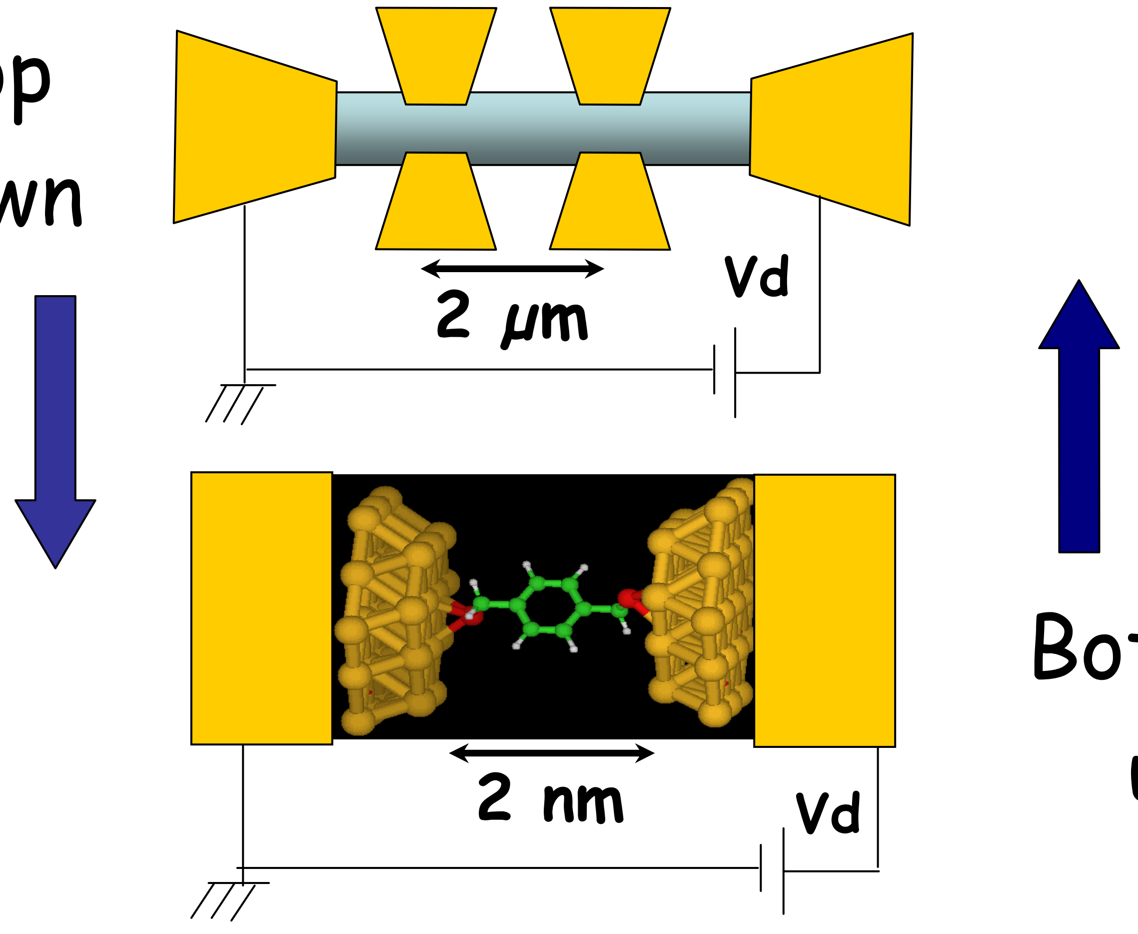
Understanding Nanoscale Conduction

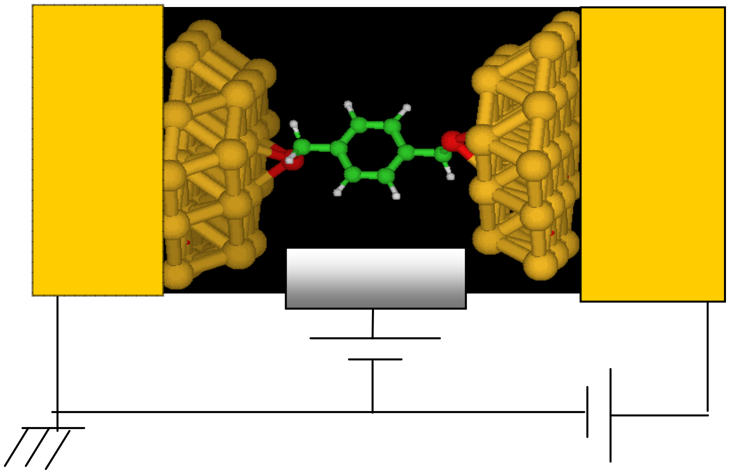
ISLPED'04

Top Down



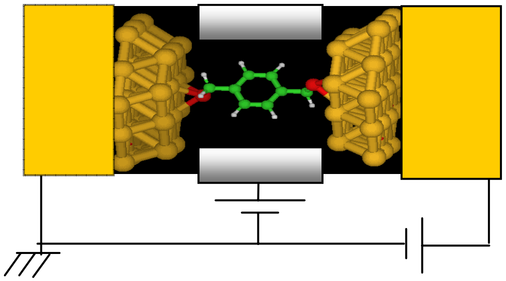
Bottom up

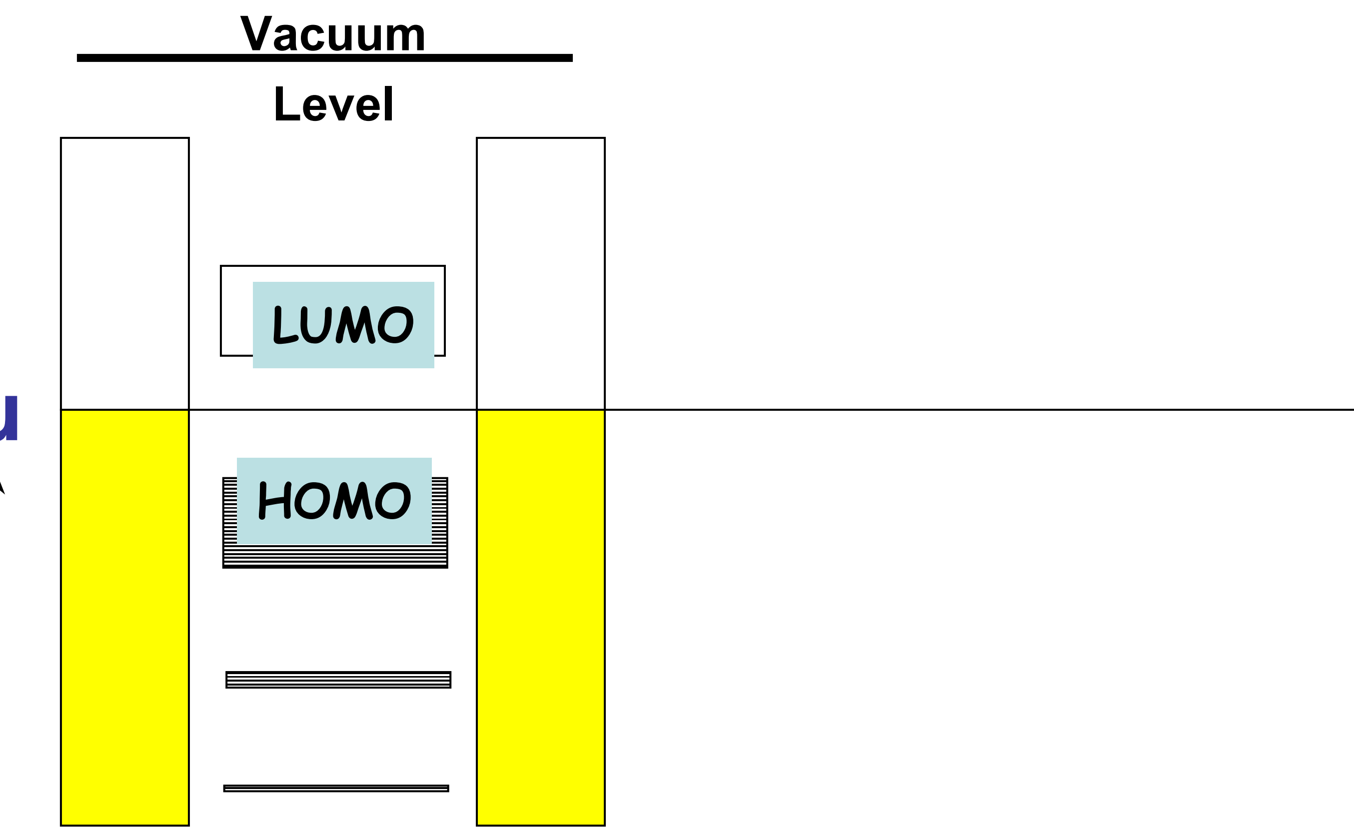
Outline



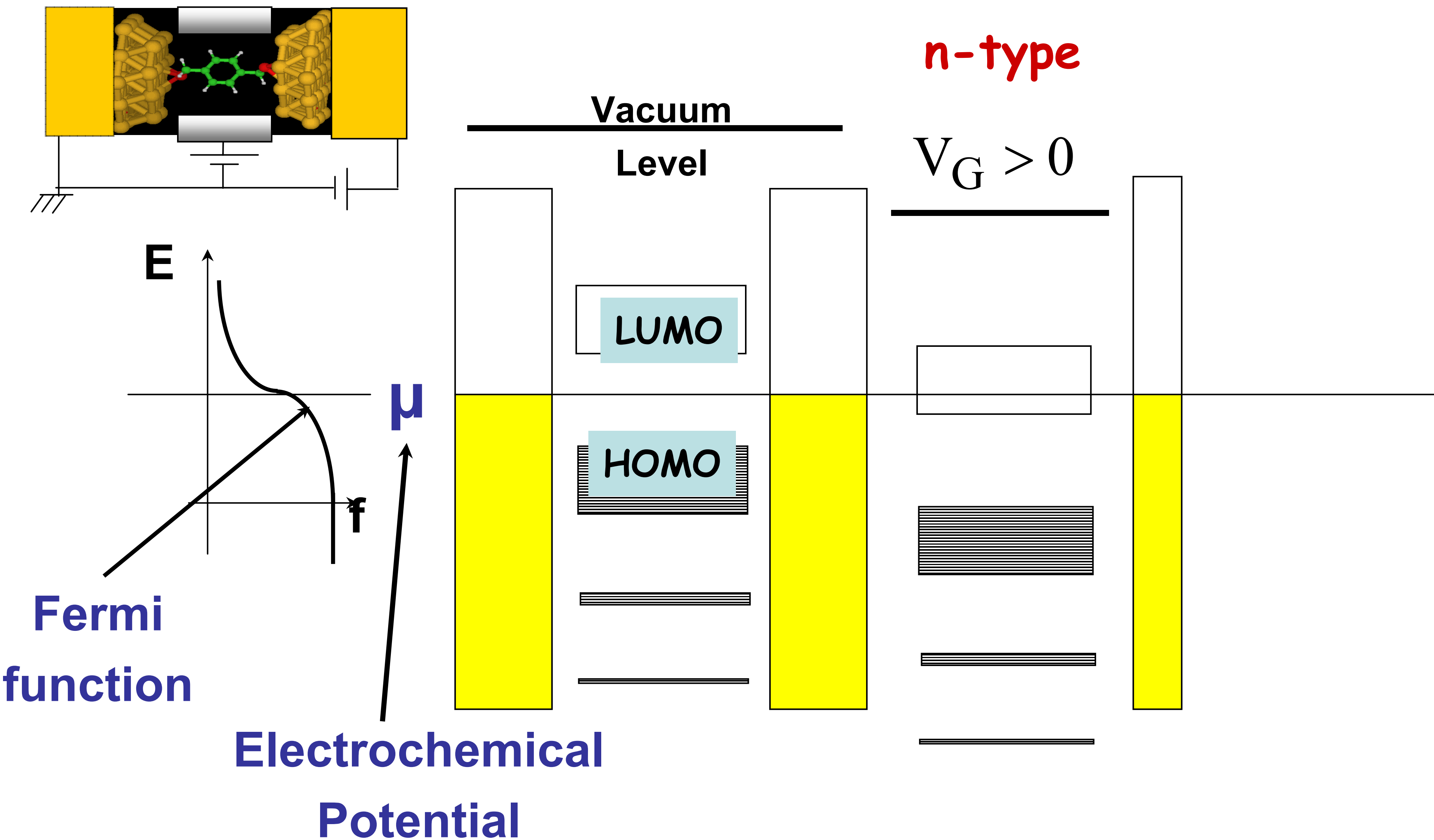
- Qualitative picture
- Quantitative models
- Examples
- Coulomb blockade
- Summary/Open questions

"Band-Diagram"

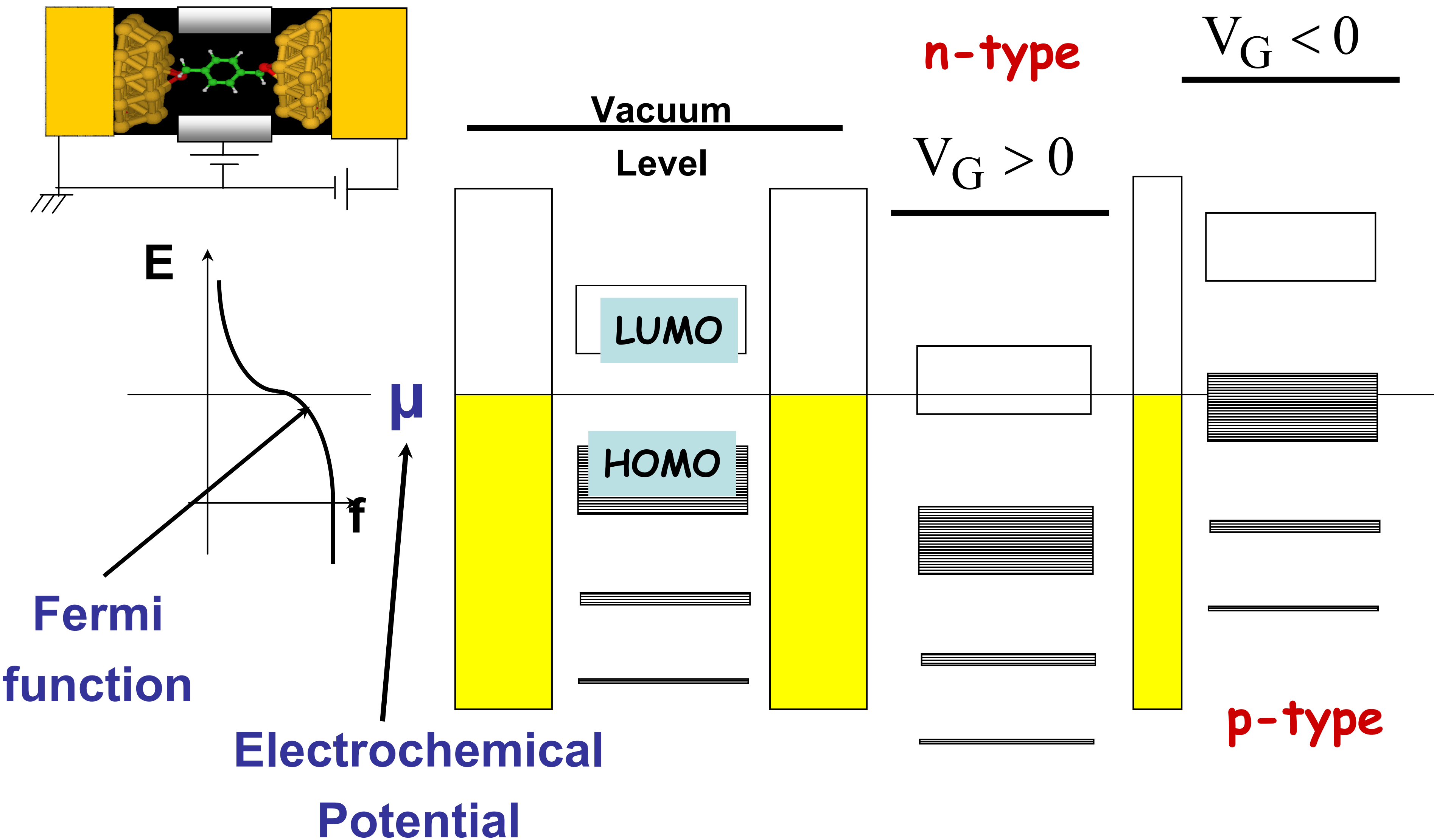




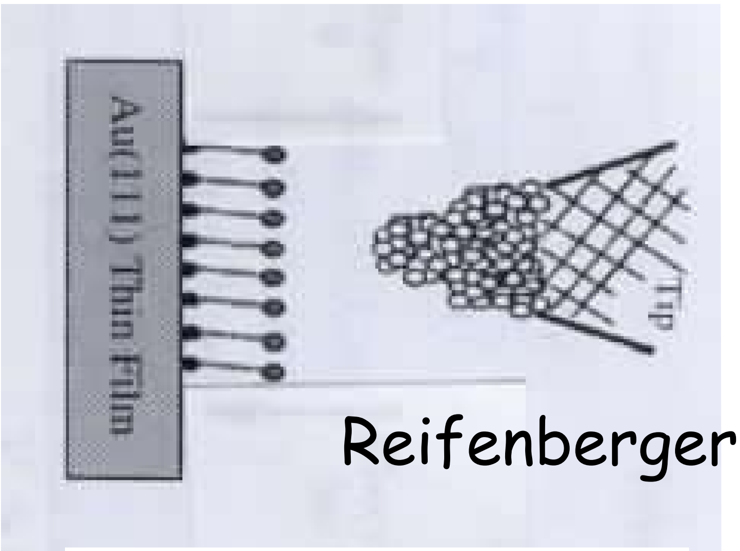
"Band-Diagram"

