Electrical Resistance: An Atomistic View

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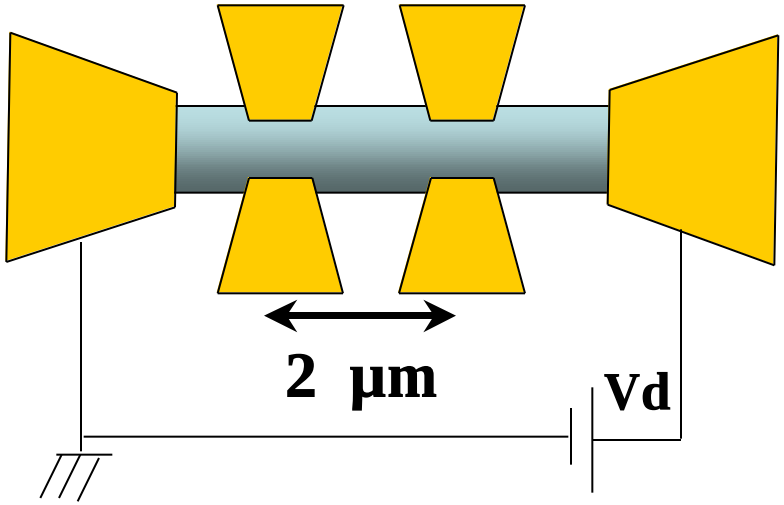
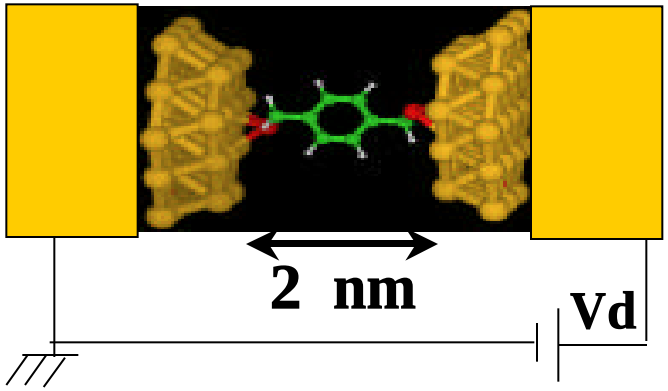
Top-down and Bottom-up

Solid-state Electronics / Mesoscopic Physics



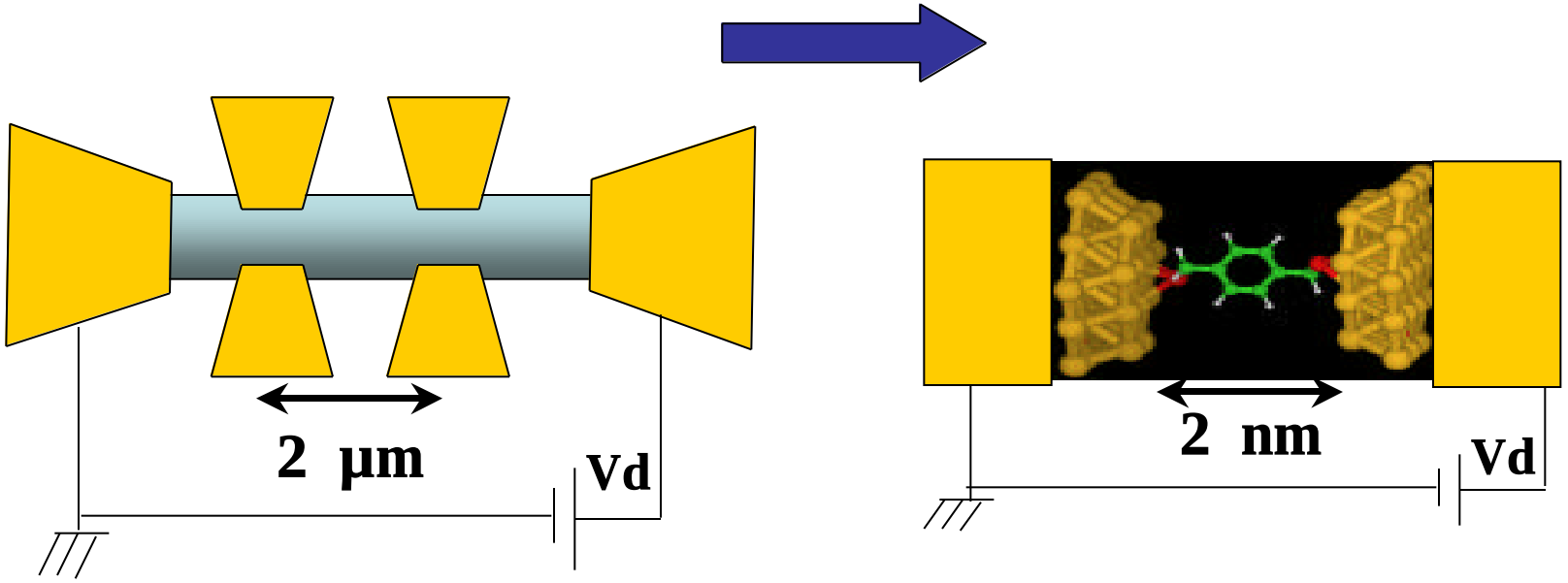
Molecular Electronics



Electrical Resistance: Top-down view

Solid-state Electronics / Mesoscopic Physics

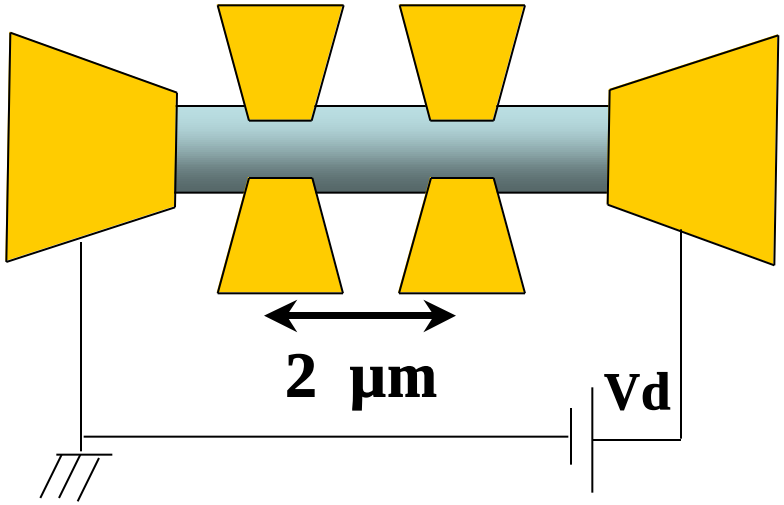
Molecular Electronics

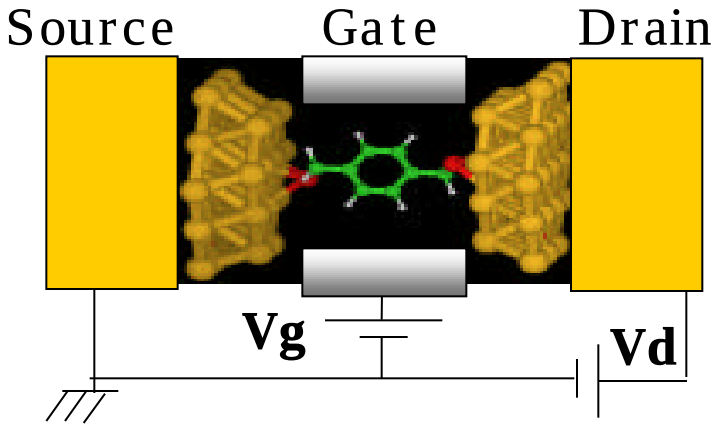


Electrical Resistance: Bottom-up view

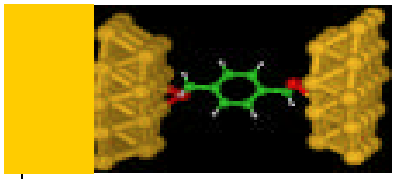
Solid-state Electronics / Mesoscopic Physics

