghosh, Datta
PRB '06

Spins don't carry equal current !!
What works for equilibrium may not work for nonequilibrium

Excitations

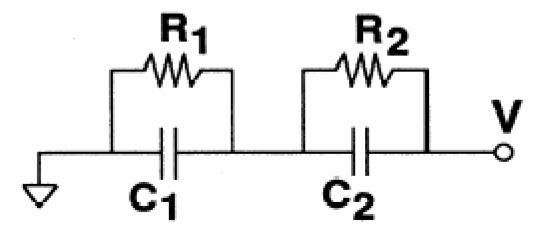


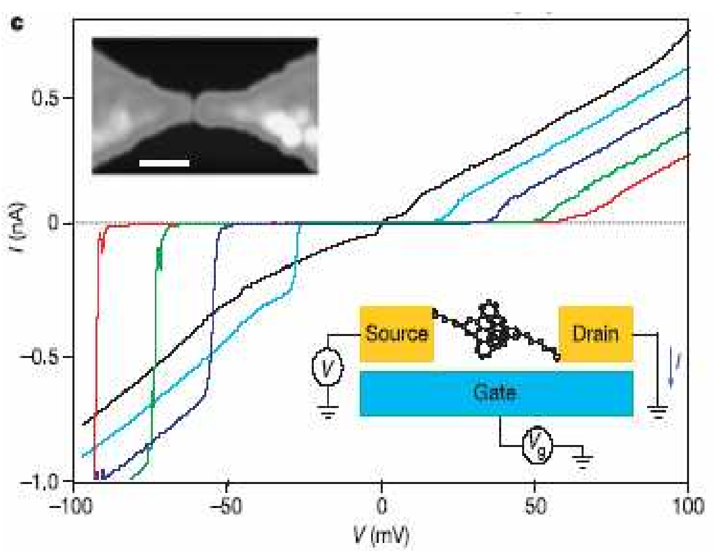
Can reorganize charge at little extra cost

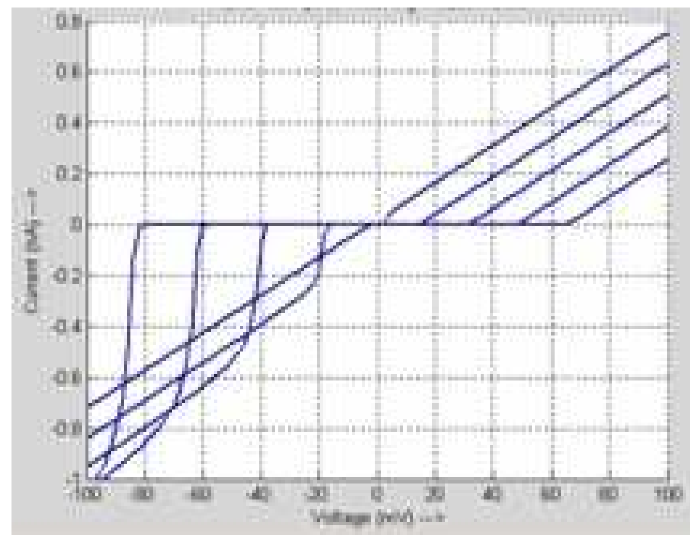
Must work in $2^N \times 2^N$ configuration space

Incoherent sum over excitations

"Orthodox" Theory
(Likharev)



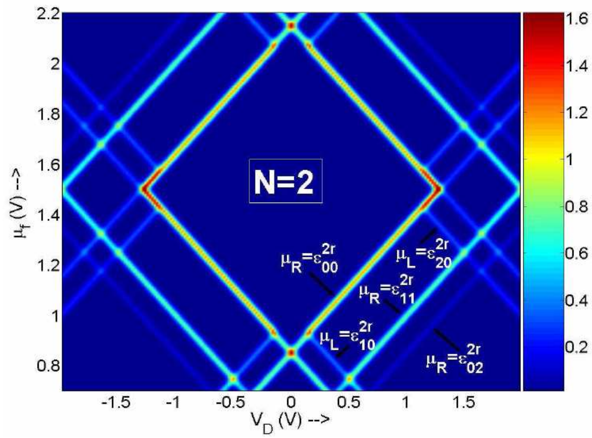




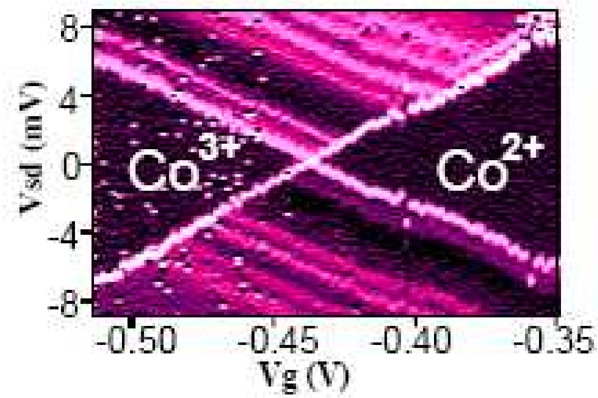
Expt.: Ralph group
(Nature '02)