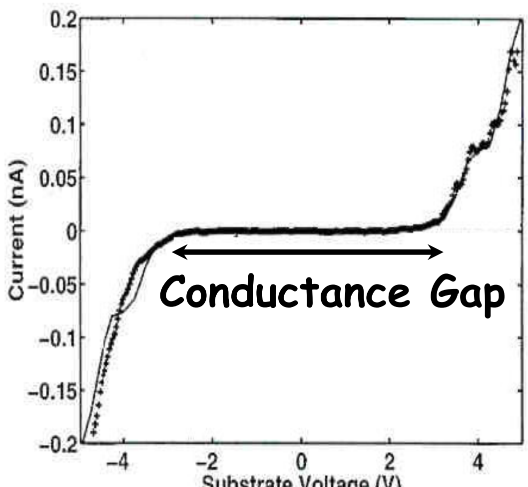


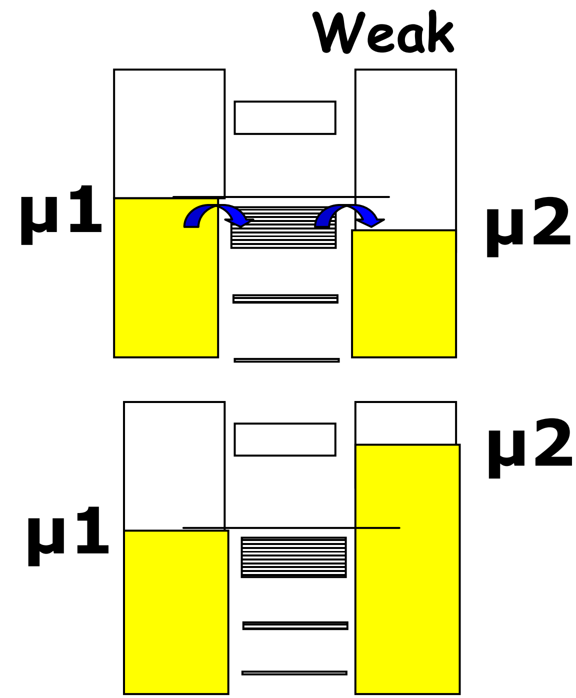
"Band-Diagram"

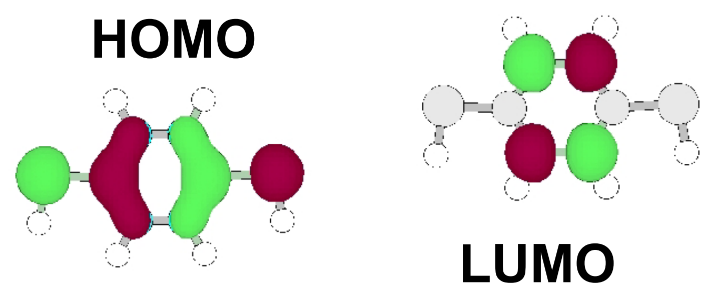


Conductance Gap = ???

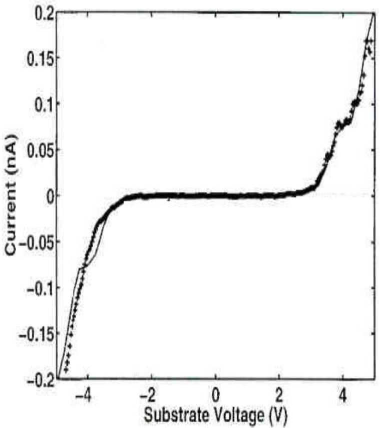






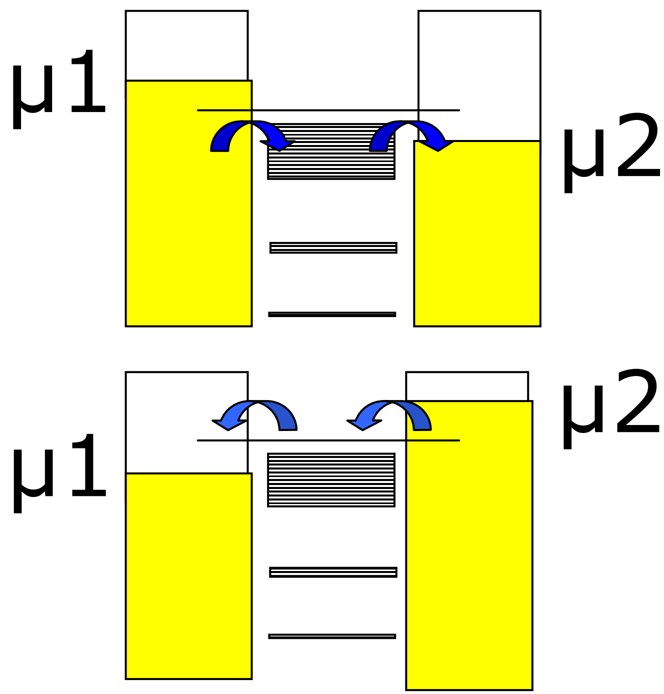


Conductance Gap = ???

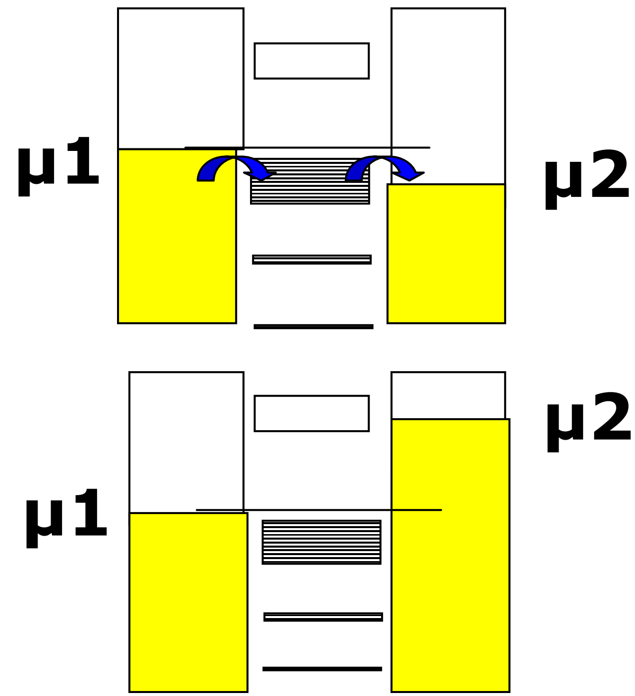


PRL 1997

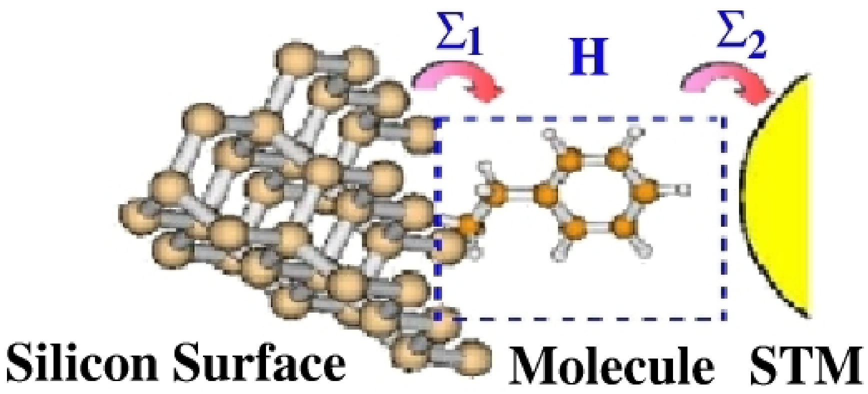
Levels move	Levels fixed
4 * (Ef - HOMO)	**LUMO - HOMO**



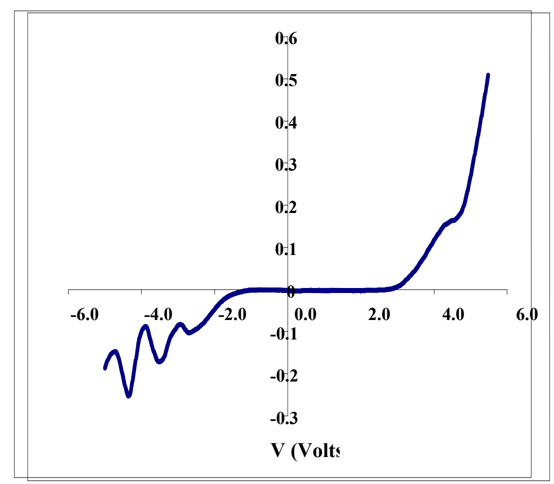
Weak

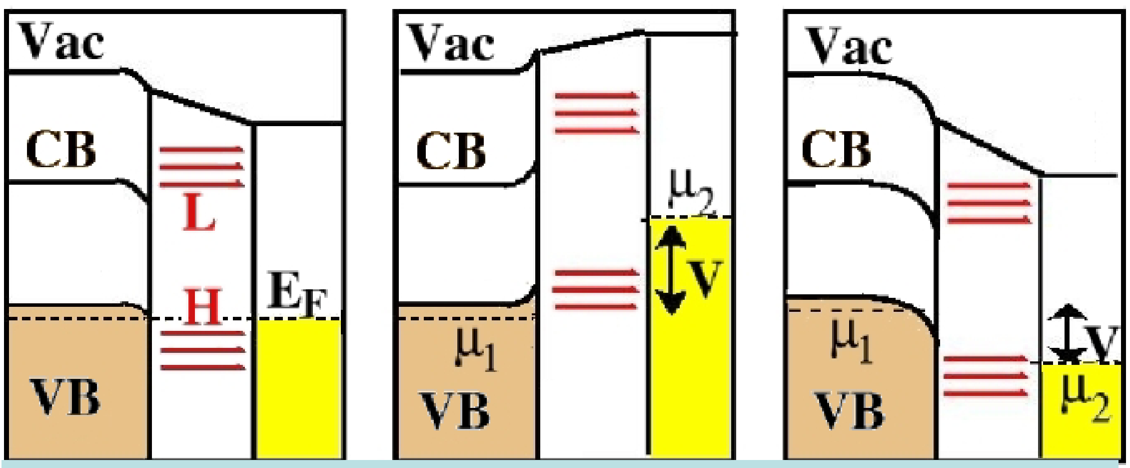


Molecular devices on silicon



Expt: Mark Hersam
Nanoletters, 01/04
Cover story

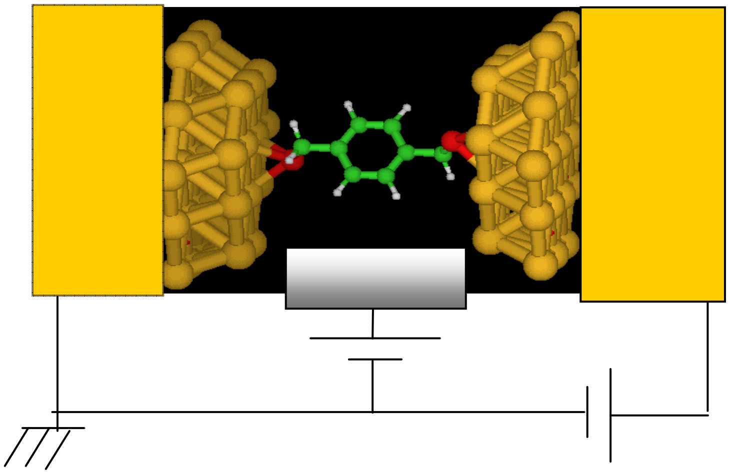




(a) V = 0 (b) V < 0 (c) V > 0

Room temperature

Outline



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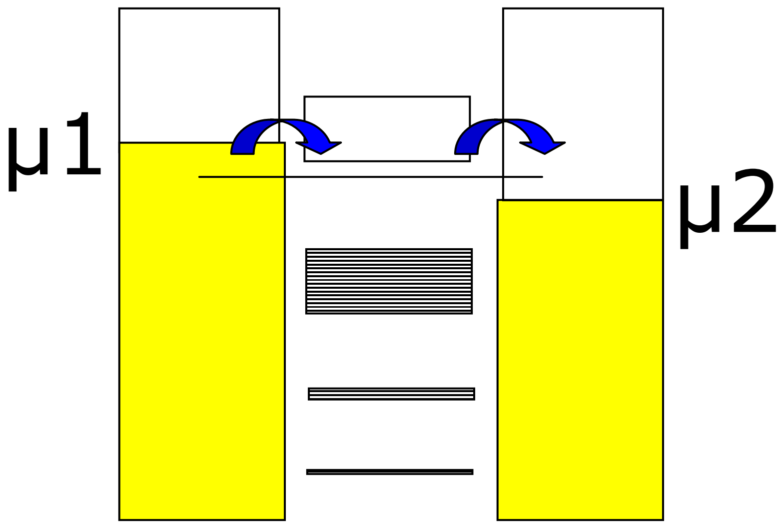
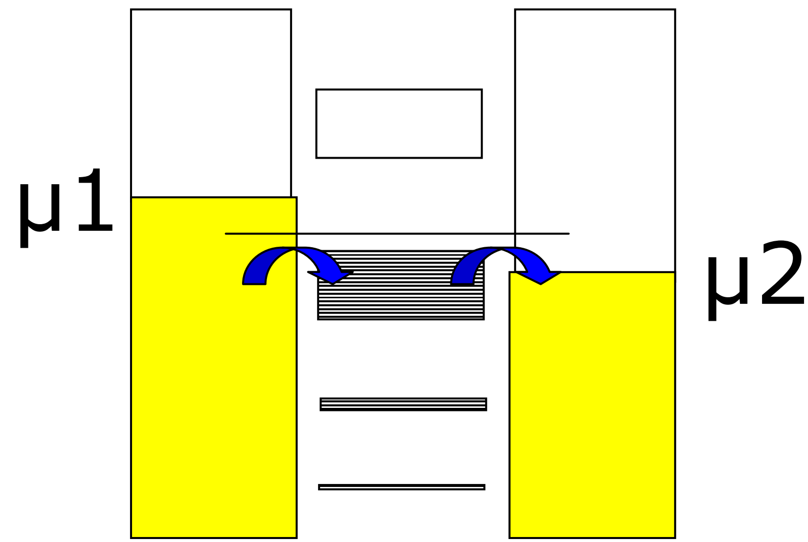
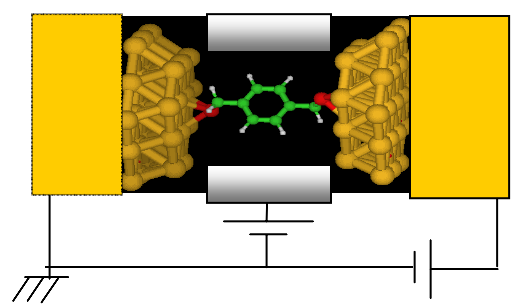
What makes electrons flow?