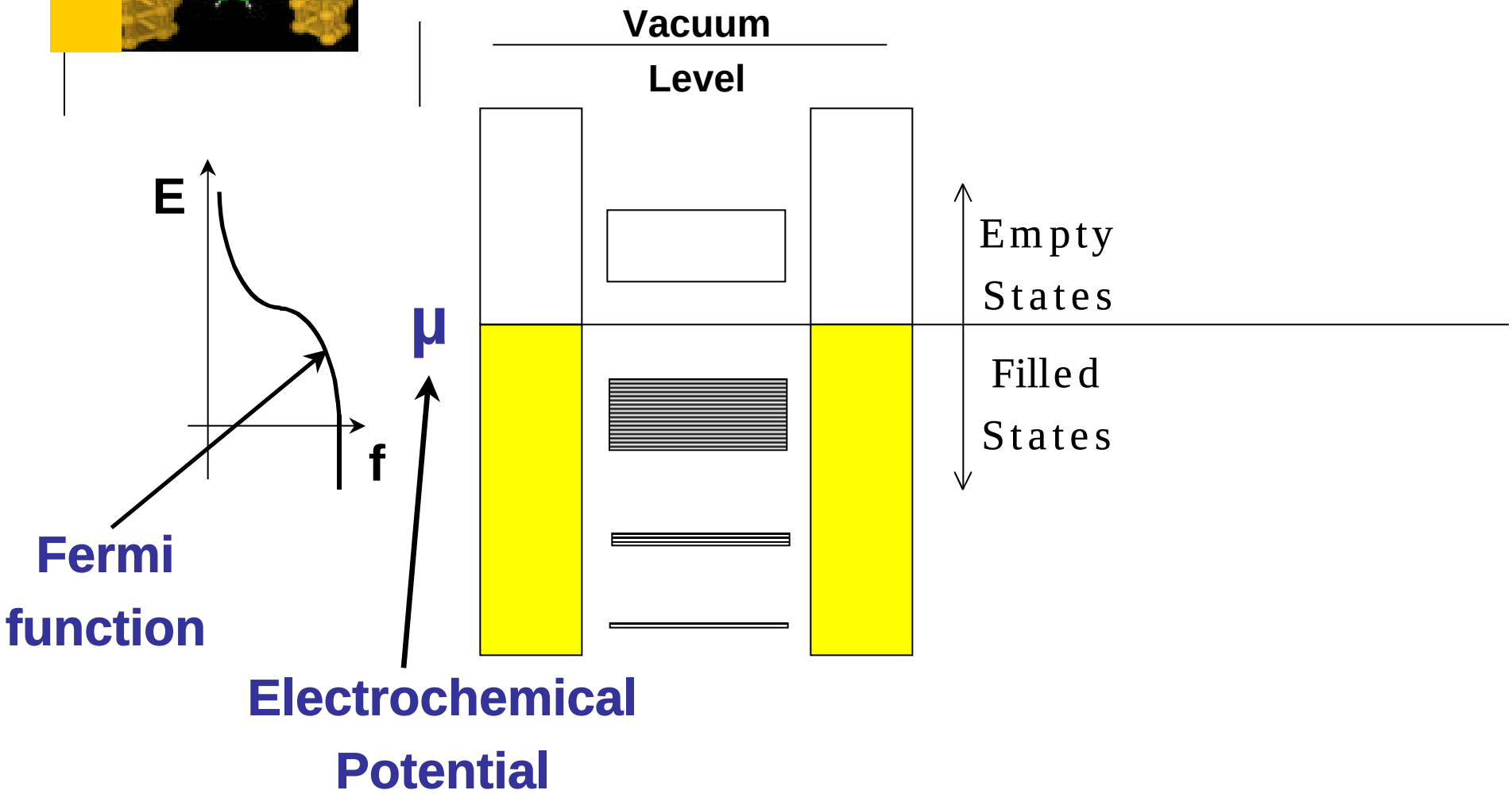
Molecular Electronics



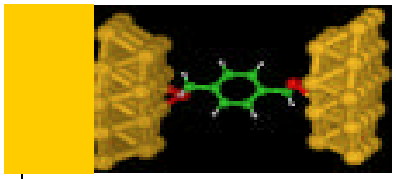


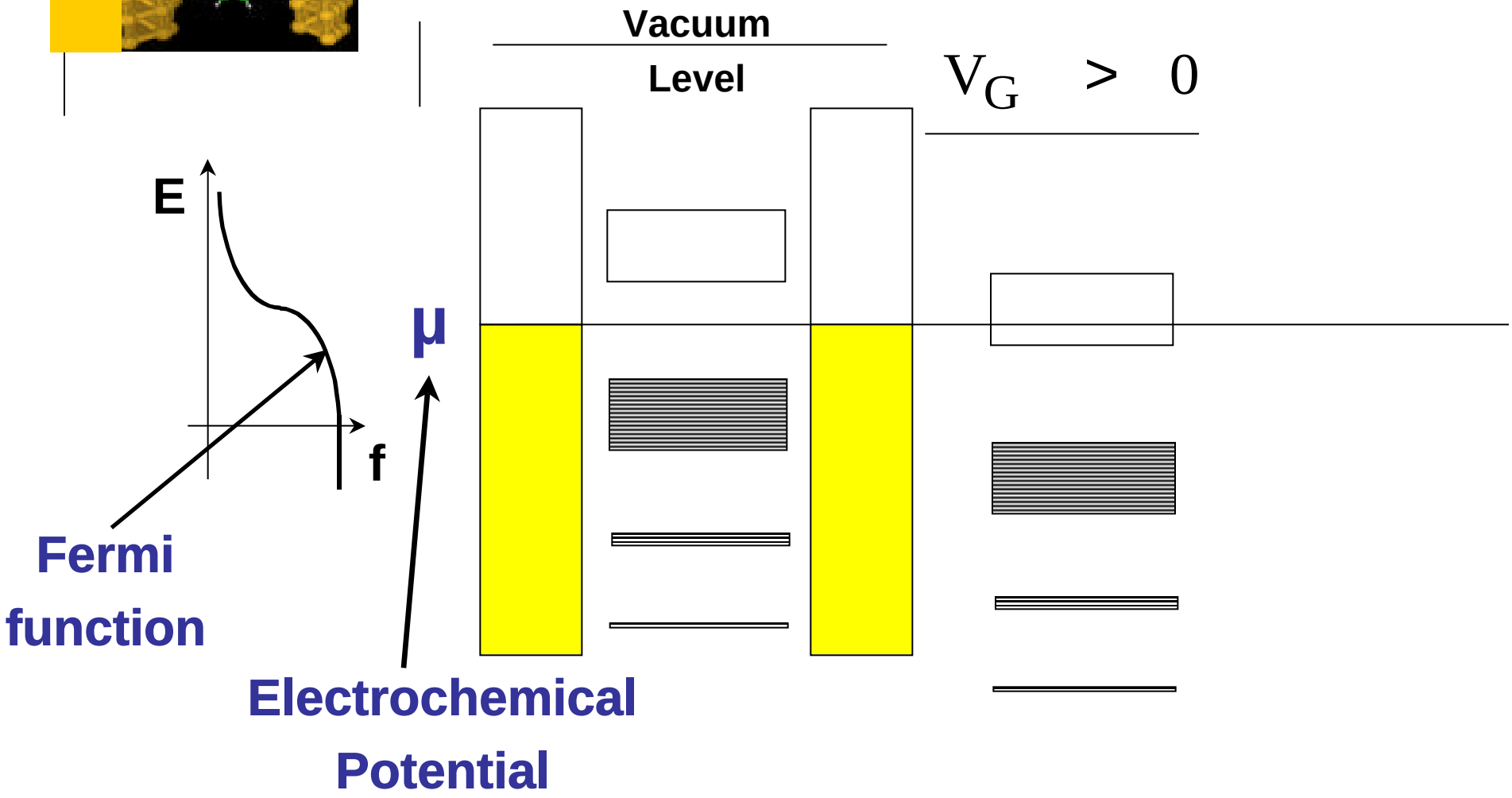
“Band - Diagram”