Theory:
Muralidharan, Miller, Kapoor, Ghosh

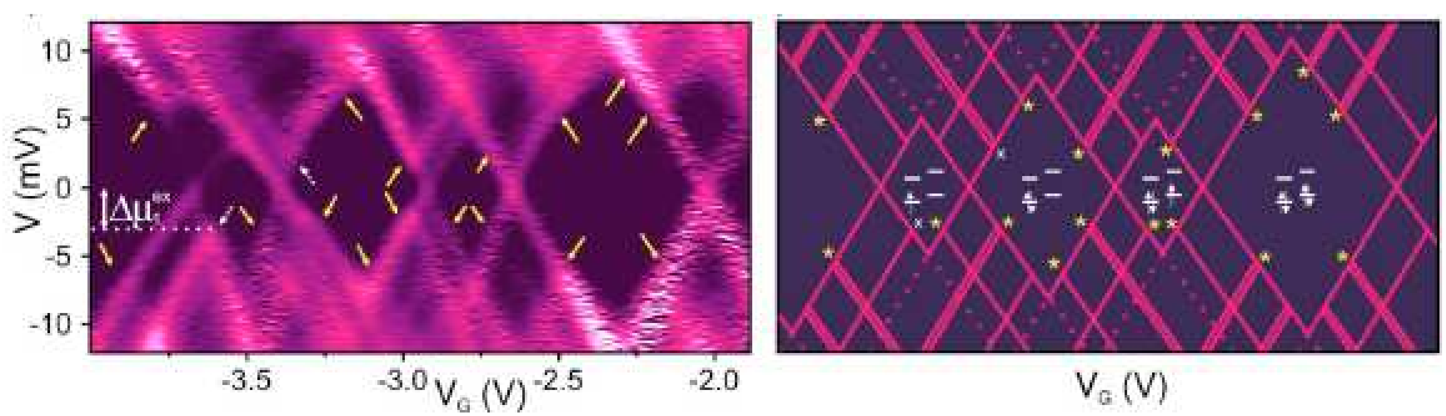
Resolvable excitations



Theory, double dot
Muralidharan, Ghosh, Datta

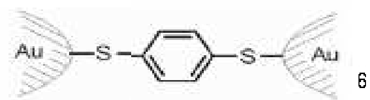


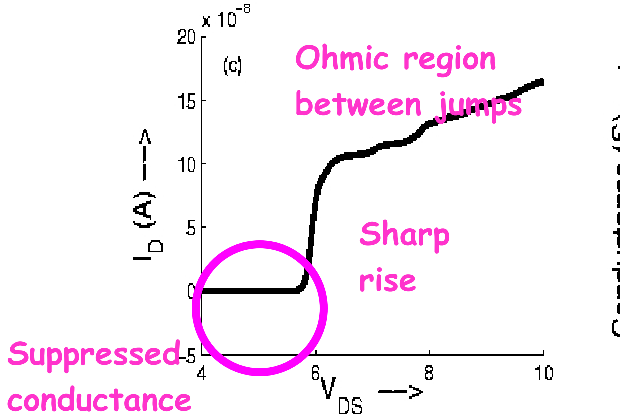
Ralph group
nanoclusters

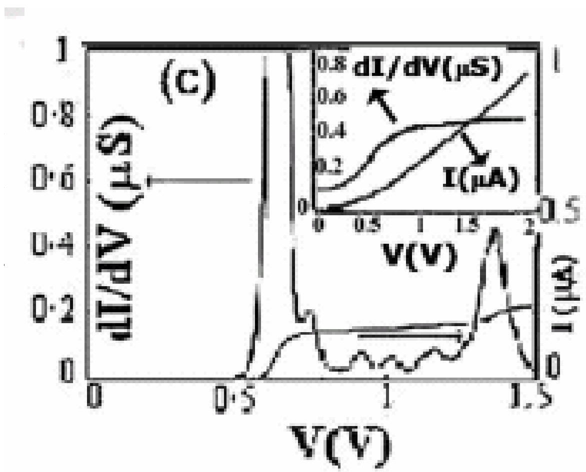


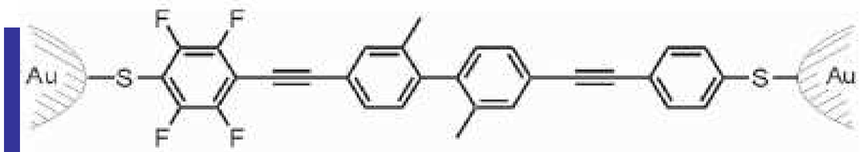
Dekker group, nanotubes

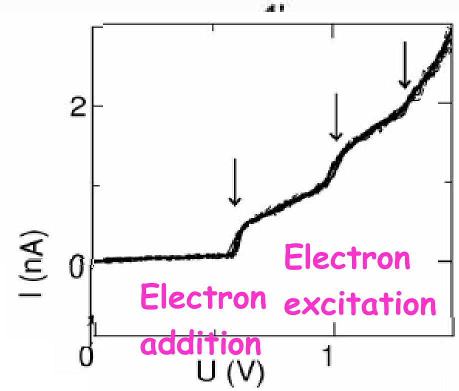
Non-equilibrium excitations

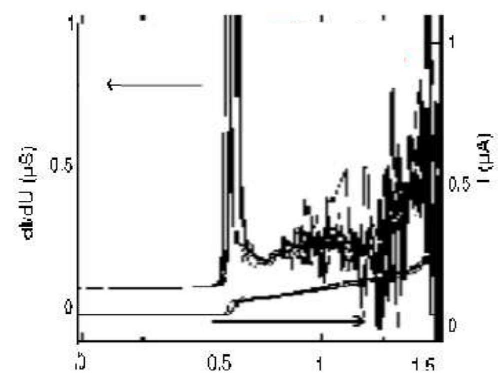












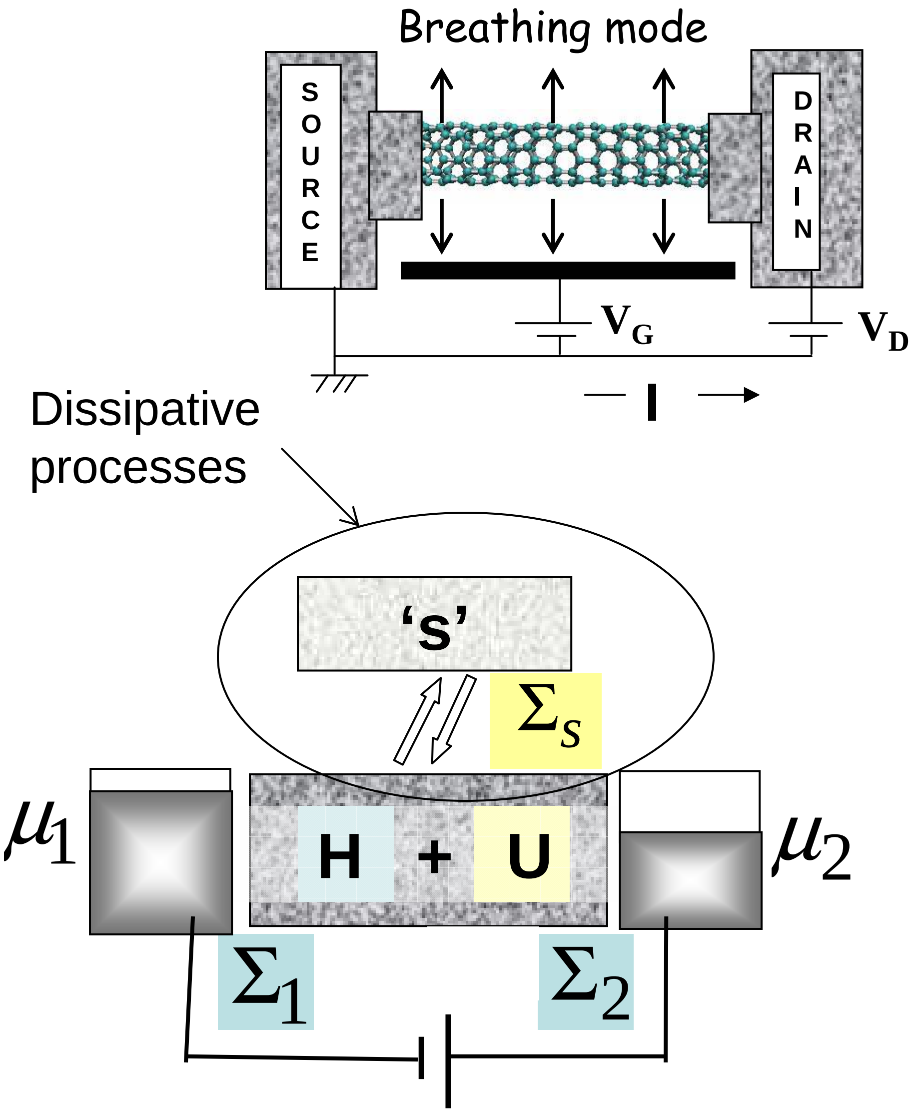
THEORY

(Muralidharan, Ghosh, Datta PRB '06)