LUMO (n-type)
Conduction



HOMO (p- type)
Conduction

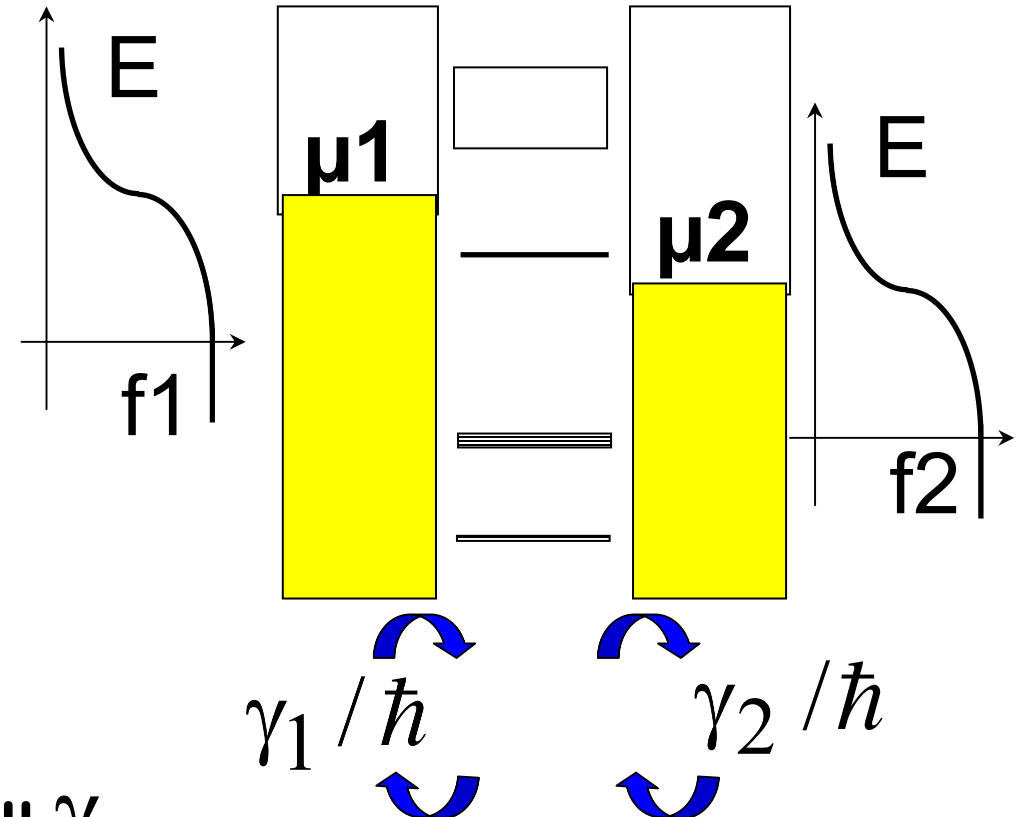


Toy model: Escape time

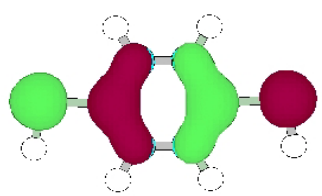
$$I_1 = q\frac{\gamma_1}{\hbar}[f_1 - N]$$

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

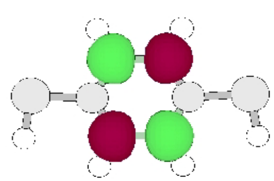
$$I = \frac{q}{\hbar}\frac{\gamma_1\gamma_2}{\gamma_1 + \gamma_2}[f_1 - f_2]$$



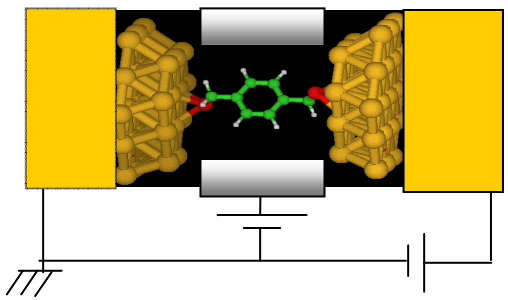
Large γ

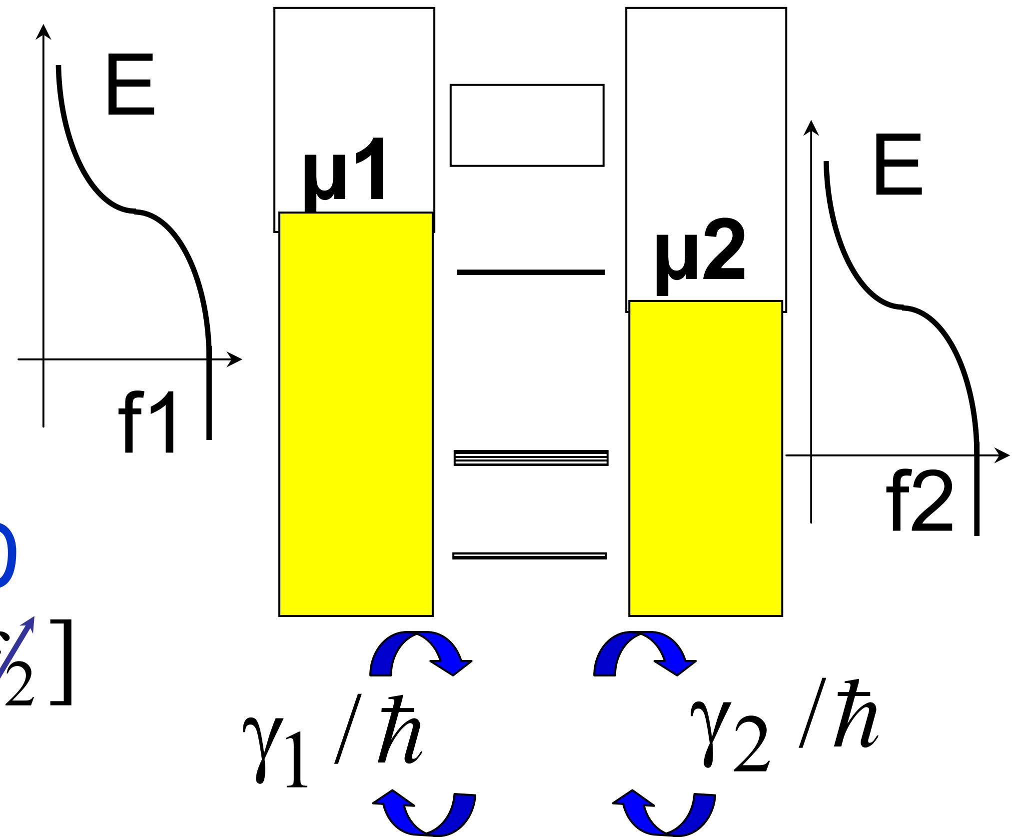


Small γ



Toy model: Max. G ?



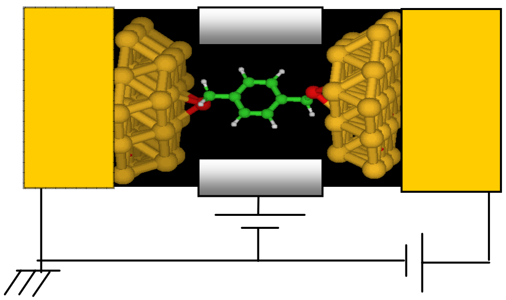


1 - 0

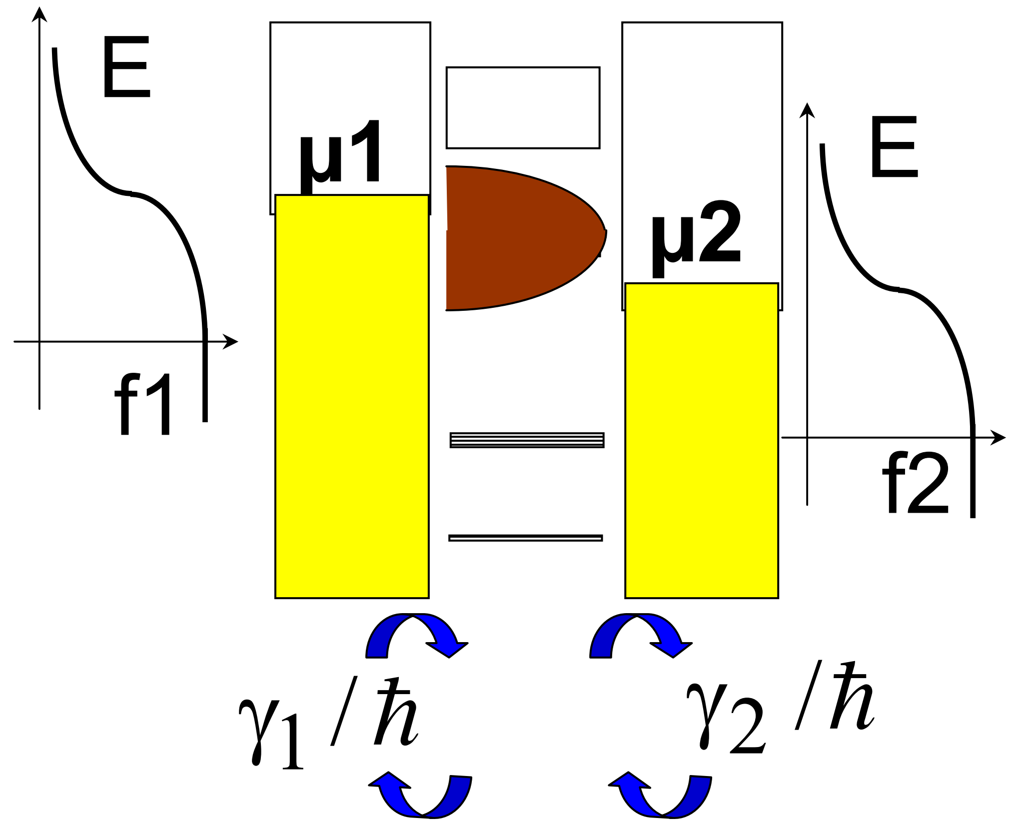
$$I = \frac{q}{\hbar} \frac{\gamma_1 \gamma_2}{\gamma_1 + \gamma_2} [f_1 - f_2]$$

$$\sim \frac{q}{2\hbar} \gamma$$

Toy model: Broadening



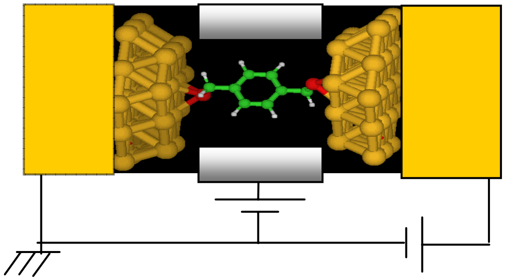
$$I \sim \frac{q\gamma}{2\hbar}\frac{qV}{\gamma}$$



Maximum conductance

$$\frac{I}{V} \sim q^2/h \sim \frac{1}{25.8\,K\Omega}$$

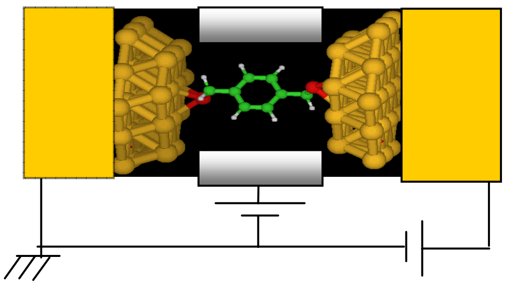
Broadening



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

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

Broadening

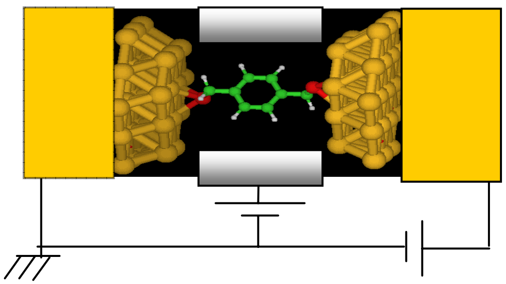


$$N = \int dE\, D(E-U)\left[\frac{\gamma_1 f_1 + \gamma_2 f_2}{\gamma_1 + \gamma_2}\right]$$

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

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

Broadening + Charging



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

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

"Poisson"

N --> U

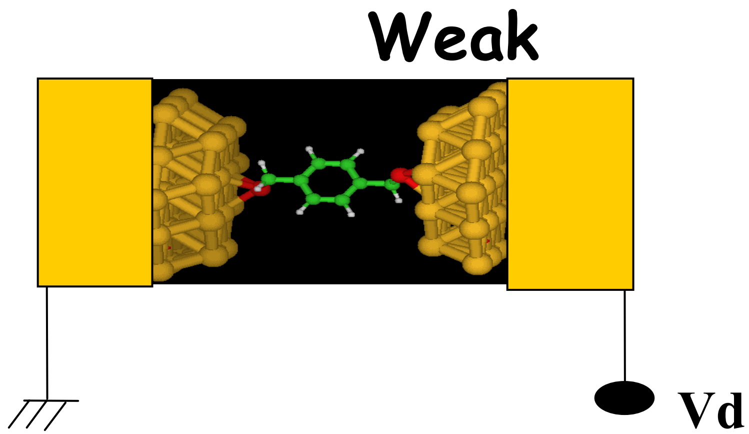
Self-Consistent Solution

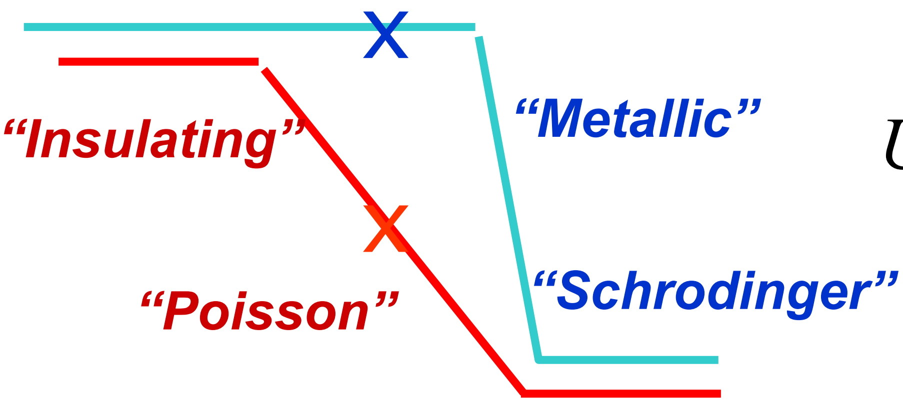
U --> N

"Schrodinger"

U --> I

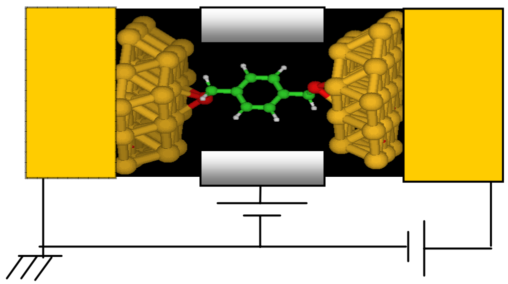
Where is the voltage drop ?