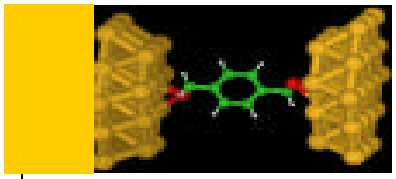


“Band - Diagram”

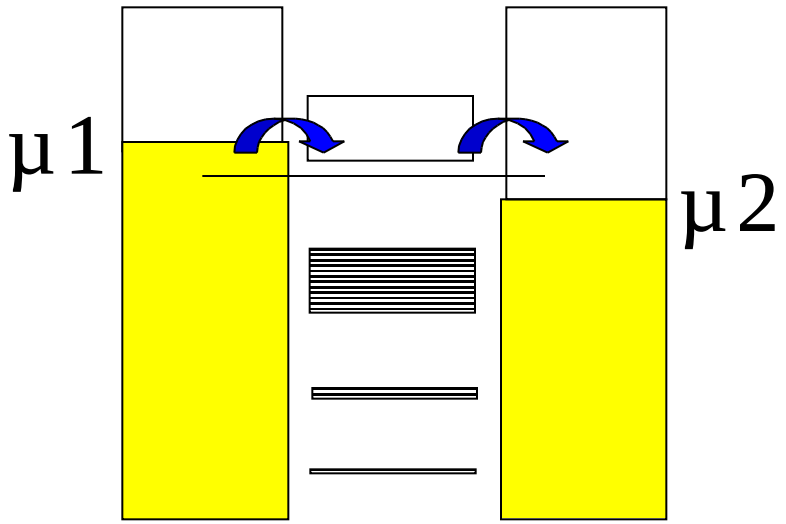




“Band-Diagram”

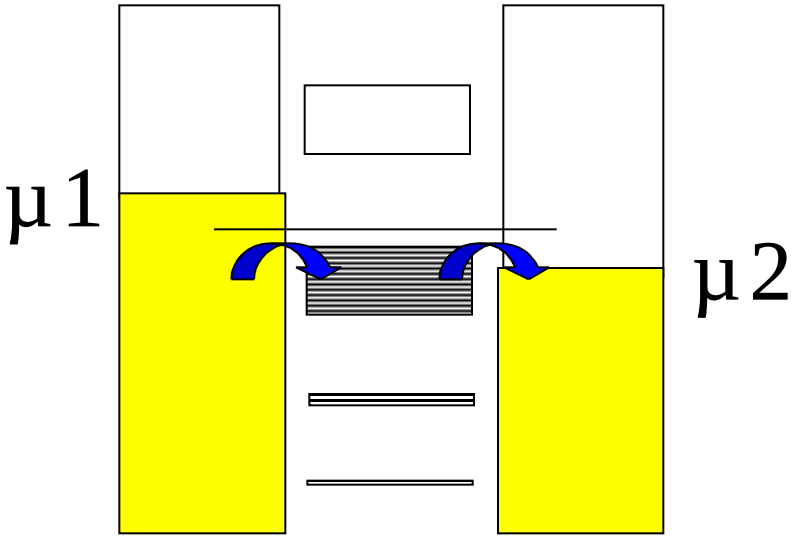


What makes electrons flow?



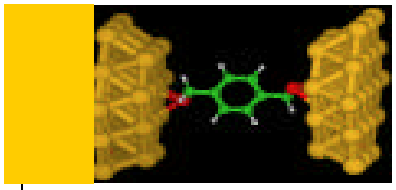
LUMO (n-type)

Conduction

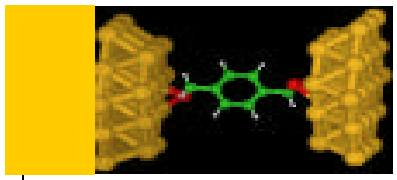


HOMO (p- type)