EXPT (Reichert et al, APL '03)

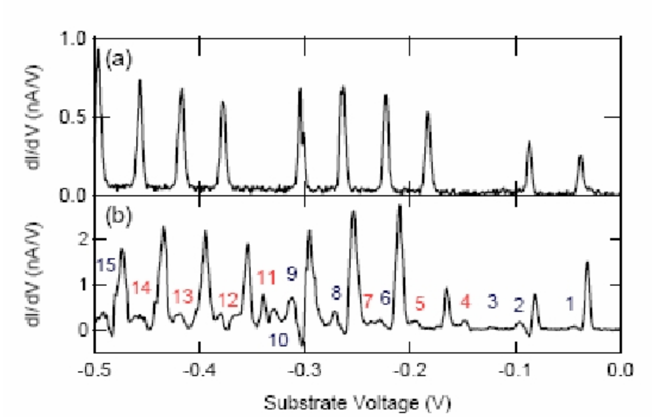
Short molecules are quantum dots

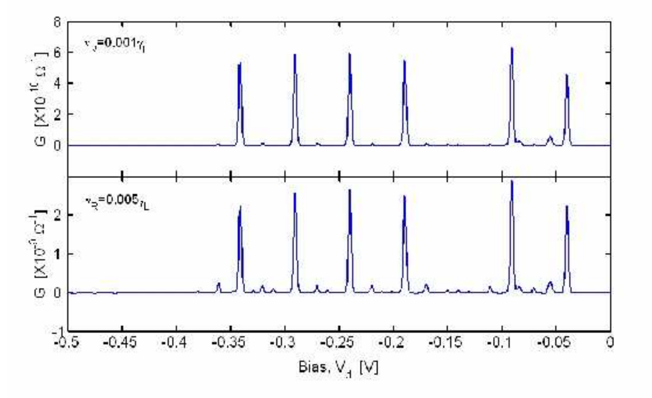
El-phonon correlation



Unified Model

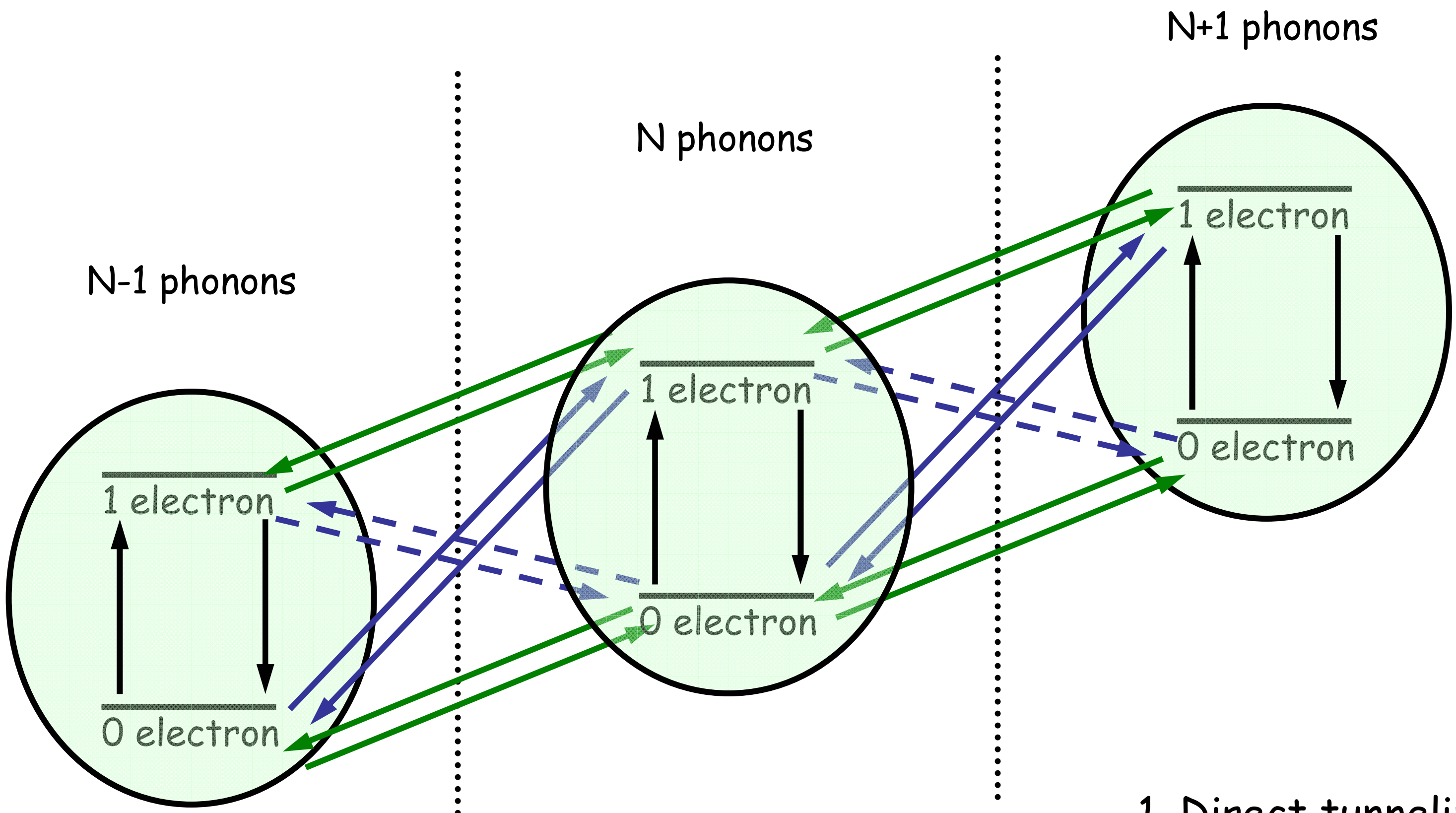
Expt. Dekker group





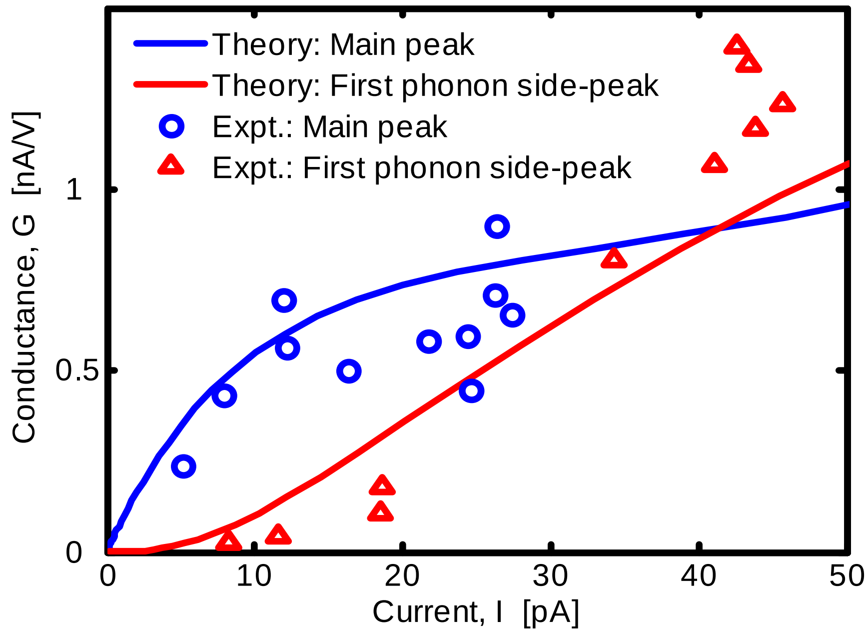
Theory Siddiqui, Ghosh, Datta

Fock space NEGF

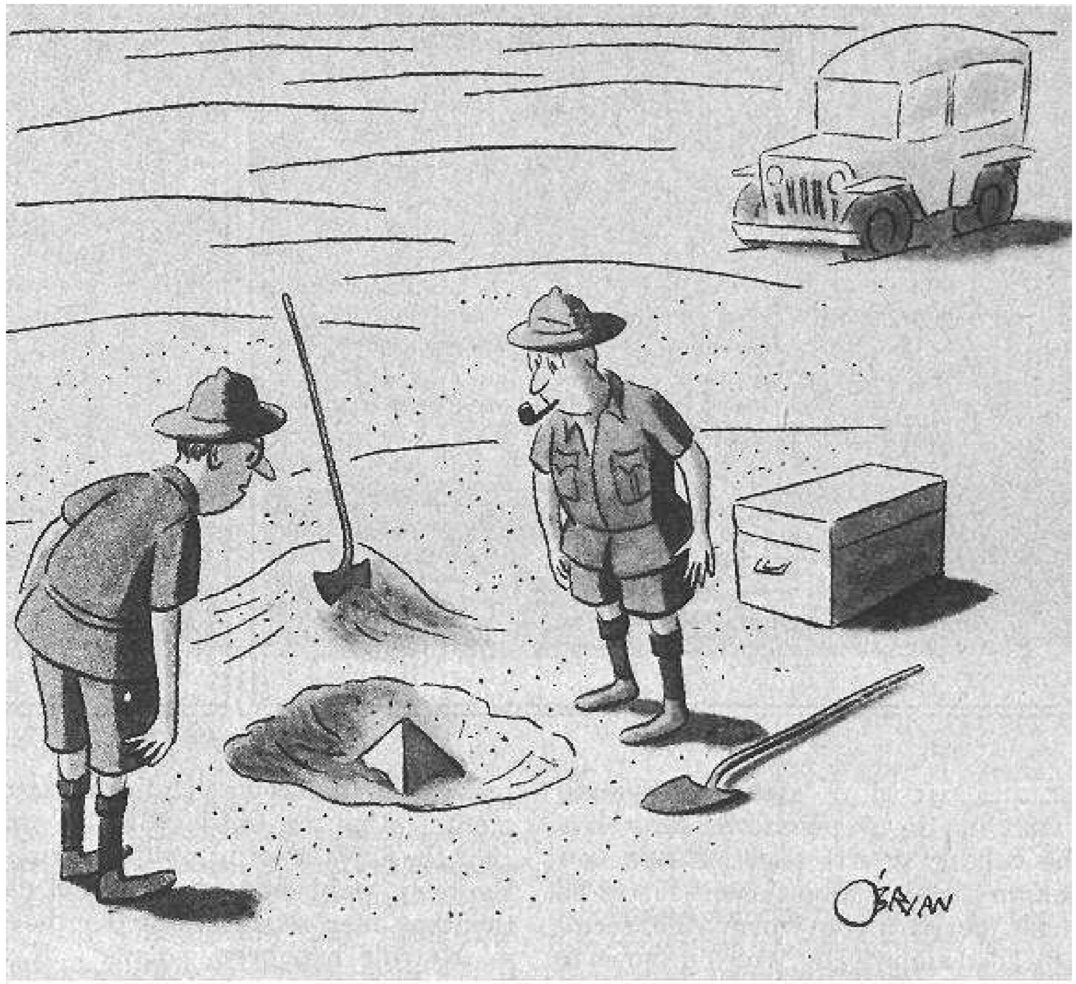


1. Direct tunneling
2. Phonon-assisted tunn.
3. Phonon bath