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

Minimal Model



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

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

"Poisson"

N --> U

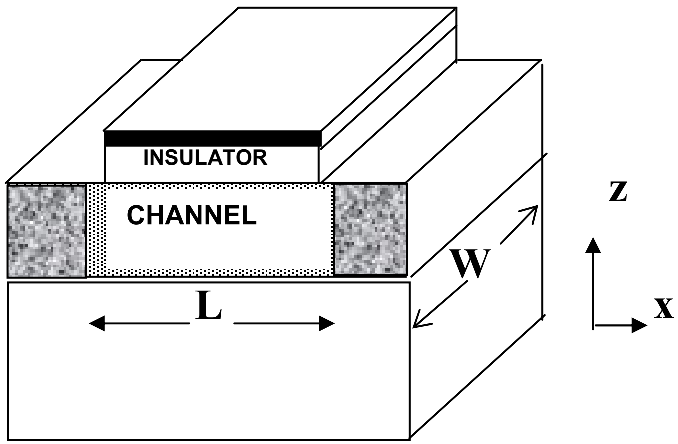
Self-Consistent Solution

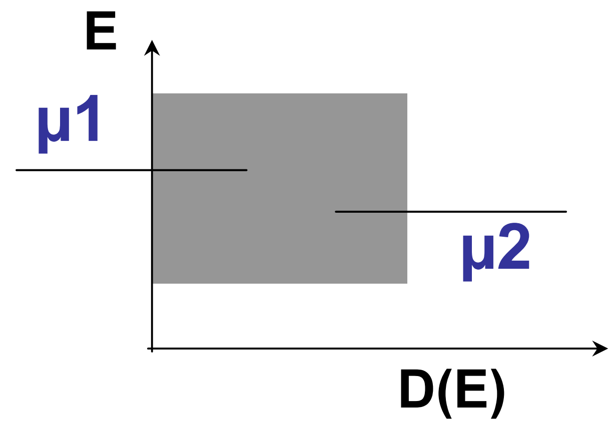
U --> N

U --> I

Nanowires / Nanotubes / Molecules

Ohm's Law ?





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

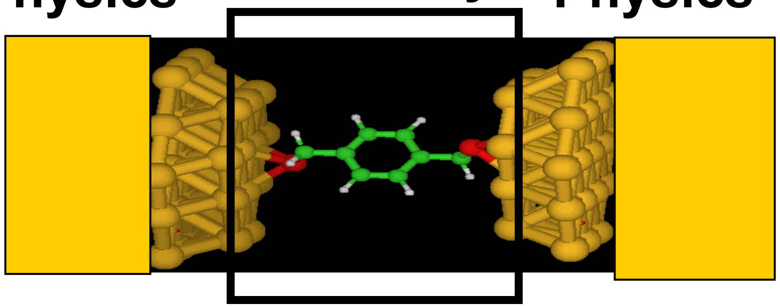
$$D(E) \sim Area \;\; x \;\; Length$$

$$\gamma \sim Velocity \; / \; Length$$

$$I \sim Area$$

Numbers --> Matrices: NEGF

Surface Physics | Quantum Chemistry | Surface Physics



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

$[\Sigma_s]$

Incoherent Scattering

www.nanohub.org

$$\varepsilon \rightarrow [H]$$

$$\gamma \rightarrow [\Gamma],\ [\Sigma]$$

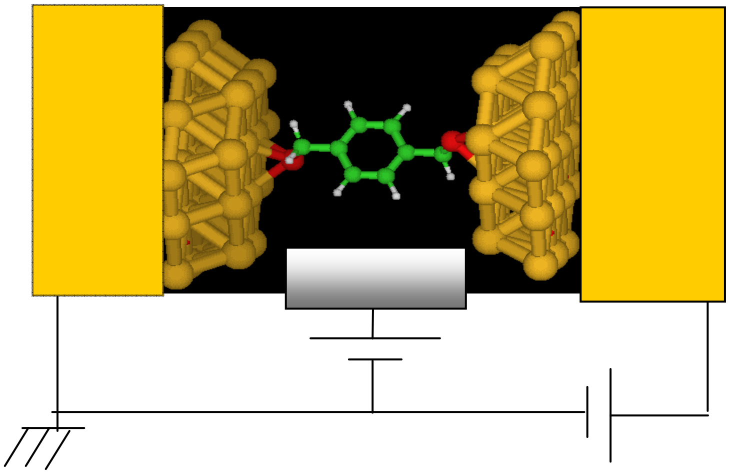
$$D(E) \rightarrow [A(E)]$$

$$U \rightarrow [U]$$

$$N \rightarrow [\rho]$$

Ghosh, Liang, Rakshit, Zahid, Damle, Paulsson

Outline



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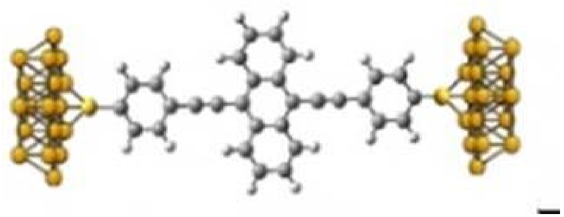
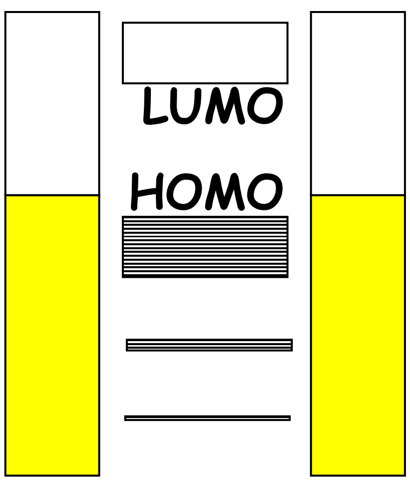
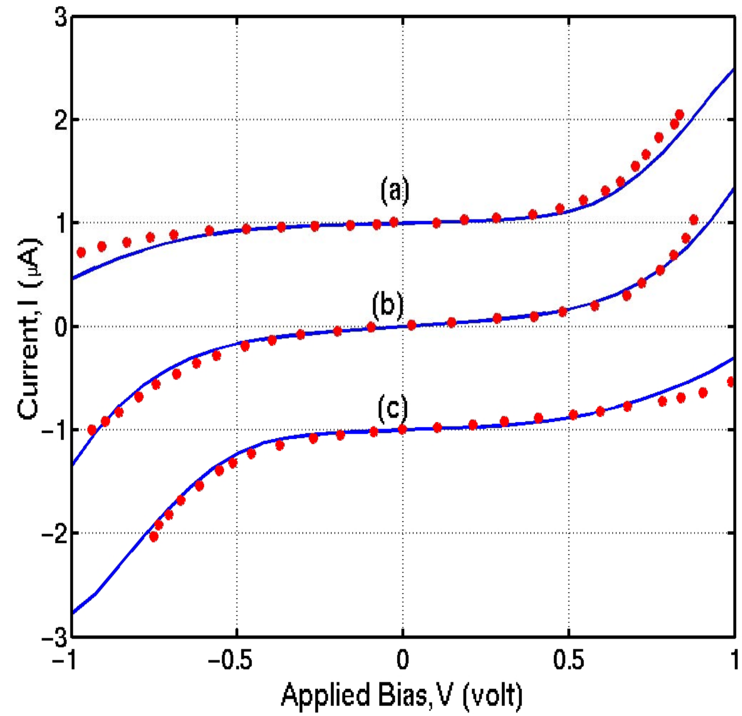
Experiment vs. Theory

Experiment:
Reichert et.al. PRL (2002)





Theory:
Zahid, Ghosh et.al.