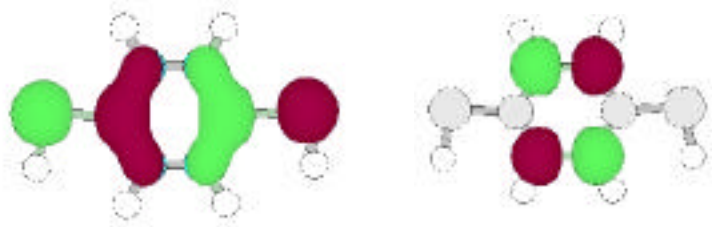
Conduction

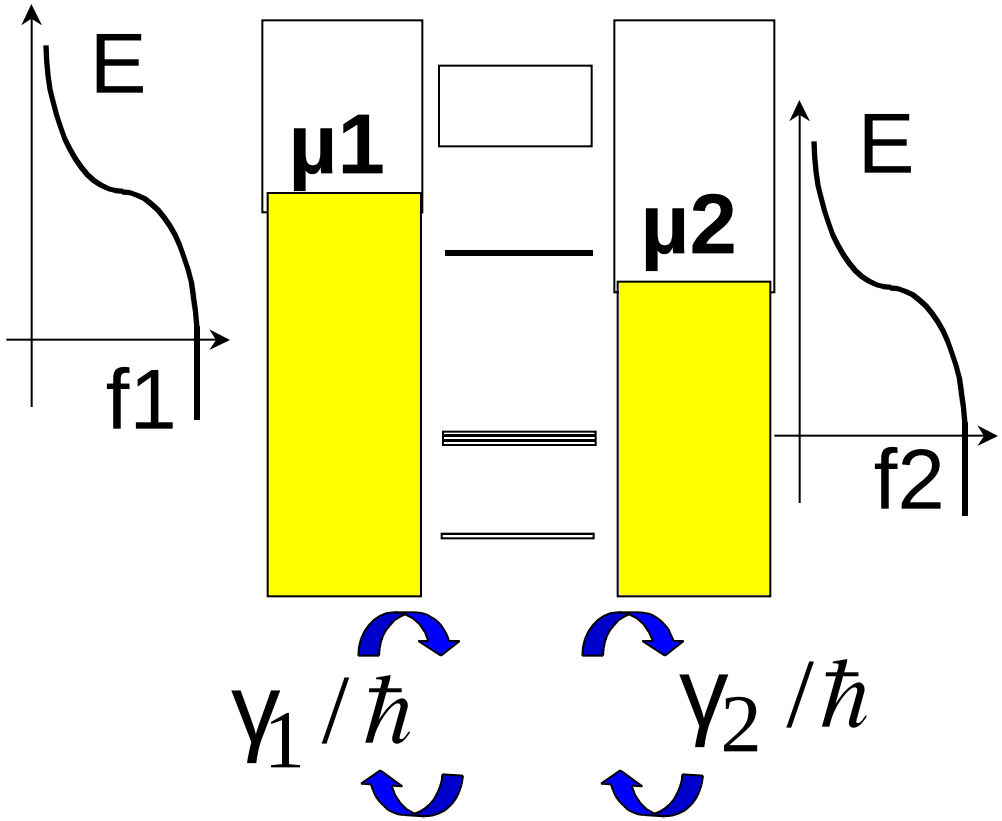


Toy model: Escape time

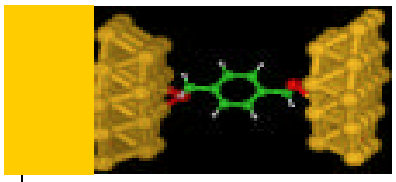


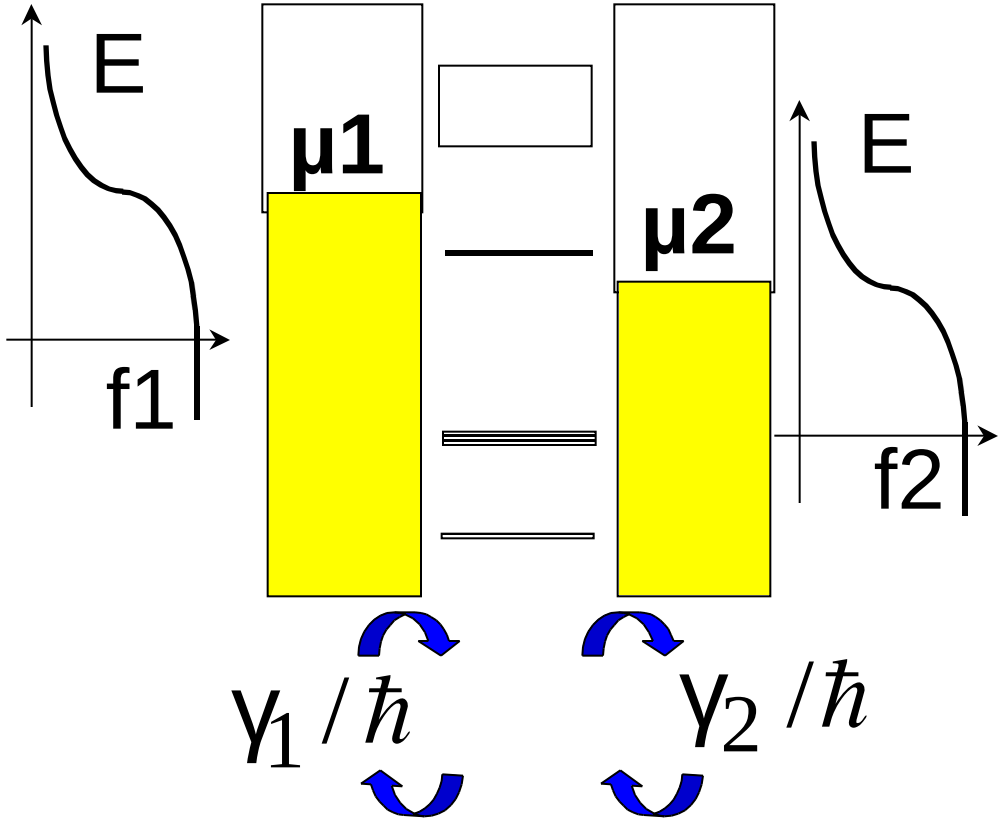
Large γ Small γ





Toy model: Escape time



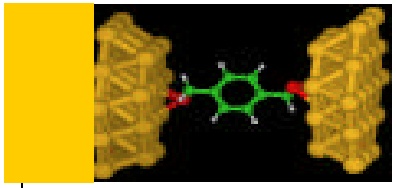


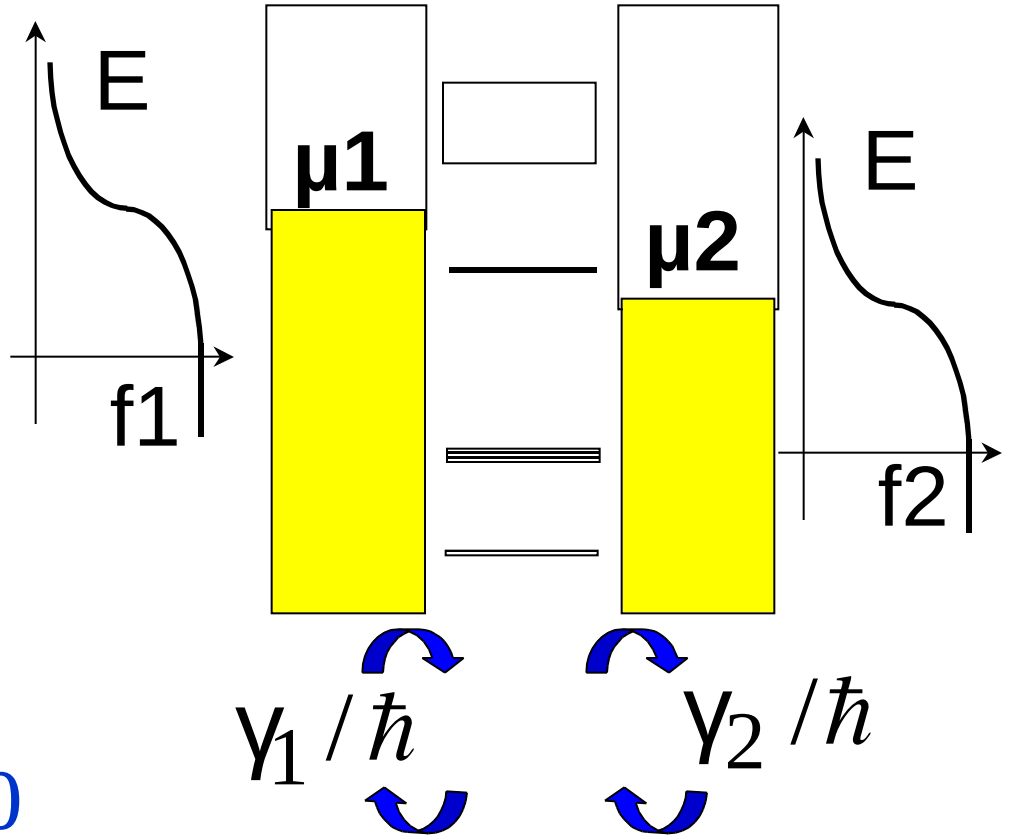
$$I_1 = q\frac{\gamma_1}{\hbar}[f_1 - N]$$

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

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

Toy model: Max. G ?