Semi-quantitative analysis of spectral signatures

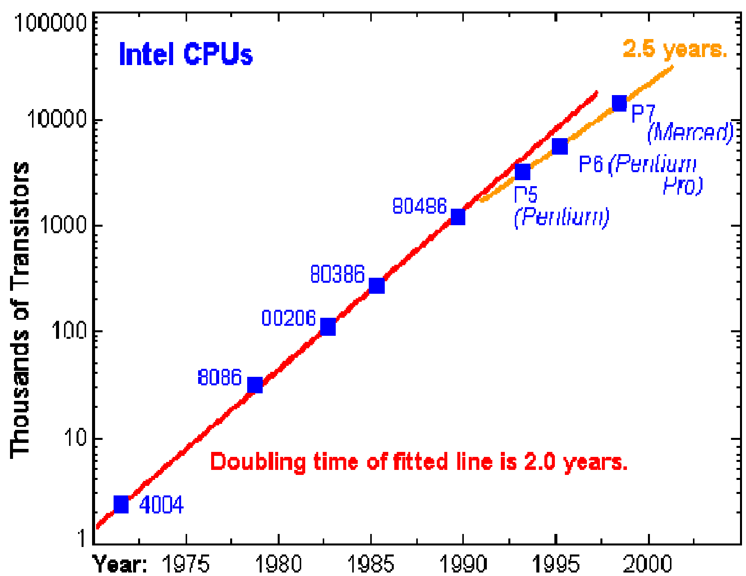


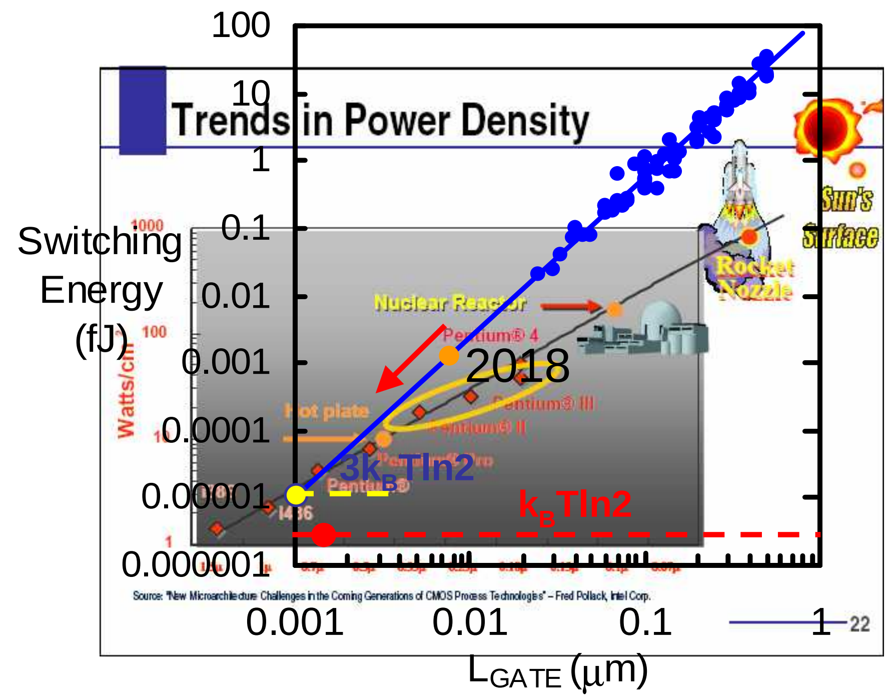
- Phonons are 'Hot' (anomalous T-dependence)
- Phonons are incoherent and correlated
- Standard PAT theory (Tien-Gordon) doesn't work



"This could be the discovery of the century. Depending, of course, on how far down it goes."

Search for new state variables





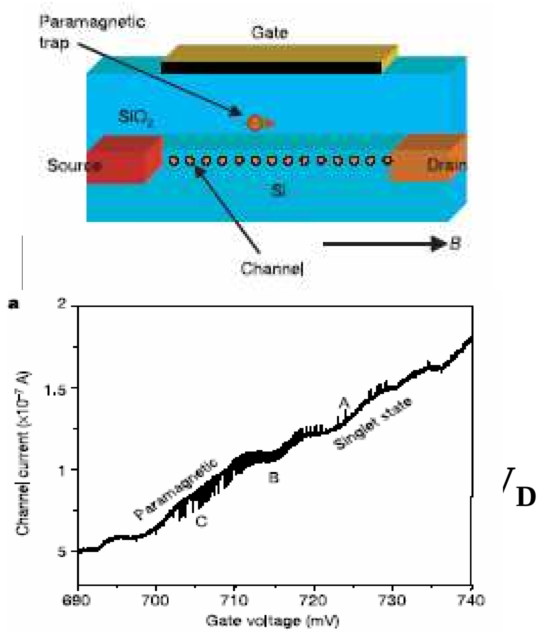
Scaling of transistor density