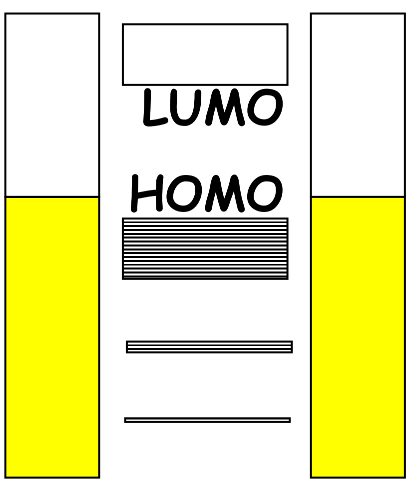


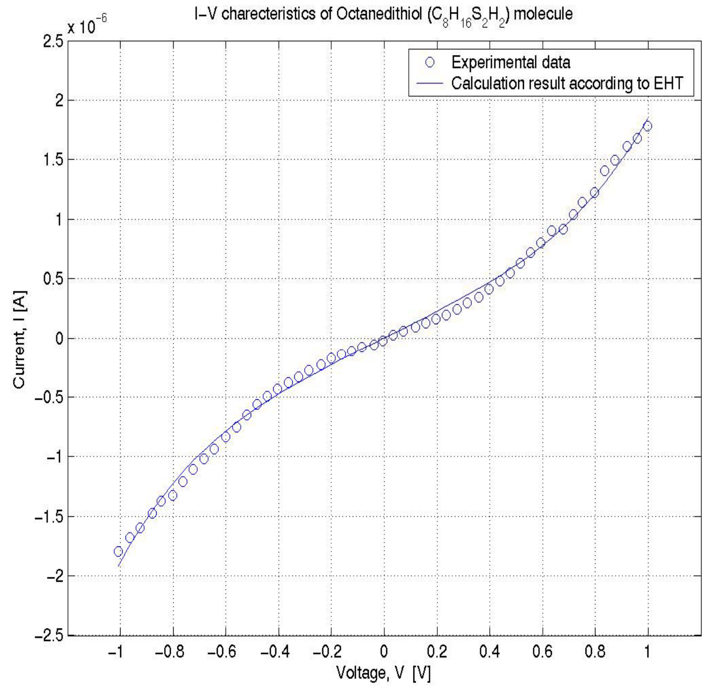
Experiment vs Theory

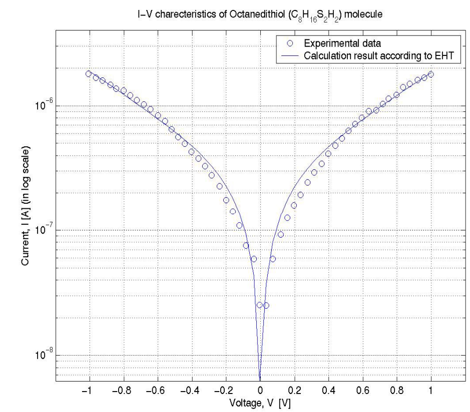
Expt: Wang, Lee and Reed

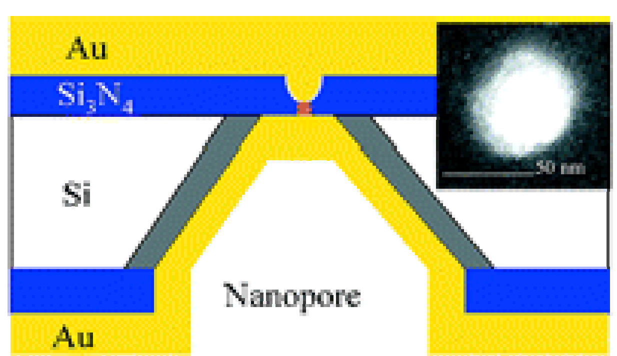
Alkane- thiols

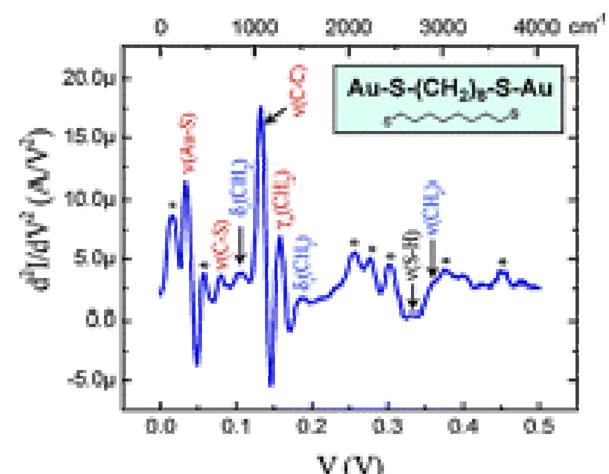
Theory: Zahid and Siddiqui



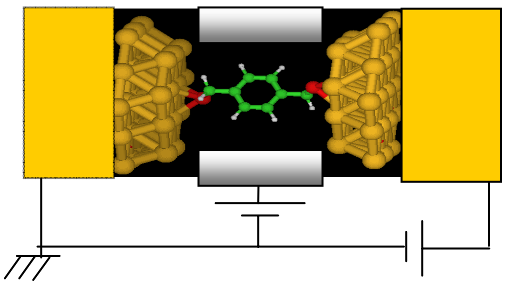








Minimal Model



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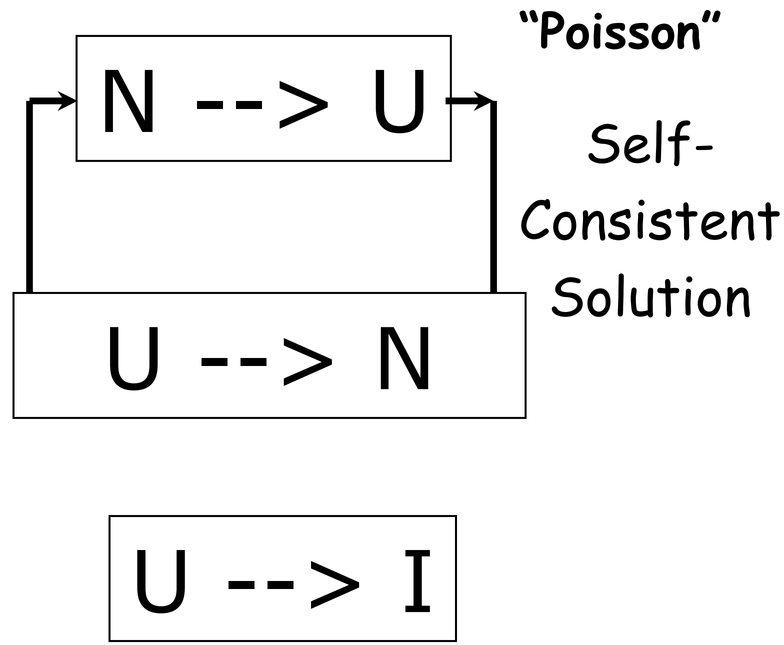
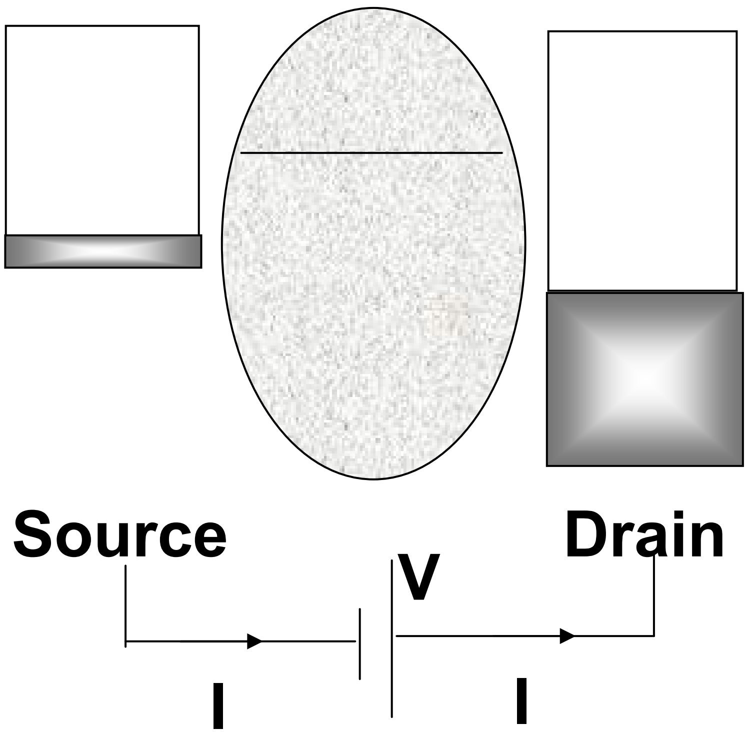
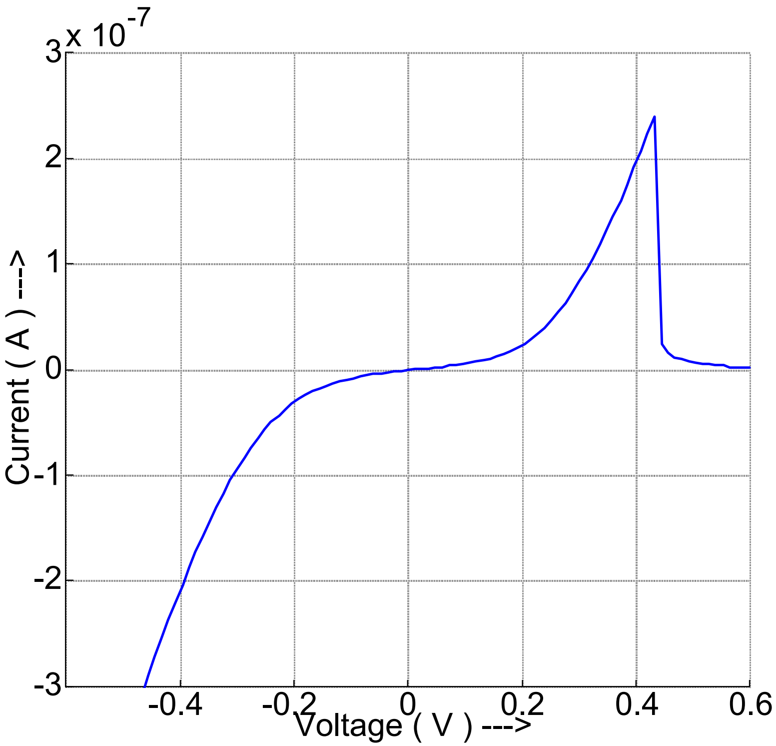


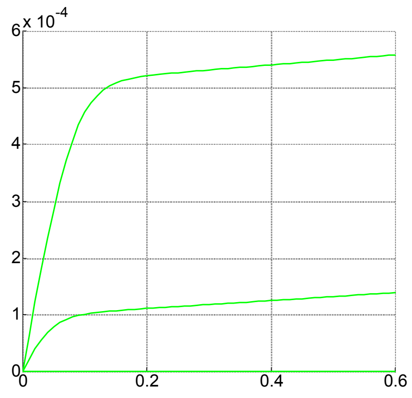
Negative Differential Resistance (NDR)





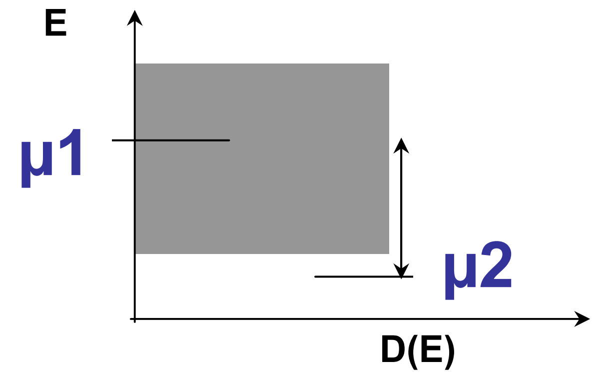
FET: Why current "saturates" ?

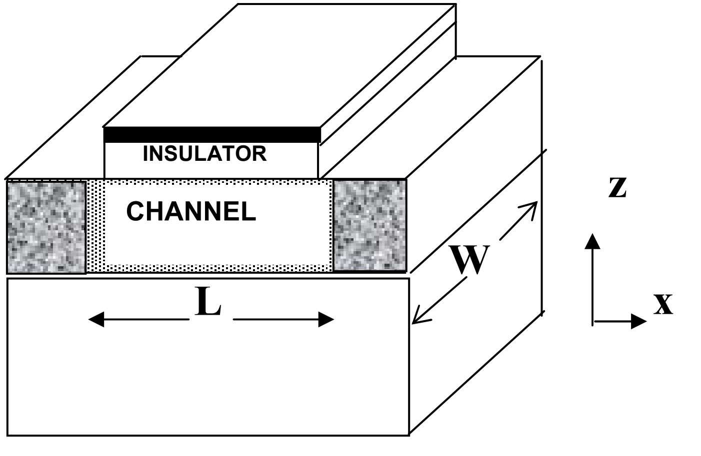
Drain current



Drain voltage

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



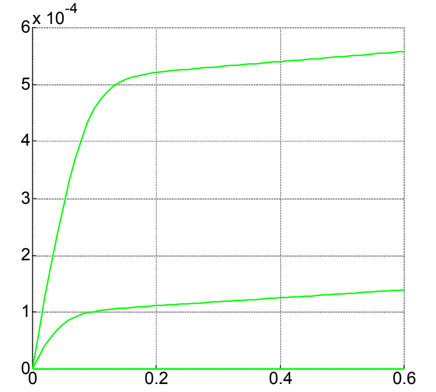


Molecular FET's ?

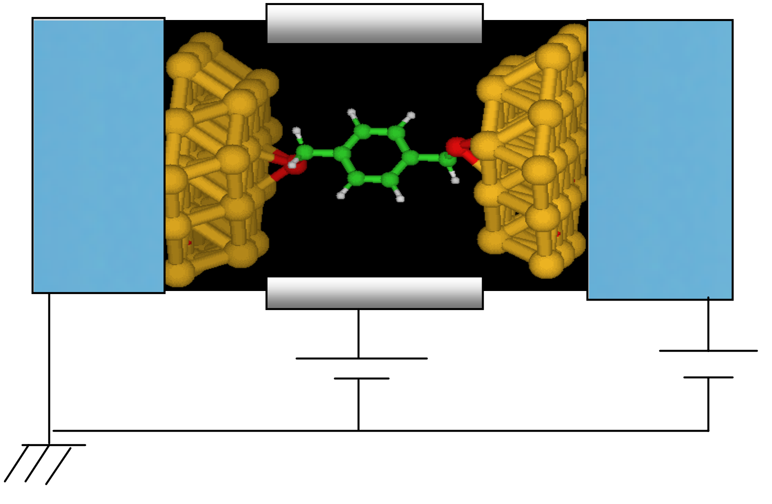
$$U = U_L + U_0(N - N_0)$$

Gate should exercise greater control than ***drain***

Drain current

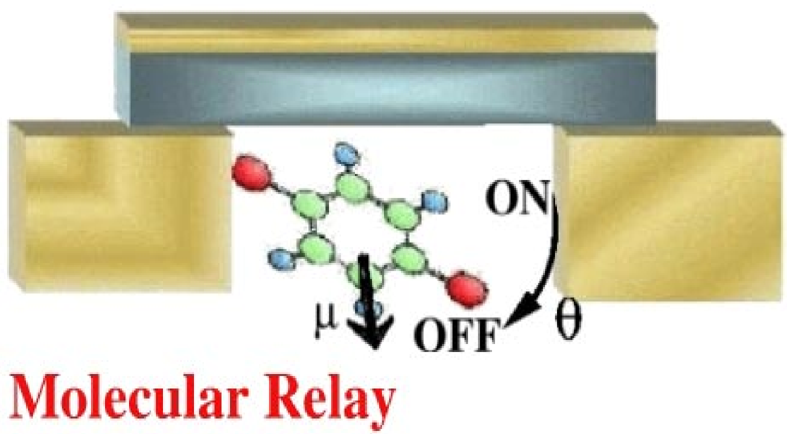


Drain voltage



Damle, Rakshit, Paulsson,
IEEE Transcations on Nanotechnology (2002)

Conformational Transistors ?



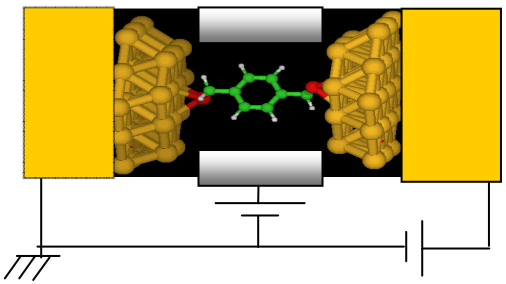
$(S_{es})_{min} = 2.3(k_BT/e) \approx 60$ mV/dec.

$(S_{conf})_{min} = 2.3(k_BT/e).(et_{ox}/\mu)$

Ghosh, Rakshit

(Nanoletters, 2004)

Minimal Model



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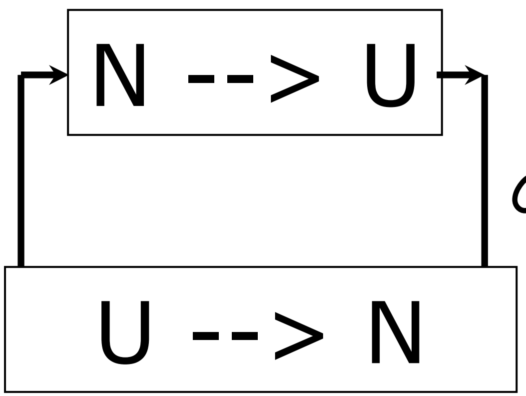
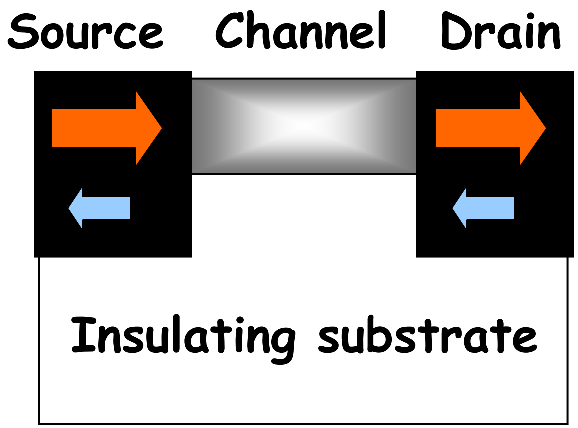


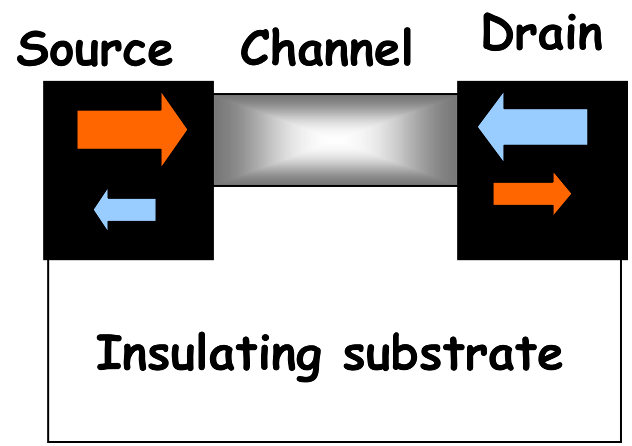
U --> I

Spin Valves



$$\alpha \text{ — } \alpha$$
$$\beta \text{ — } \beta$$

$$I_P \sim \frac{\alpha.\alpha}{\alpha+\alpha} + \frac{\beta.\beta}{\beta+\beta} = \frac{\alpha+\beta}{2}$$

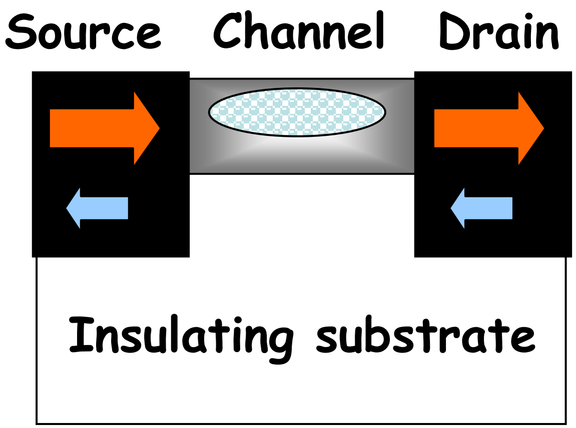


$$\alpha \text{ — } \beta$$
$$\beta \text{ — } \alpha$$

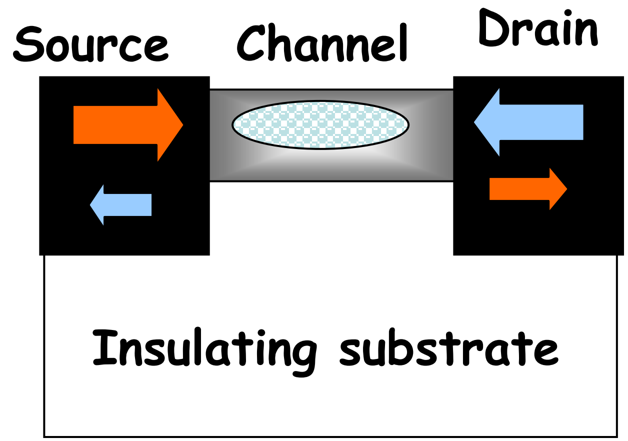
$$I_{AP} \sim \frac{2\alpha\beta}{\alpha+\beta}$$

$$= \left(\frac{\alpha+\beta}{2}\right) - \frac{(\alpha-\beta)^2}{2(\alpha+\beta)}$$