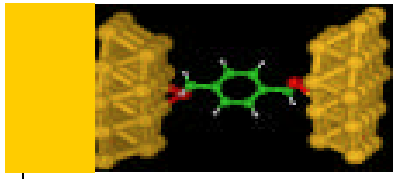




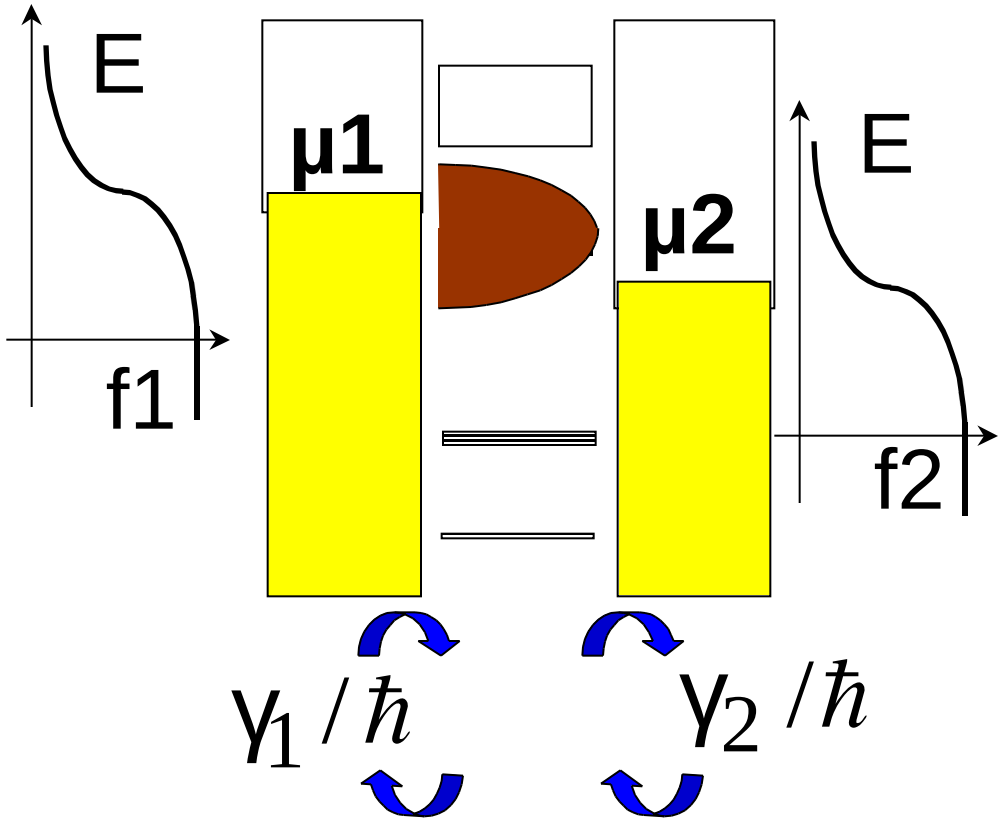
$$I = \frac{q}{\hbar}\frac{\gamma_1\gamma_2}{\gamma_1+\gamma_2}[f_1 - f_2]$$

1 - 0

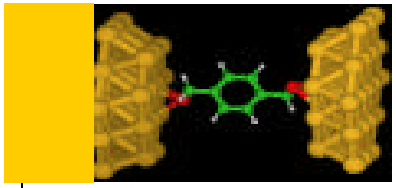
Toy model: Broadening

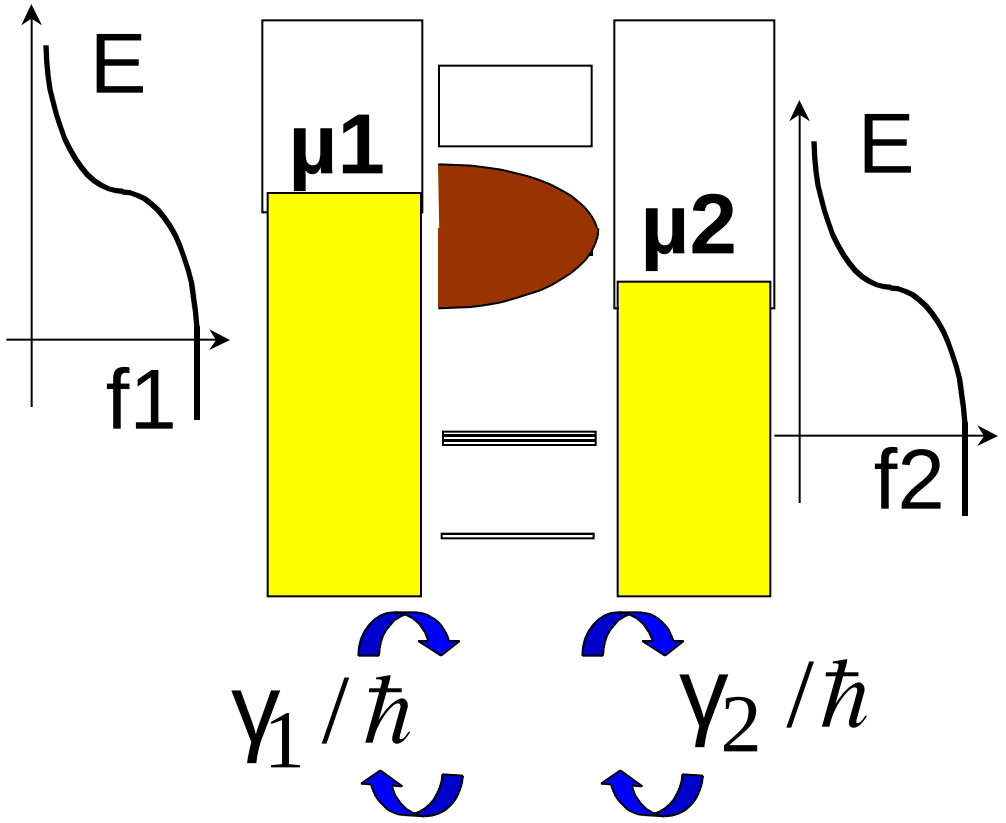


$$I \sim \frac{q}{\hbar}\,\frac{\gamma_1\gamma_2}{\gamma_1+\gamma_2}\,\frac{qV}{\gamma_1+\gamma_2}$$



Toy model: Broadening



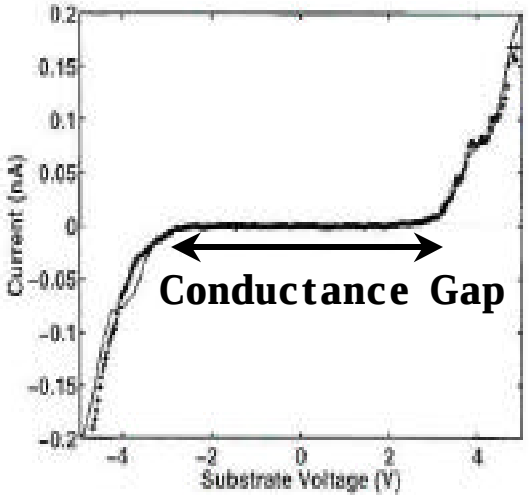


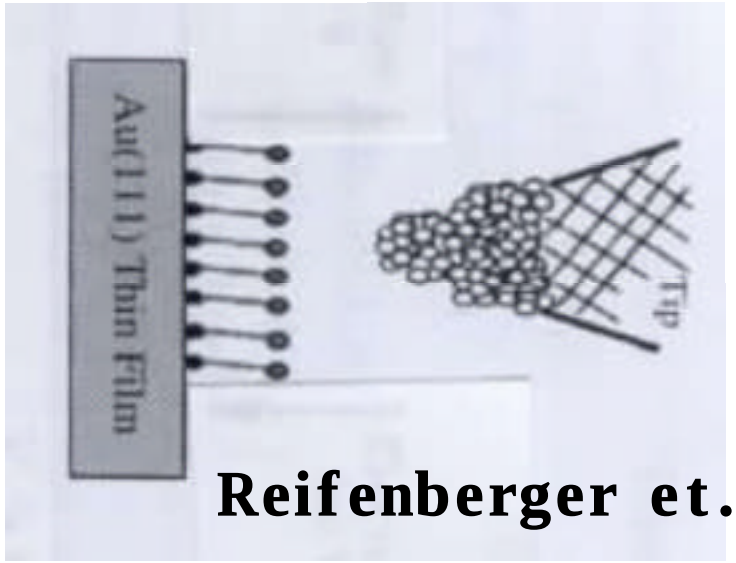
$$I \sim \frac{q}{\hbar}\frac{\gamma_1\gamma_2}{\gamma_1+\gamma_2}\frac{qV}{\gamma_1+\gamma_2}$$