(Moore's Law)

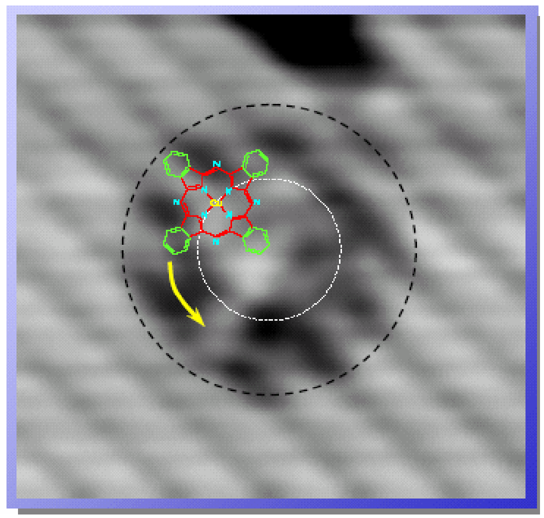
Present day CMOS
$E = 10^4 k_B T$

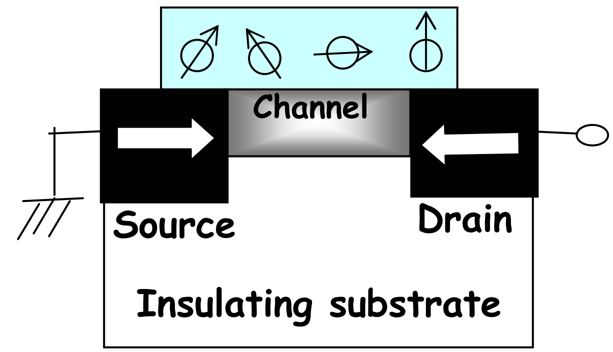
Scaling of energy
Single electron operation
$E = 3k_B T\ln 2$

Novel non-charge based computation
(Dynamic switching, interacting systems)

Coupling FETs with molecular variables







S. Datta, APL '05

Charge Coupling

(Characterization)

Vibronic Coupling

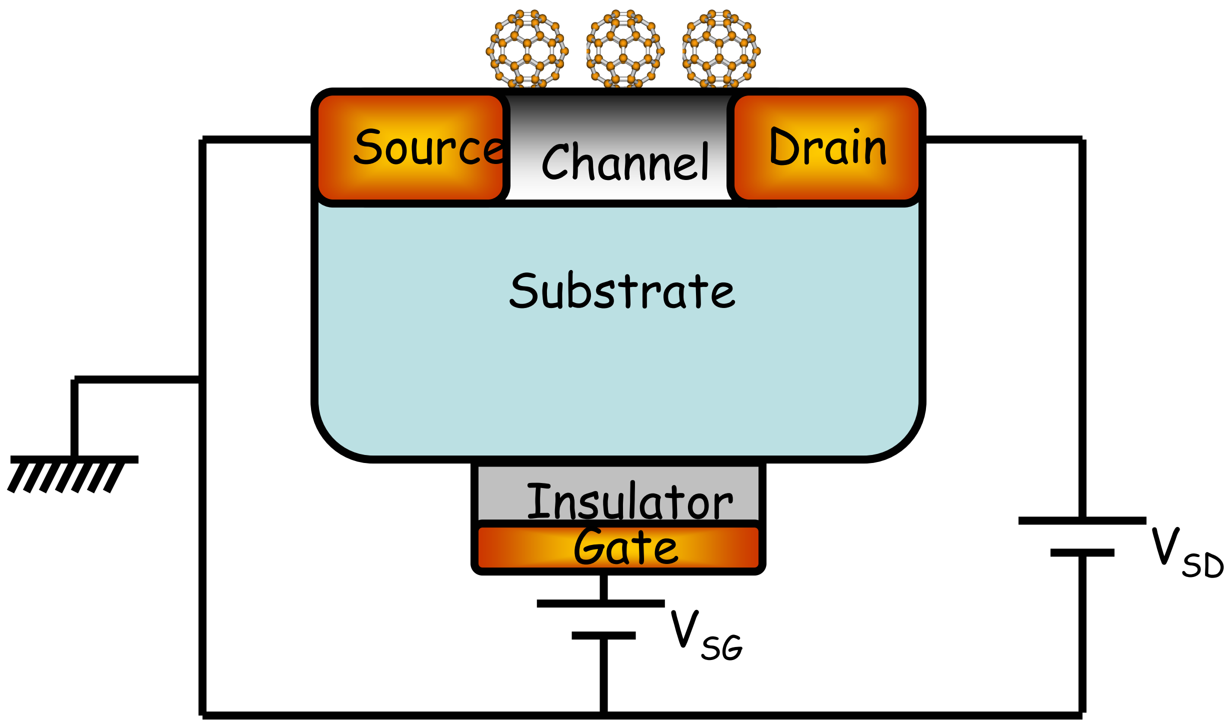
(Heat sinking,

ratchets/motors)