Spintronics

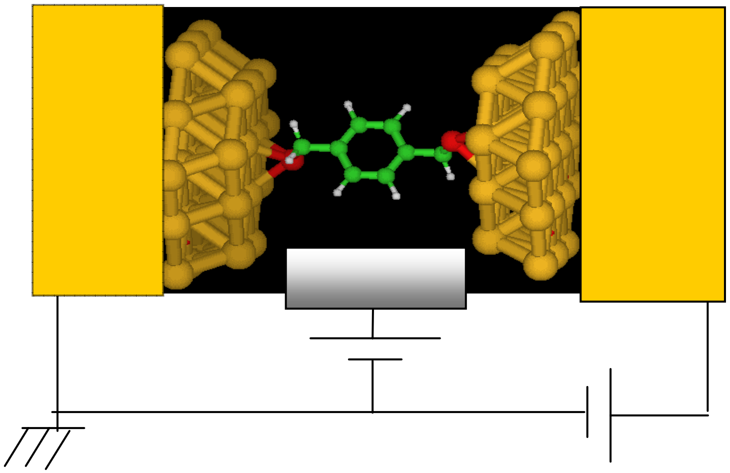


$$\alpha \text{ --- } \alpha$$
$$\beta \text{ --- } \beta$$



$$\alpha \text{ --- } \beta$$
$$\beta \text{ --- } \alpha$$

Outline



- Qualitative picture
- Quantitative models
- Examples
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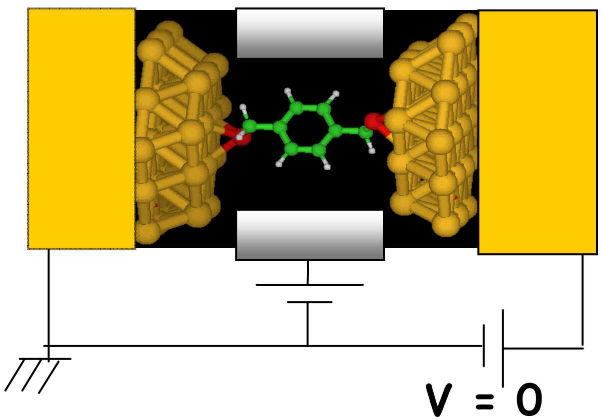
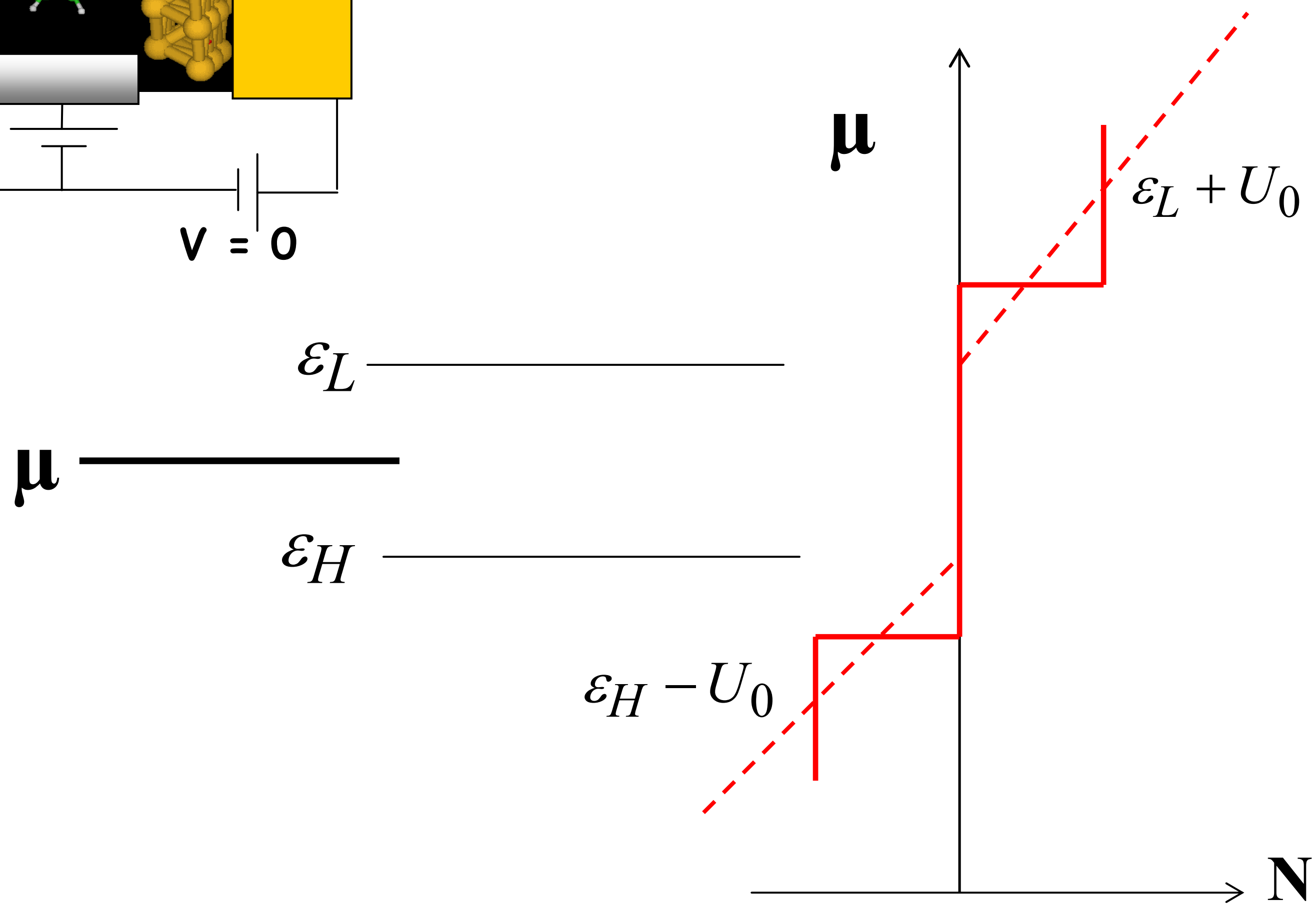
- Summary/Open questions

Electron addition and removal

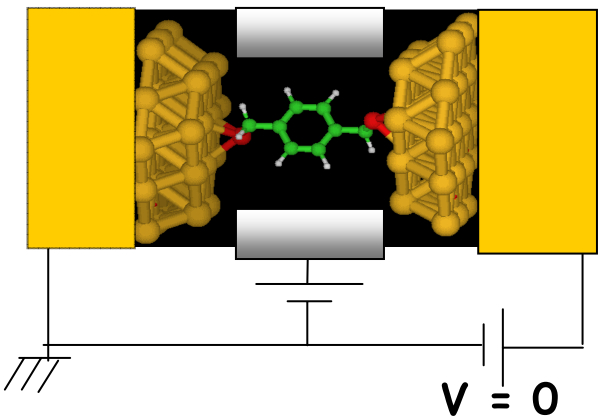


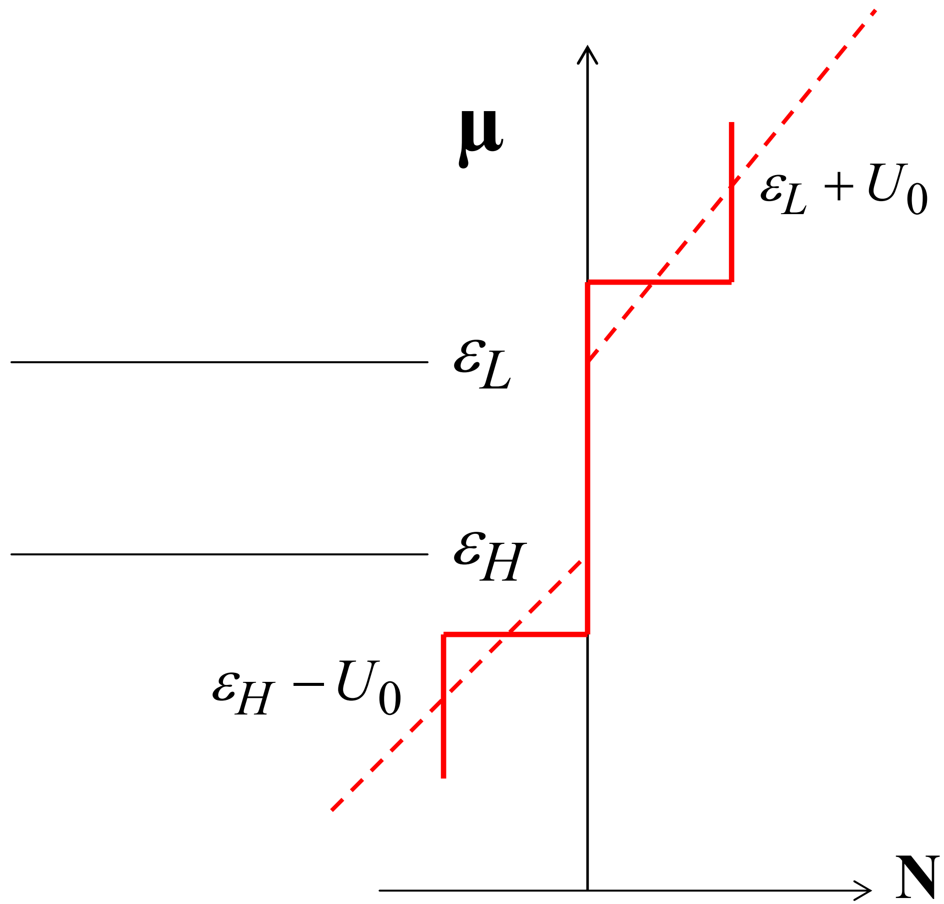
$$U = U_L + U_0 \, \Delta N$$



Self-interaction correction

$$U_j = U_L + U_0(\Delta N - \Delta n_j)$$

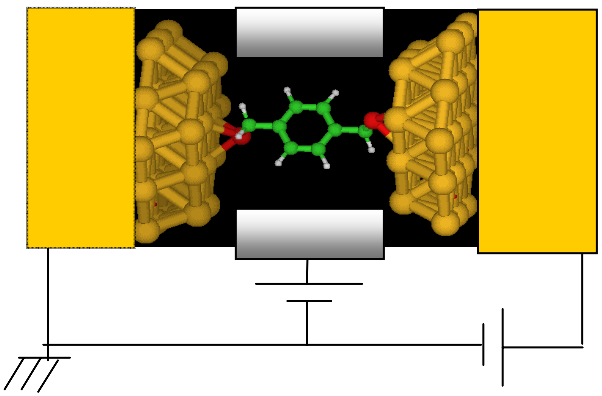




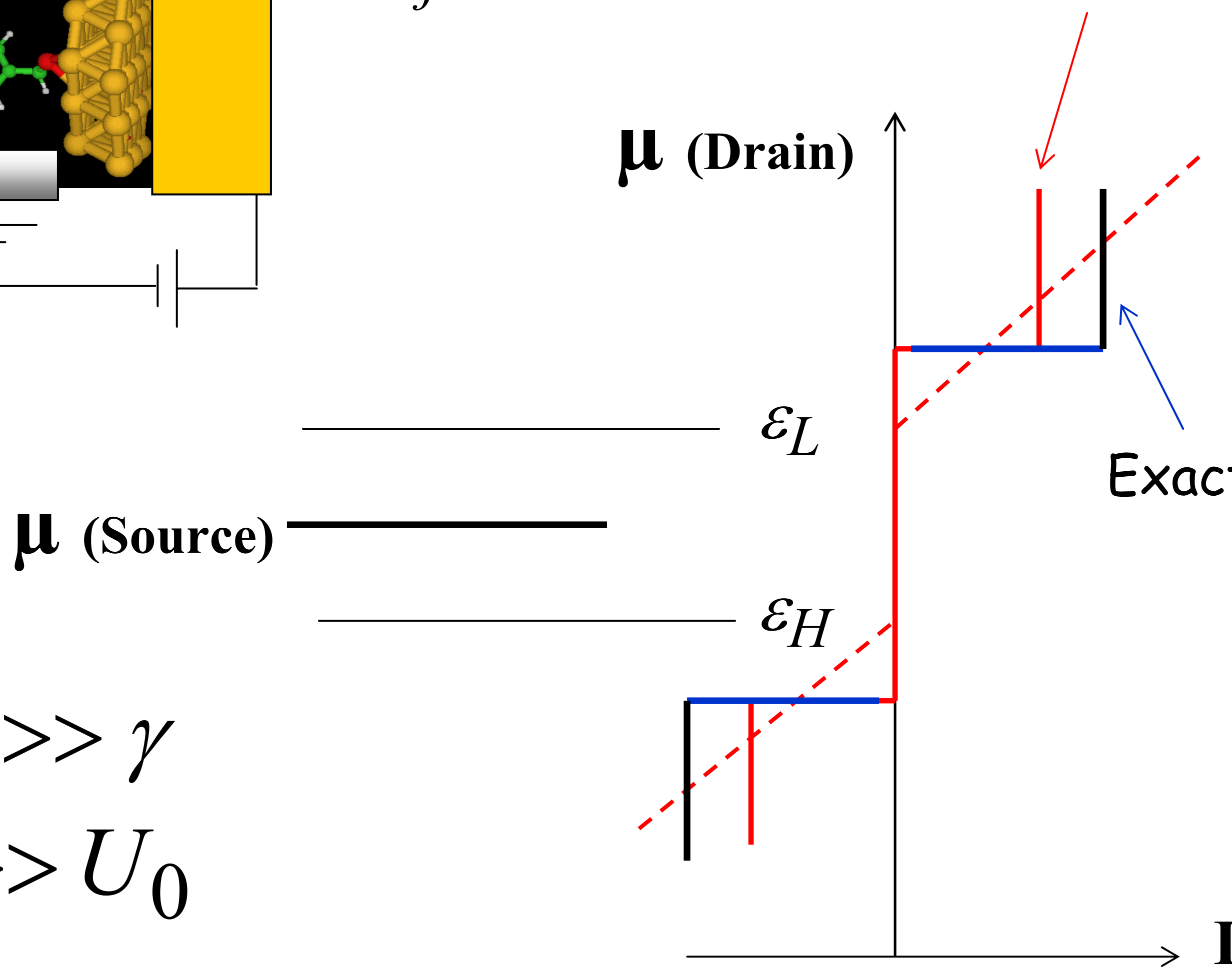
CB: $U_0 >> \gamma$

SCF: $\gamma >> U_0$

Non-equilibrium



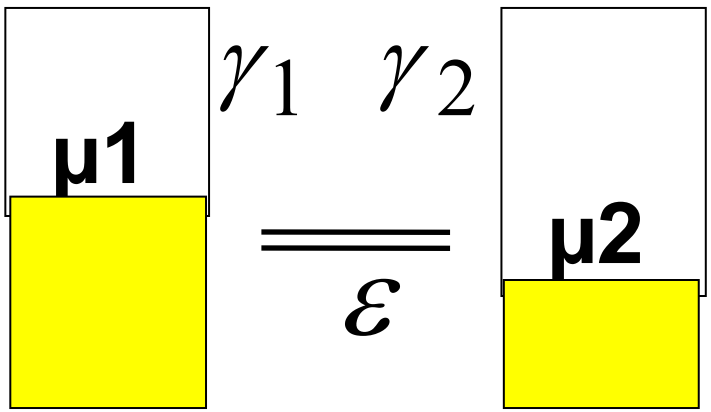
$$U_j = U_L + U_0(\Delta N - \Delta n_j)$$