Maximum conductance

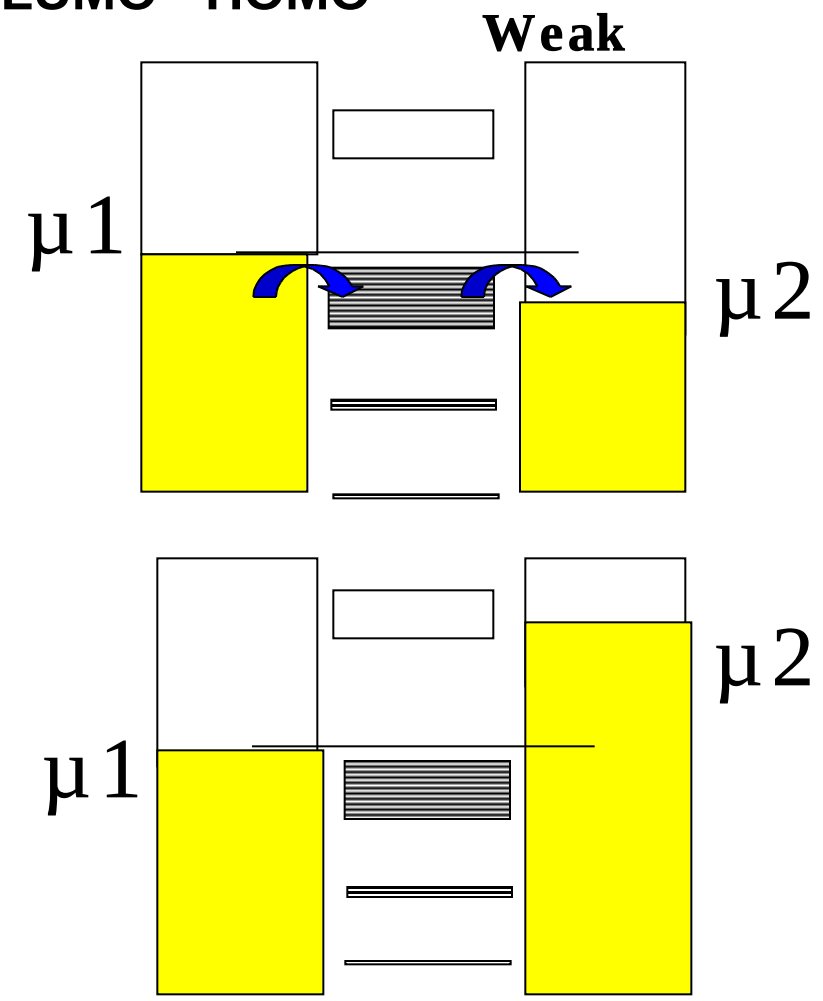
$$\frac{I}{V} \sim 2q^2/h \sim \frac{1}{12.9\,K\Omega}$$

Conductance Gap = ???

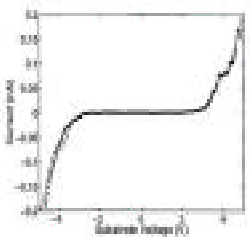




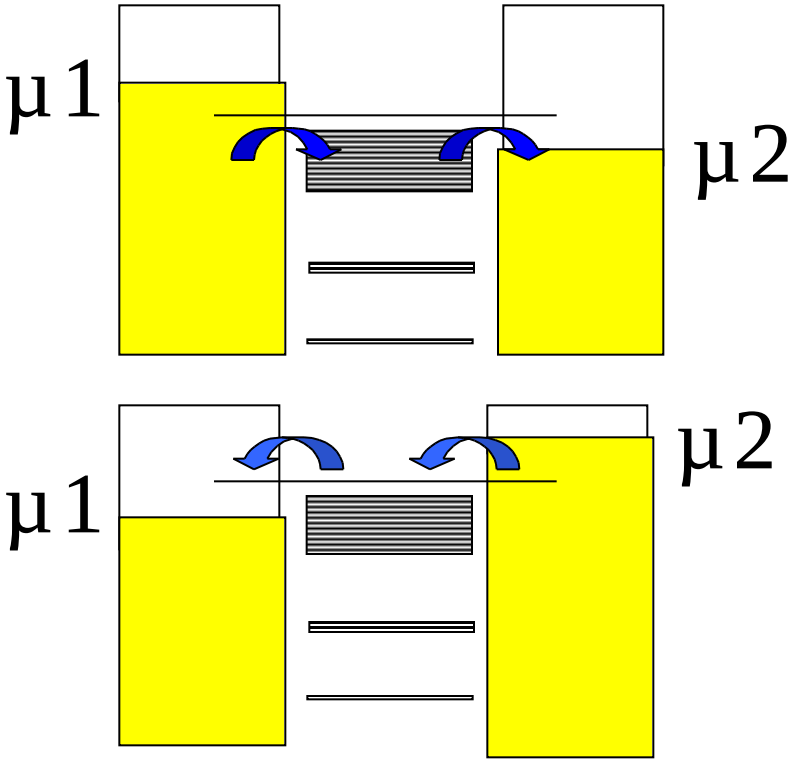
LUMO - HOMO



Conductance Gap = ???

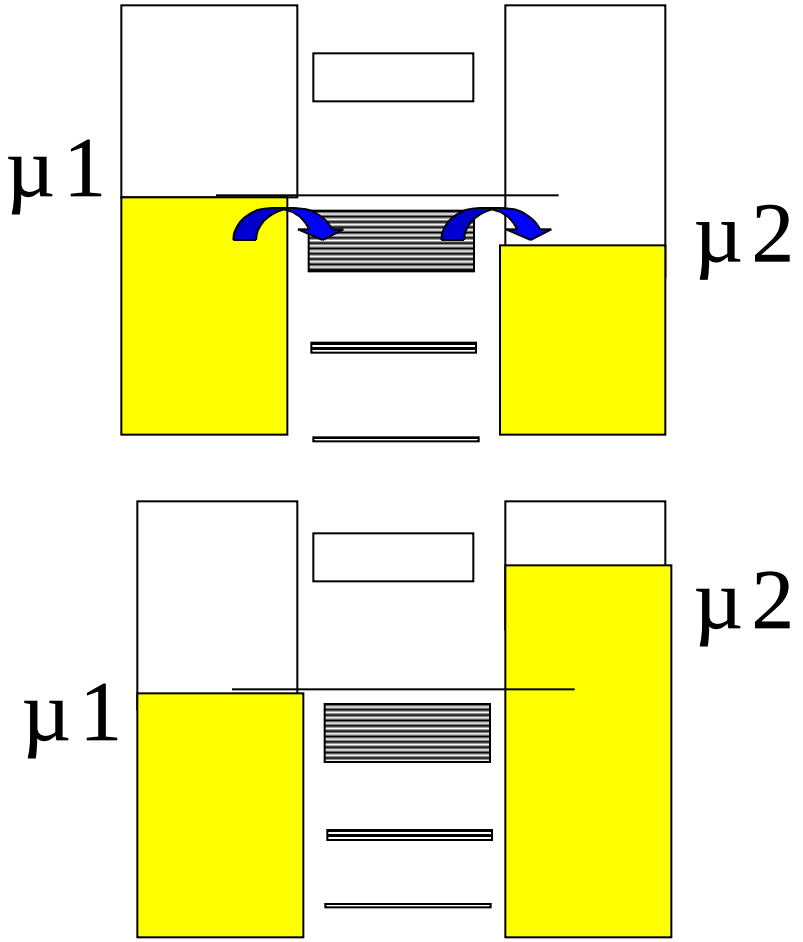


4 * (Ef - HOMO)