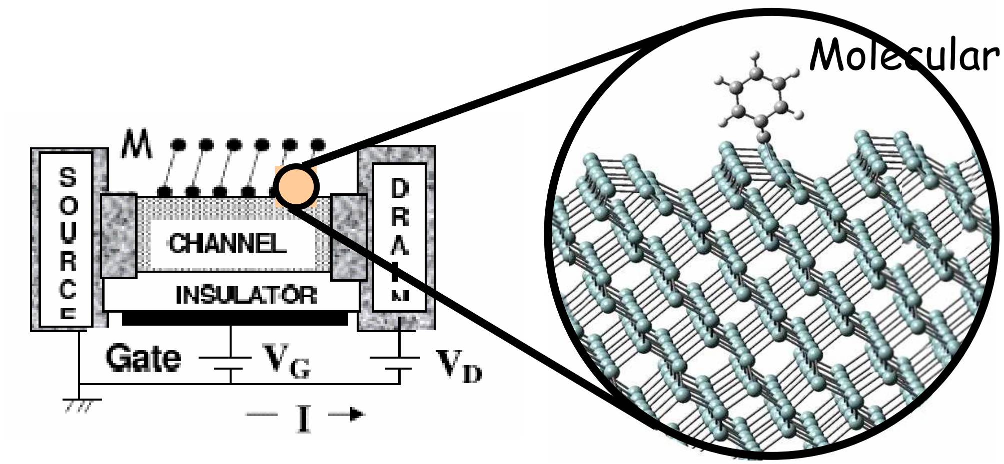
Spin Coupling

Molecular NVM

Combining dimensions: dots and wires

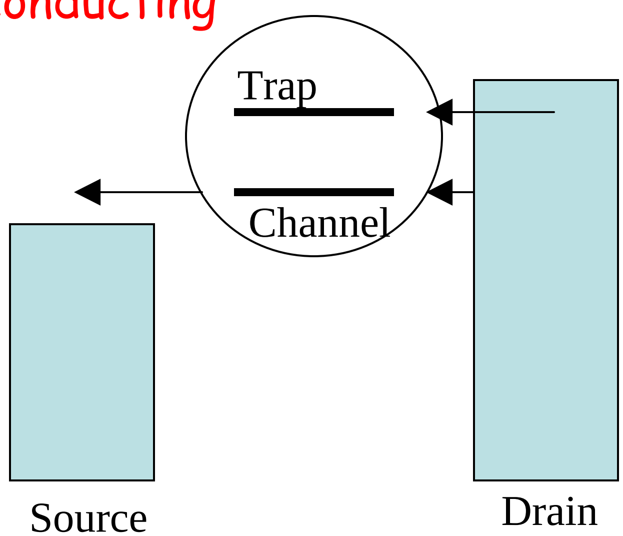


Trap-channel correlation

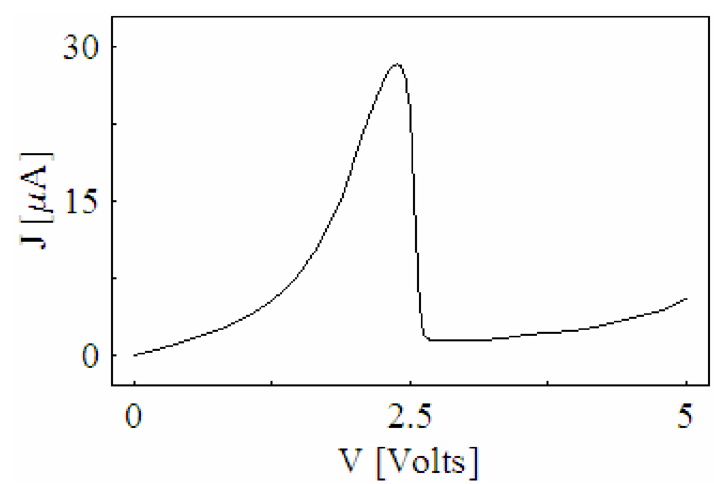


Molecules create localized 'trap' centers in silicon

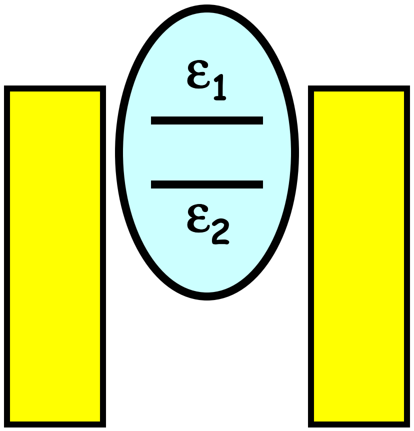
A trapped electron blocks channel from conducting