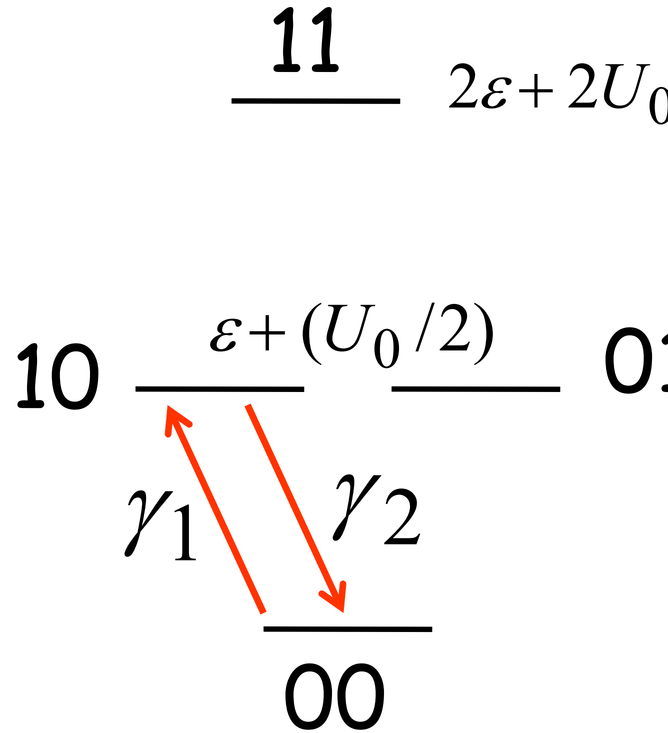
CB: $U_0 >> \gamma$

SCF: $\gamma >> U_0$

One-electron vs. Multielectron

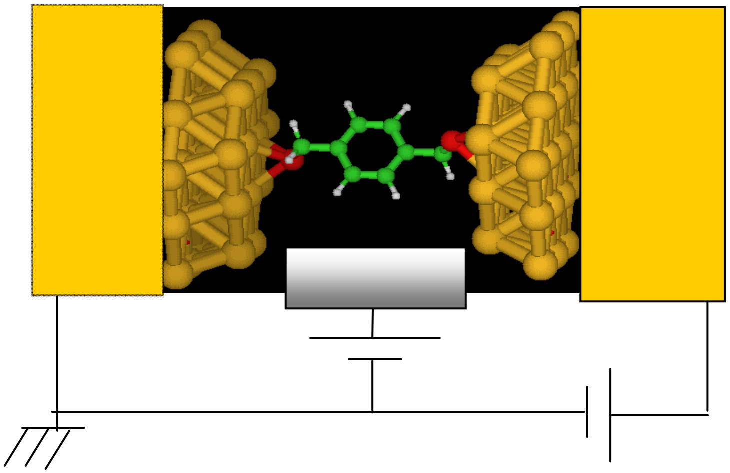


$$U_{scf} = \partial U_{ee} / \partial N$$
$$= U_0 (N - N_0)$$



$$U_{ee} = (U_0/2)\,(N - N_0)^2$$

Outline



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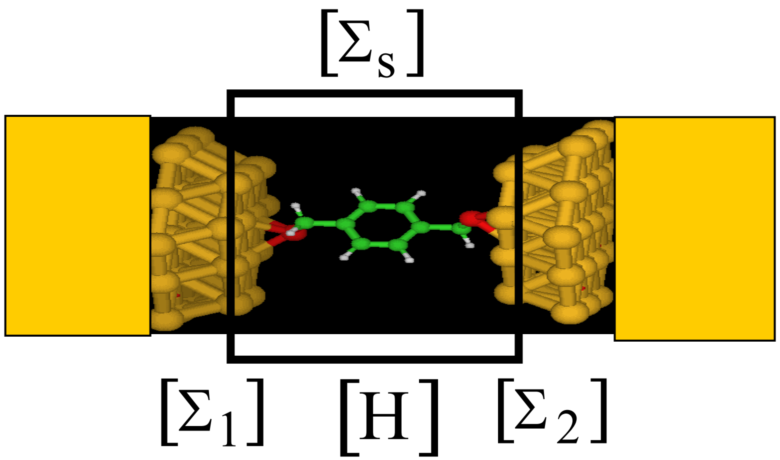
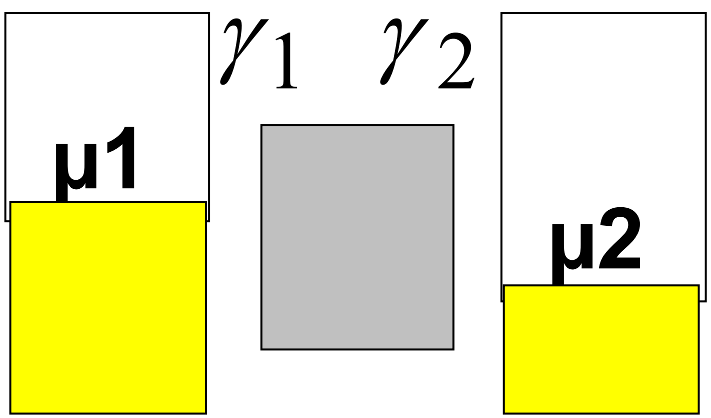
Summary



$$U = U_L + U_0 \Delta N$$

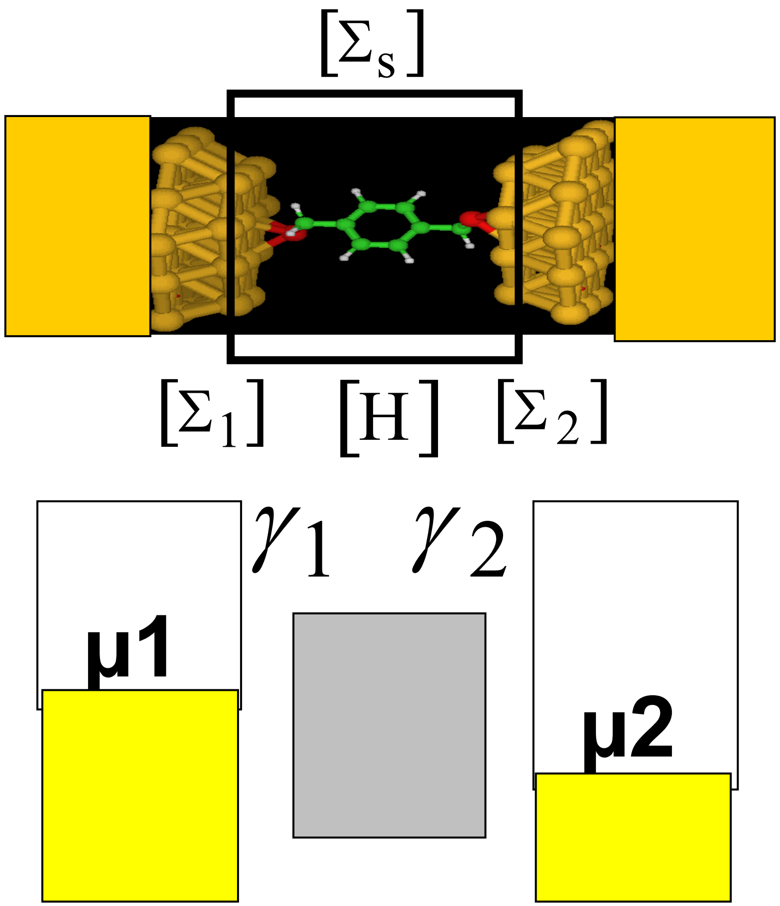
SCF: $\gamma >> U_0$

CB: $U_0 >> \gamma$



Nanotechnology, 15, S433 (2004)

Summary / Open questions



$$U = U_L + U_0 \Delta N$$

SCF: $\gamma >> U_0$

CB: $U_0 >> \gamma$

$\gamma \sim U_0$: ?????

Cooperative Phenomena ?

Nanotechnology, <u>15</u>, S433 (2004)

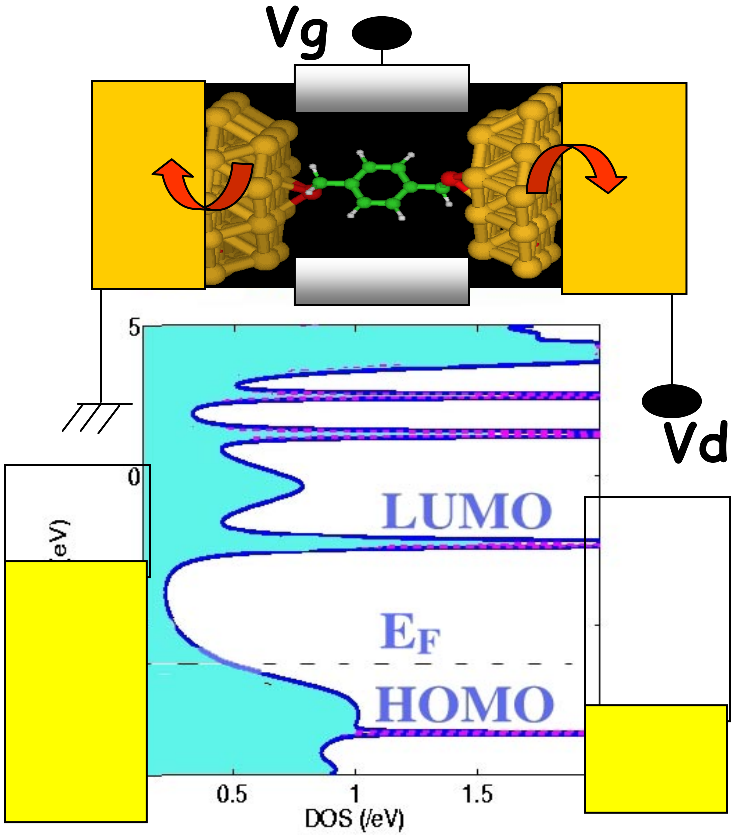
Inflow / Outflow

$$\hbar\frac{d}{dt}N + \gamma_1 N = \gamma_1 f_1$$

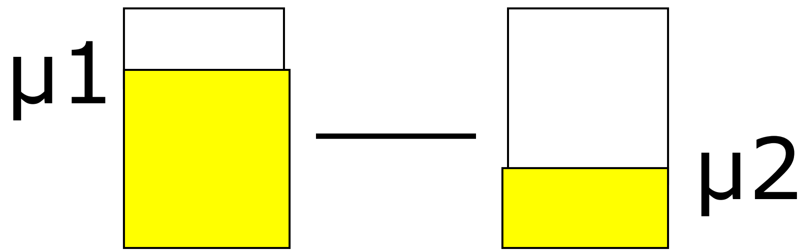
Out   In

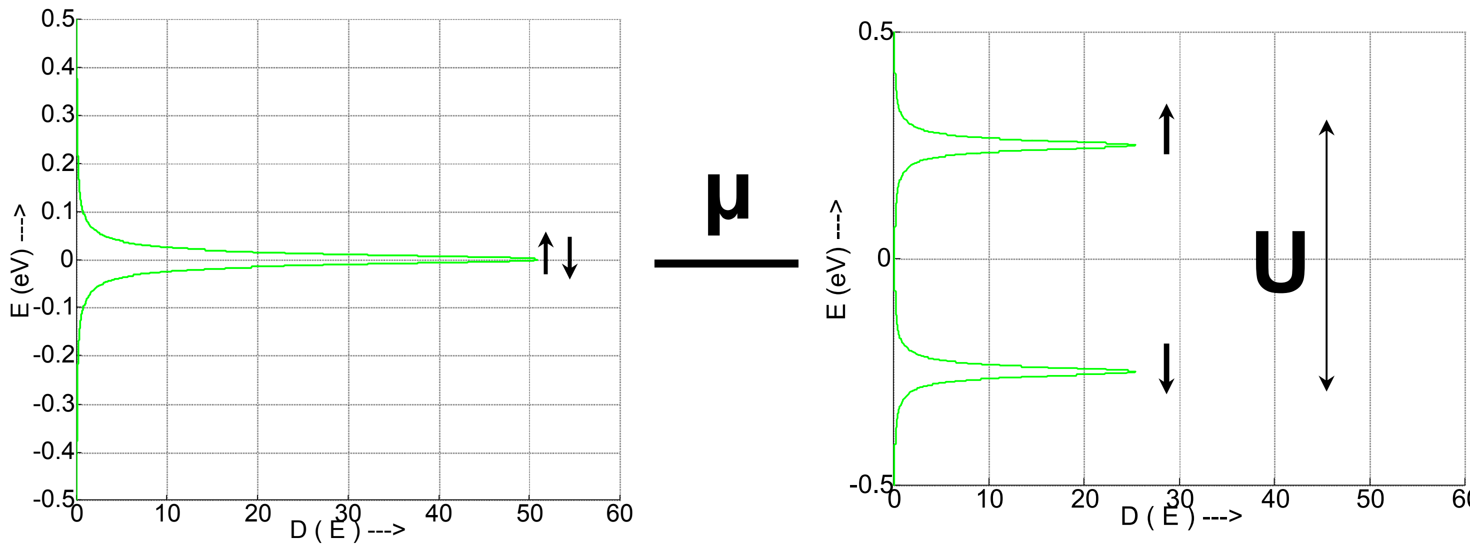
$$i\hbar\frac{d}{dt}\psi - H\psi - \Sigma_1\psi = S_1$$

$$i\hbar\frac{d}{dt}\begin{Bmatrix}\psi_L\\ \psi\\ \psi_R\end{Bmatrix} = \begin{bmatrix}H_L & \tau^+ & 0\\ \tau & H & \tau\\ 0 & \tau^+ & H_R\end{bmatrix}\begin{Bmatrix}\psi_L\\ \psi\\ \psi_R\end{Bmatrix}$$



Coulomb blockade $(\Gamma << U)$

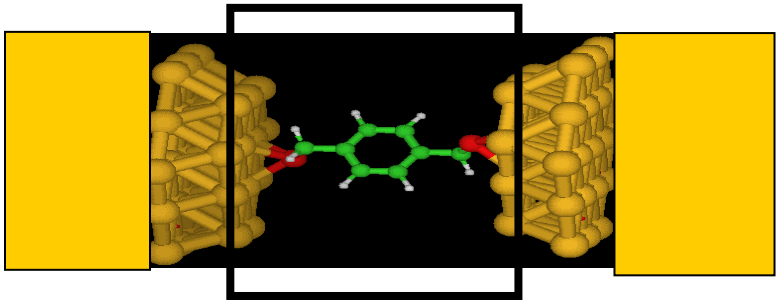




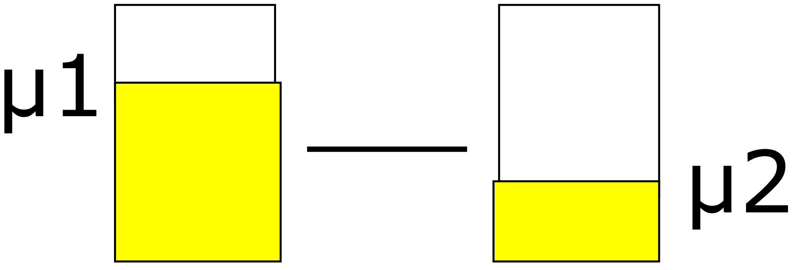
$$\Gamma \quad << \quad U \quad \sim \quad q^2 / 4\pi\varepsilon R$$

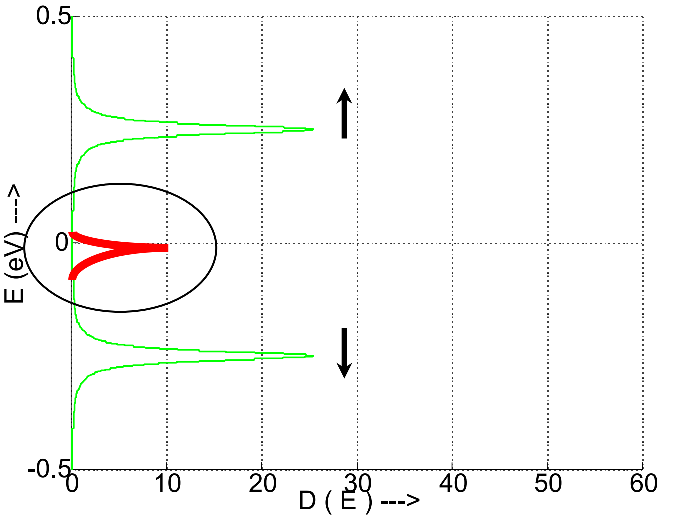
Kondo Resonance $(\Gamma \sim U)$

$[\Sigma_P]$



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





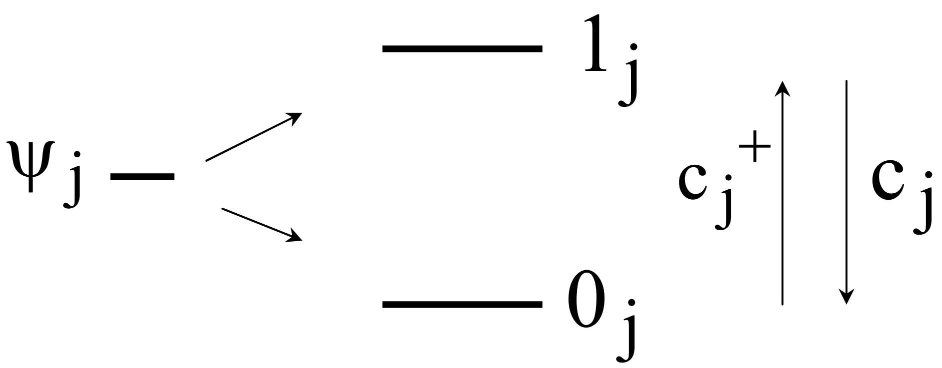
In

$$i\hbar \frac{d}{dt}\psi - H\psi - \Sigma\,\psi = S$$

Out

Σ, S **depend on 'f'**

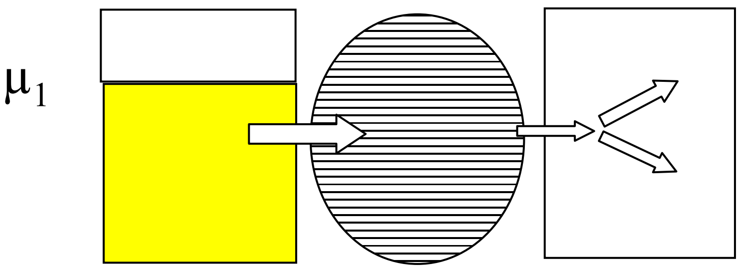
Second quantization

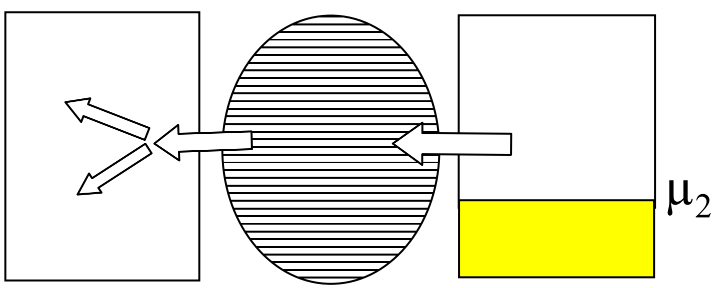


$$i\hbar\frac{d}{dt}\begin{Bmatrix} c_L \\ c \\ c_R \end{Bmatrix} = \begin{bmatrix} H_L & \tau^+ & 0 \\ \tau & H & \tau \\ 0 & \tau^+ & H_R \end{bmatrix} \begin{Bmatrix} c_L \\ c \\ c_R \end{Bmatrix}$$

$$i\hbar\frac{d}{dt}c - Hc - \Sigma c = S \quad + \quad U\, d^+ d c$$

Pauli blocking?