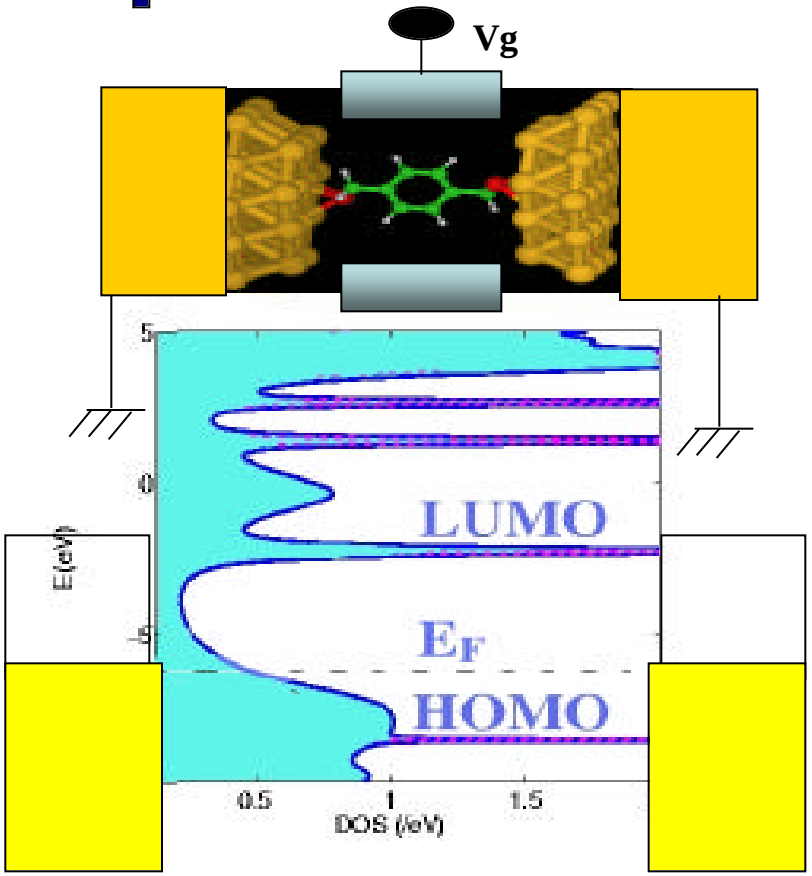


LUMO - HOMO

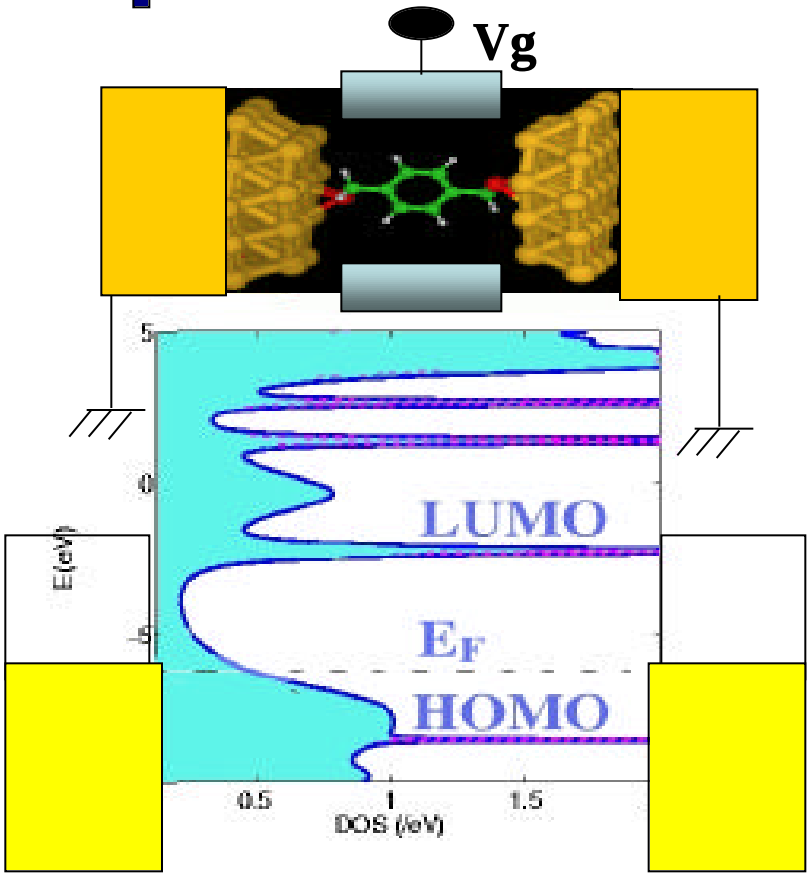
Weak

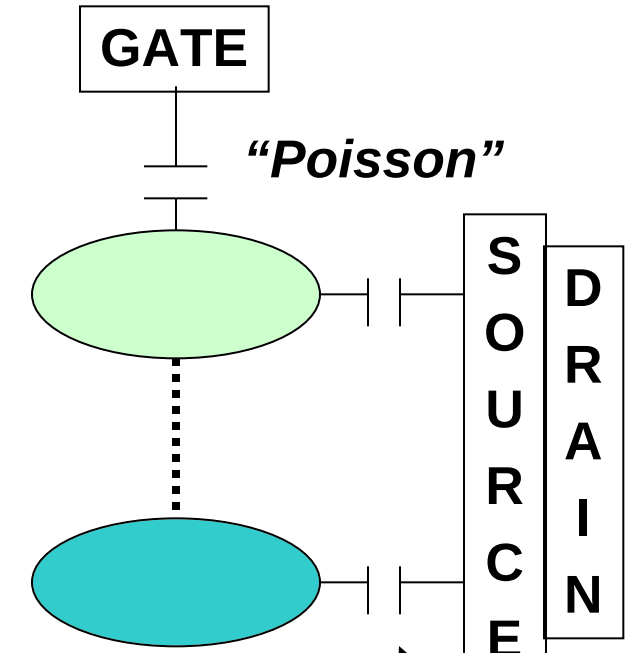


Equilibrium



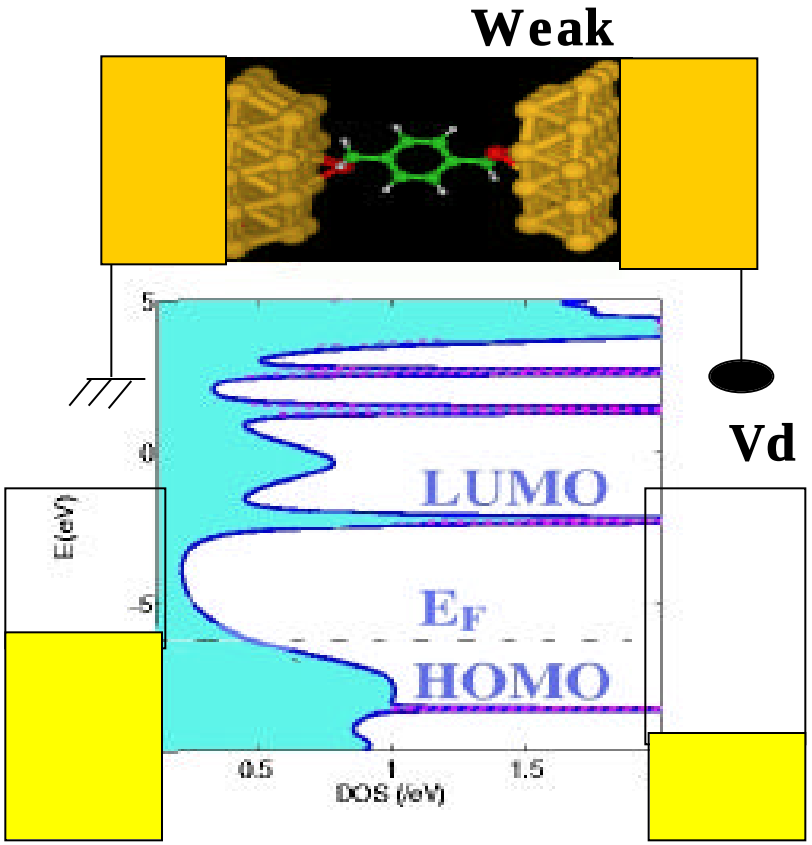
“Quantum Capacitance”