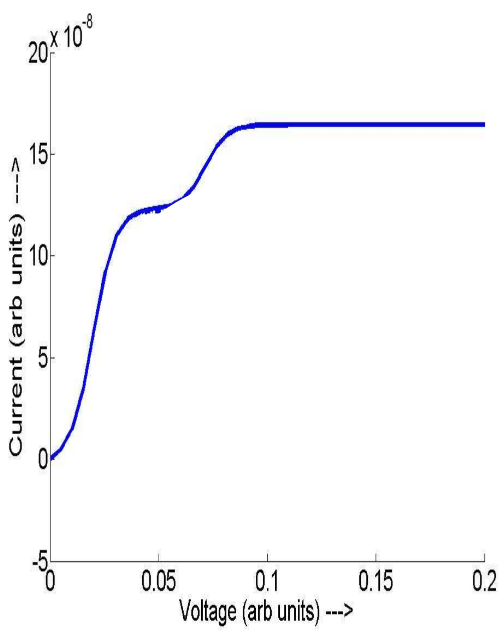


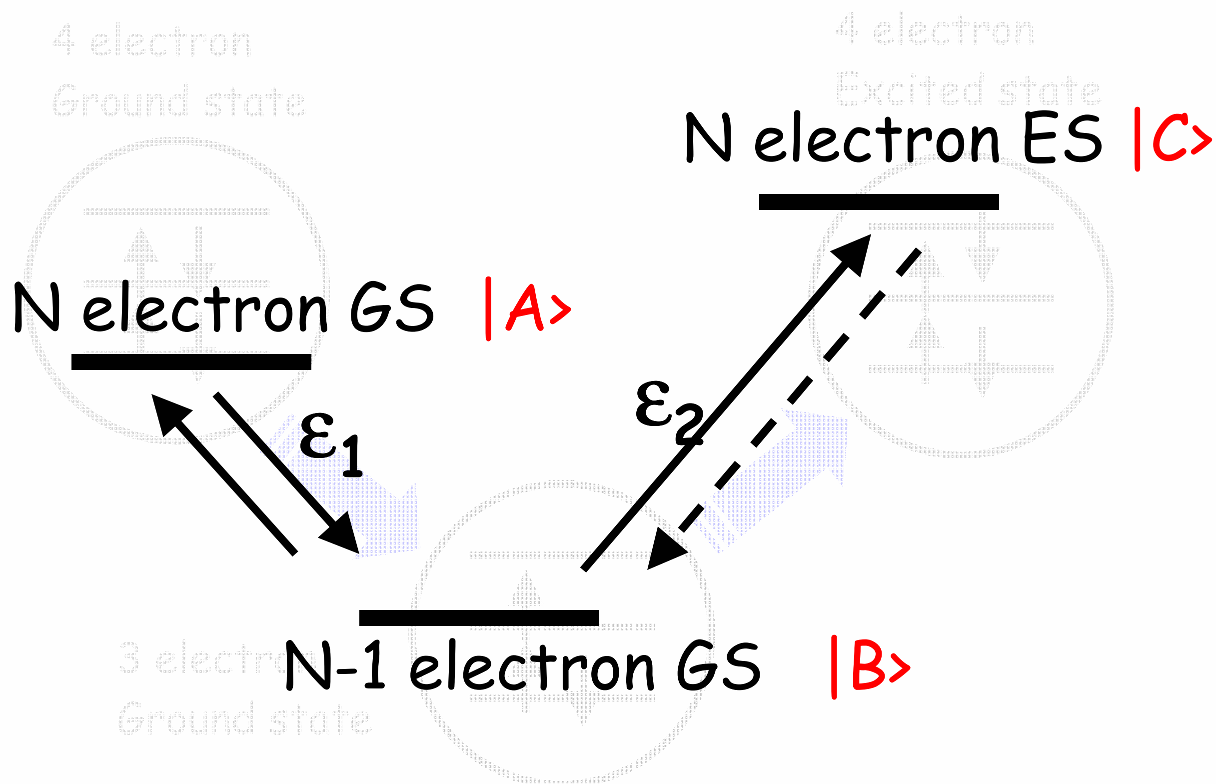
Eviction of channel level from conduction window creates NDR