$$\hbar \frac{d}{dt} N + (\gamma_1 + \gamma_2) N = \gamma_1 f_1 + \gamma_2 f_2$$

Out   In

$$i\hbar \frac{d}{dt} \psi - H\psi - (\Sigma_1 + \Sigma_2)\psi = S_1 + S_2$$

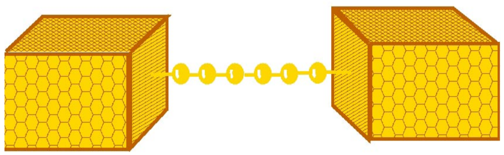
$$|1'\rangle = \exp[-iHt/\hbar]|1\rangle$$

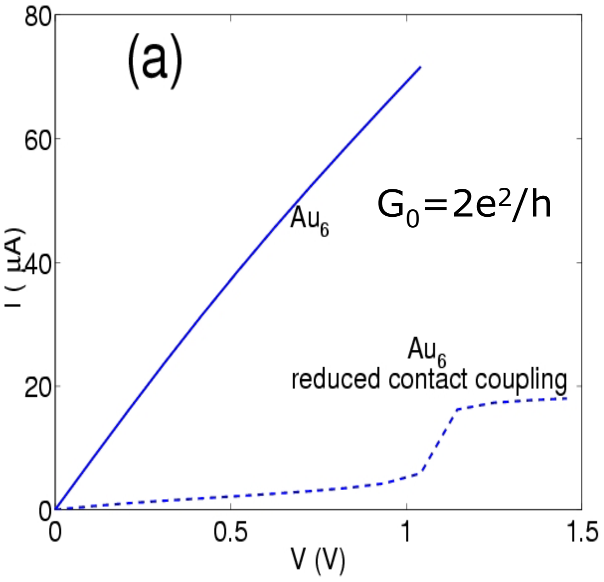
$$|2'\rangle = \exp[-iHt/\hbar]|2\rangle$$

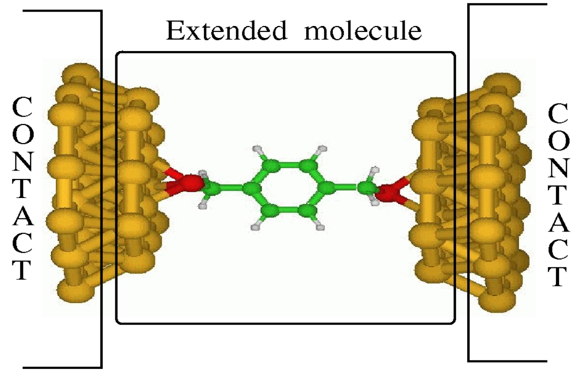
$$\langle 1' | 2' \rangle = \langle 1 | 2 \rangle$$

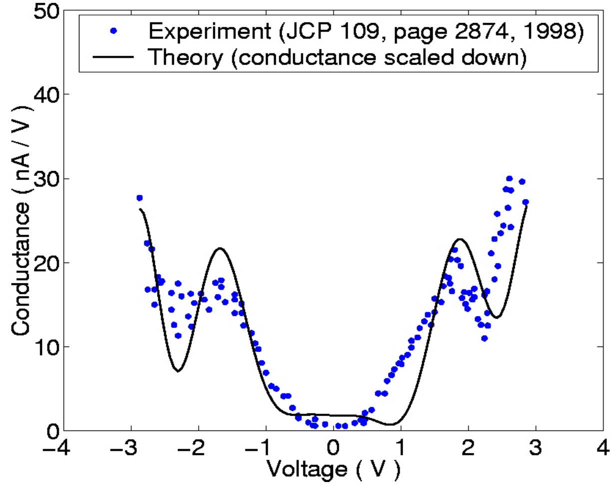
NOT applicable to phase-breaking processes

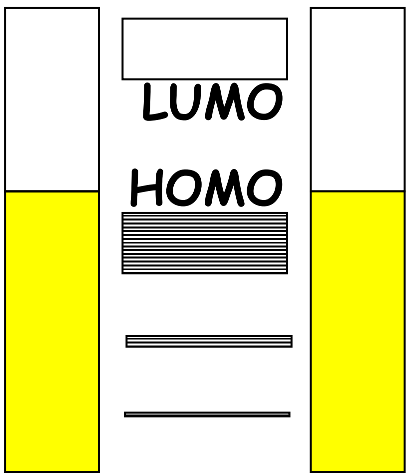
Experiment vs Theory









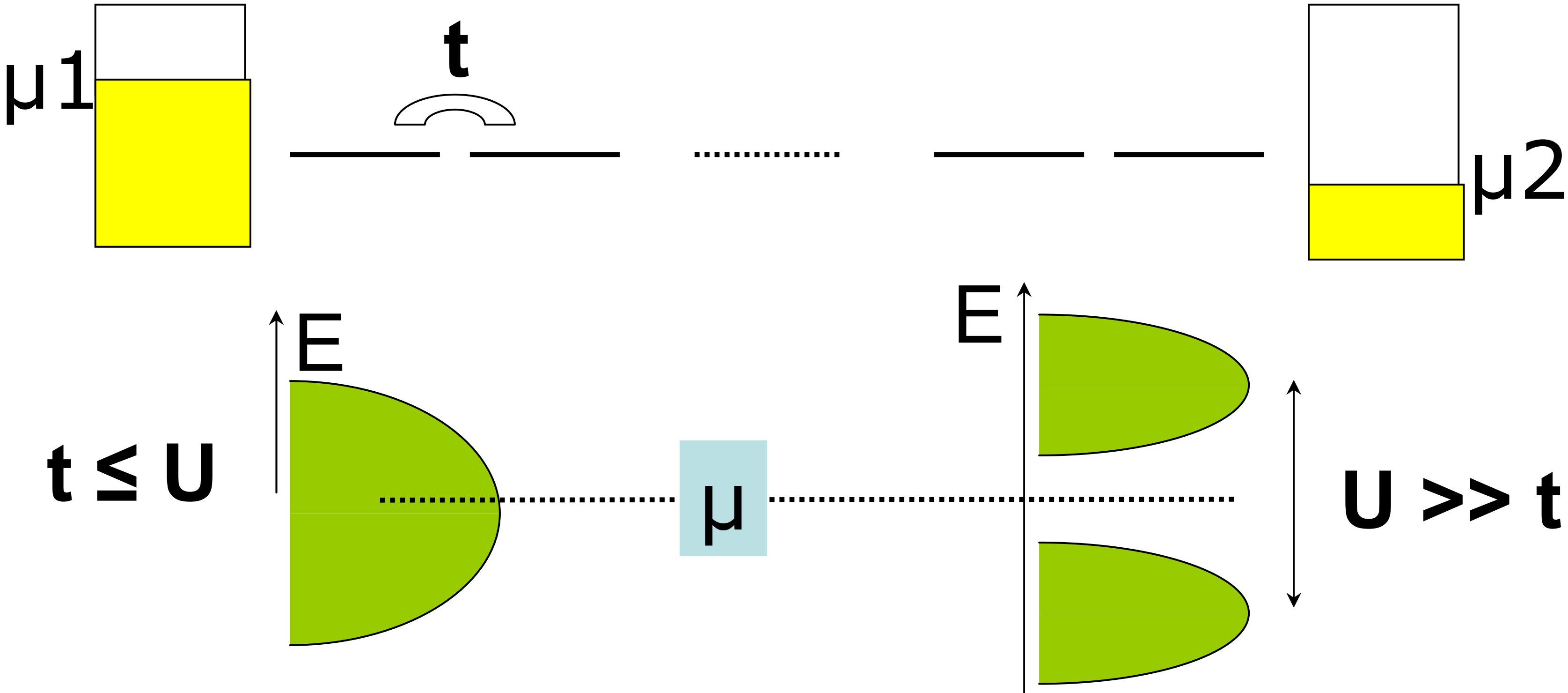


Expt: Reifenberger, Kubiak et.al.

Theory: Damle, Ghosh et.al.
PRB 64, 201403 R (2001)

Solid state <--> Molecular

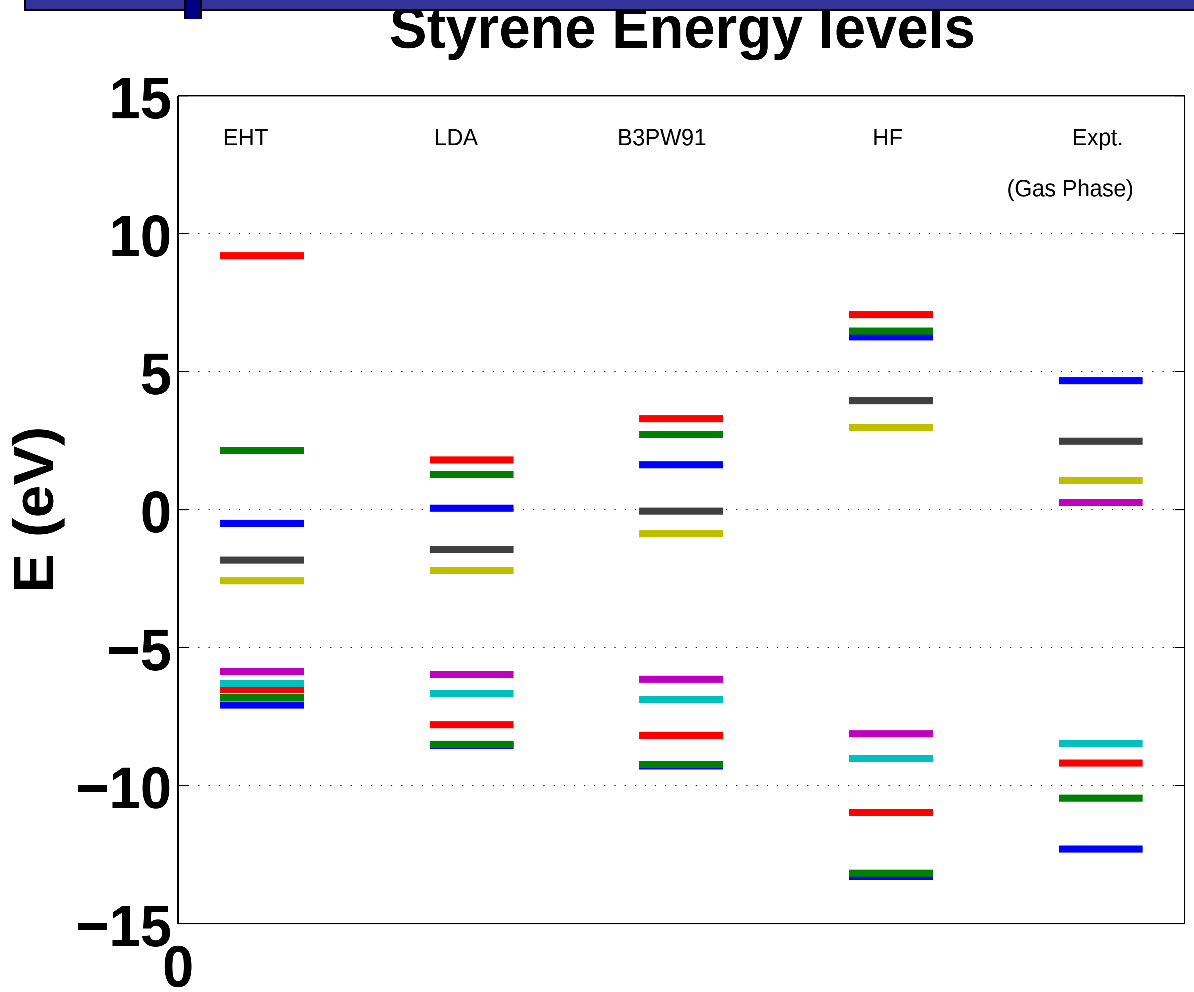
$$t \leftrightarrow \Gamma$$

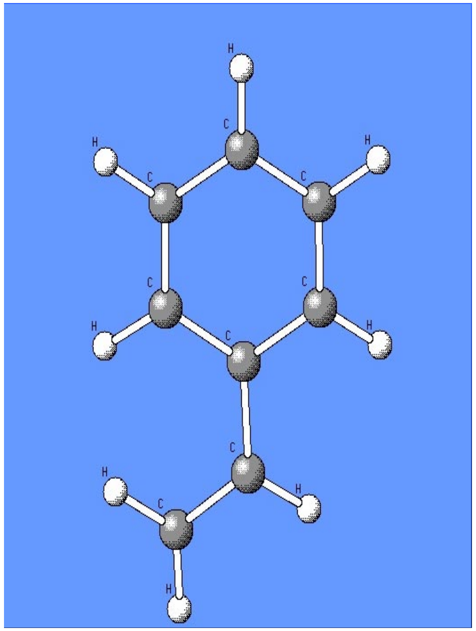


Band limit ⟷ **Solids** ⟷ **Atomic limit**

Scf method ⟷ "Molecules" ⟷ **Coulomb blockade**

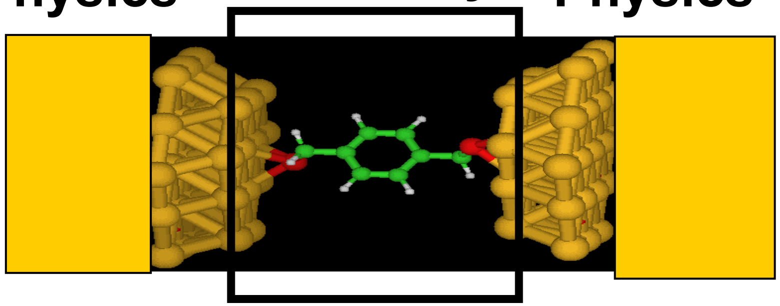
Energy Levels: Styrene





Real (?) Models

Surface Physics | Quantum Chemistry | Surface Physics



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

Incoherent Scattering, $[\Sigma_s]$

Closed System

Open System, Out-of-equilibrium