Understanding NDR in terms of state filling



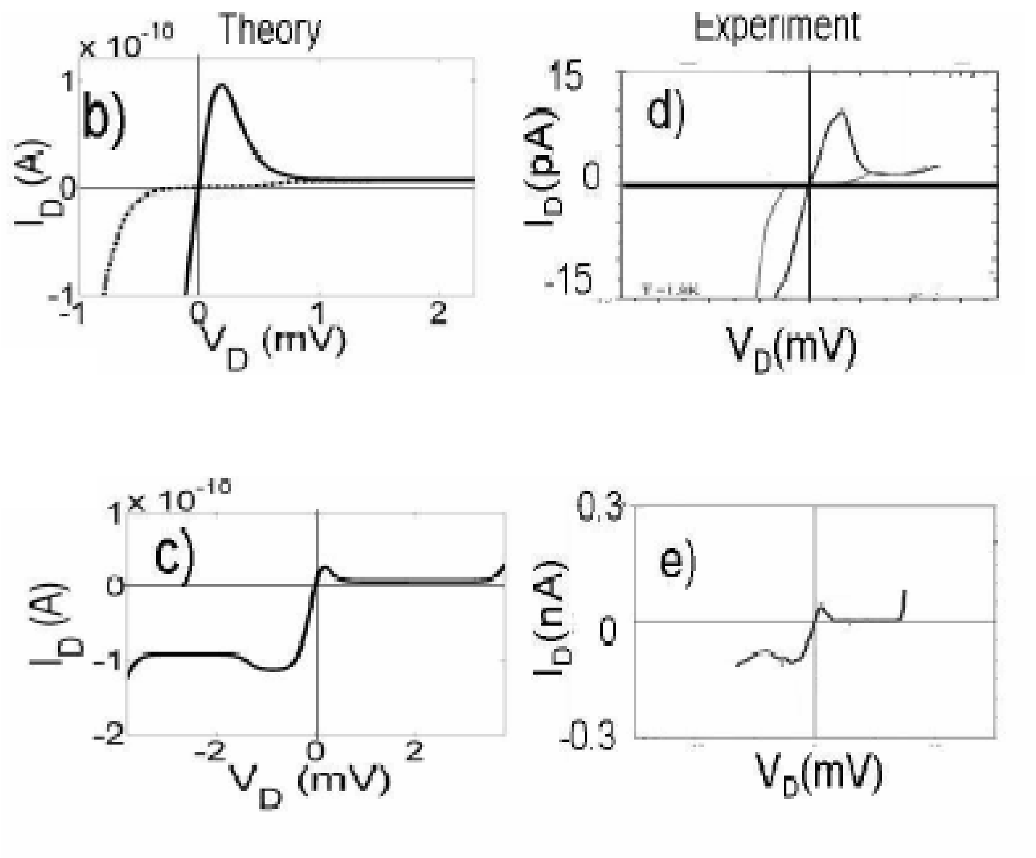




'Dark' state emptied slowly compared to other transitions in the system

$$t^{R}_{CB} > t^{R}_{AB}$$

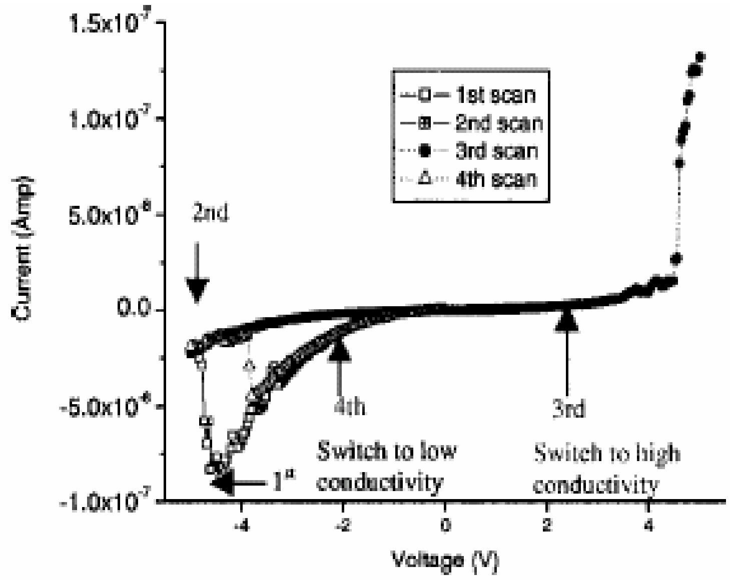
Pauli Spin Blockade



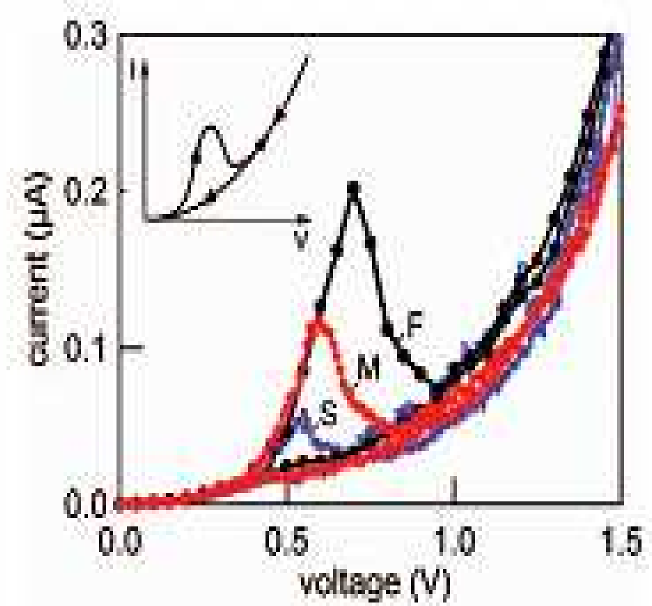
Theory
(Muralidharan, Datta)

Experiments
(Tarucha et al)

Hysteresis



Harriott group, UVA
(Switching with memory)



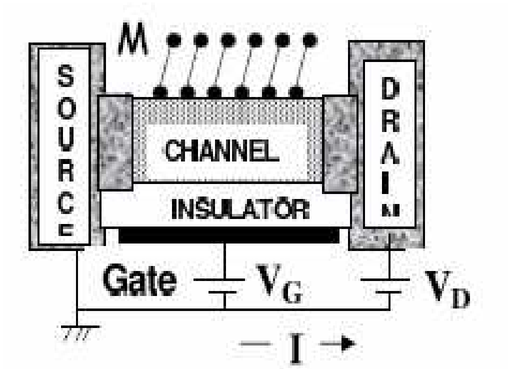
Kiehl group, Minnesota
(sweep rate dependence)

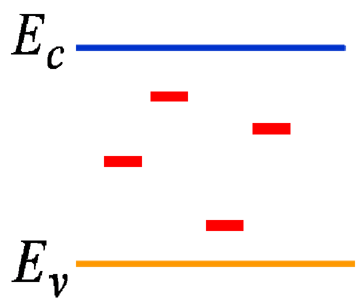
Voltage swept faster than trap escape time

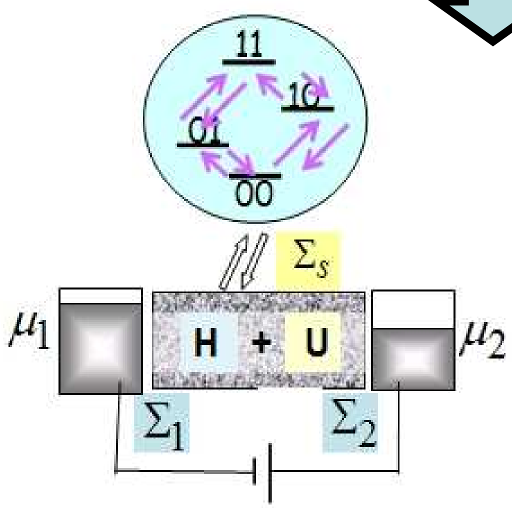
Time-dependent correlated scattering

Sweep faster than escape time for time-resolved experiments

Stochastic filling/emptying of trap creates 2-state random noise



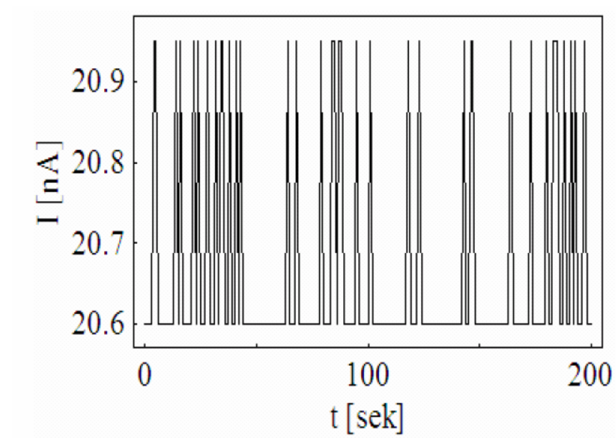




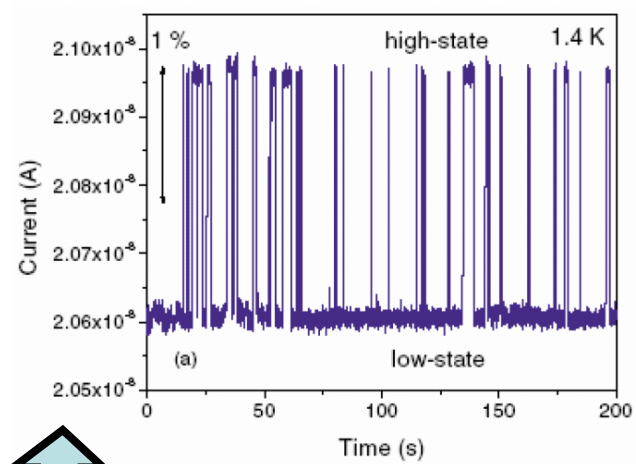
Rate equations for dot

NEGF equations for channel

Theory



Expt



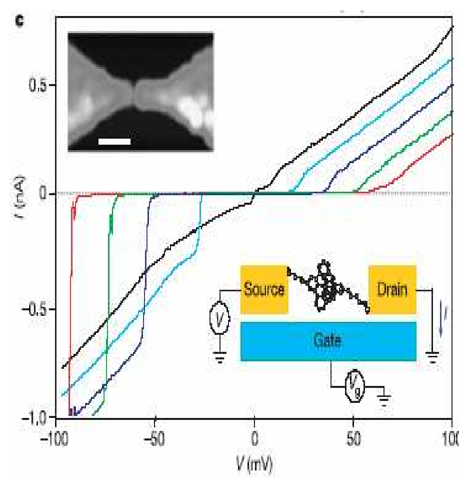
Summary

Unified treatment of conduction

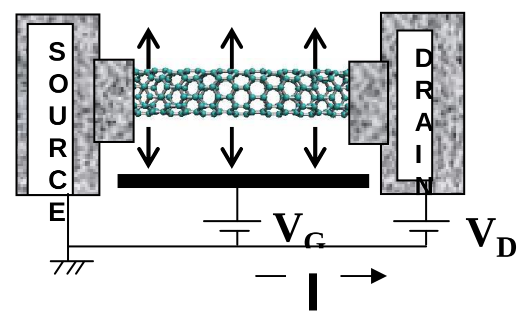
Quantitative Benchmarking

Hybrid systems

Strong Coupling



Coulomb Blockade



"Hot" Phonons

Technology of the future will need understanding that is atomistic and interdisciplinary