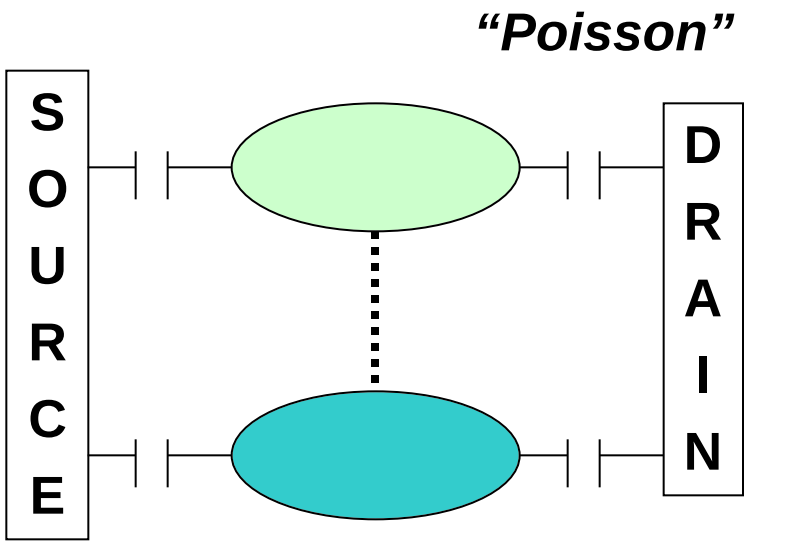




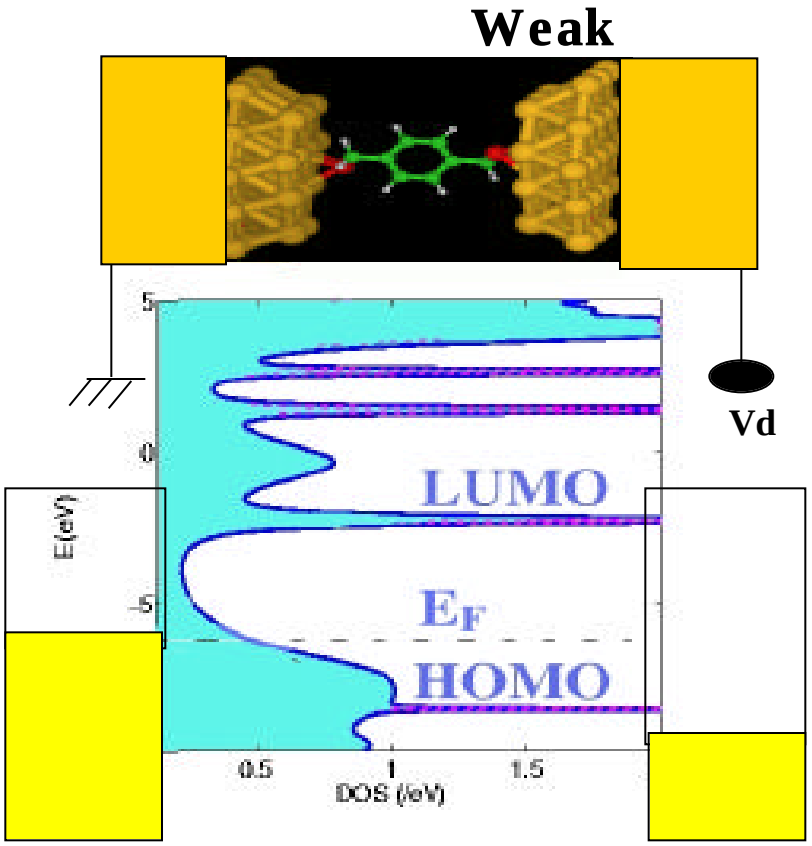
$$C_Q = q^2 D_0$$

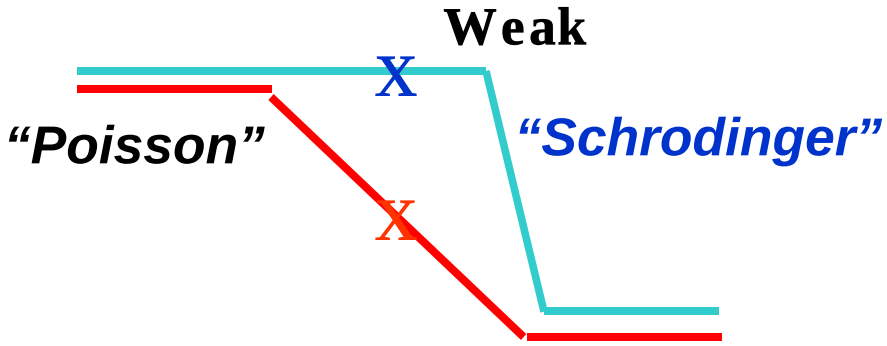
“Schrodinger” vs. “Poisson”

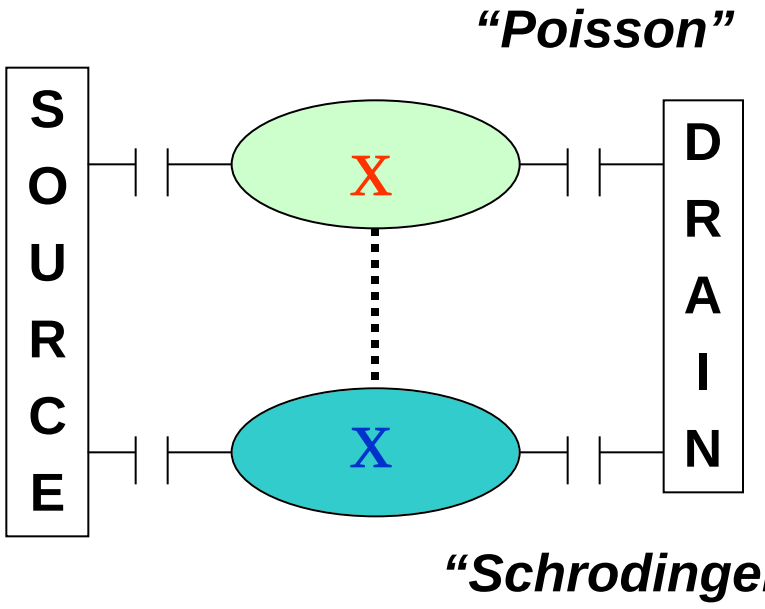




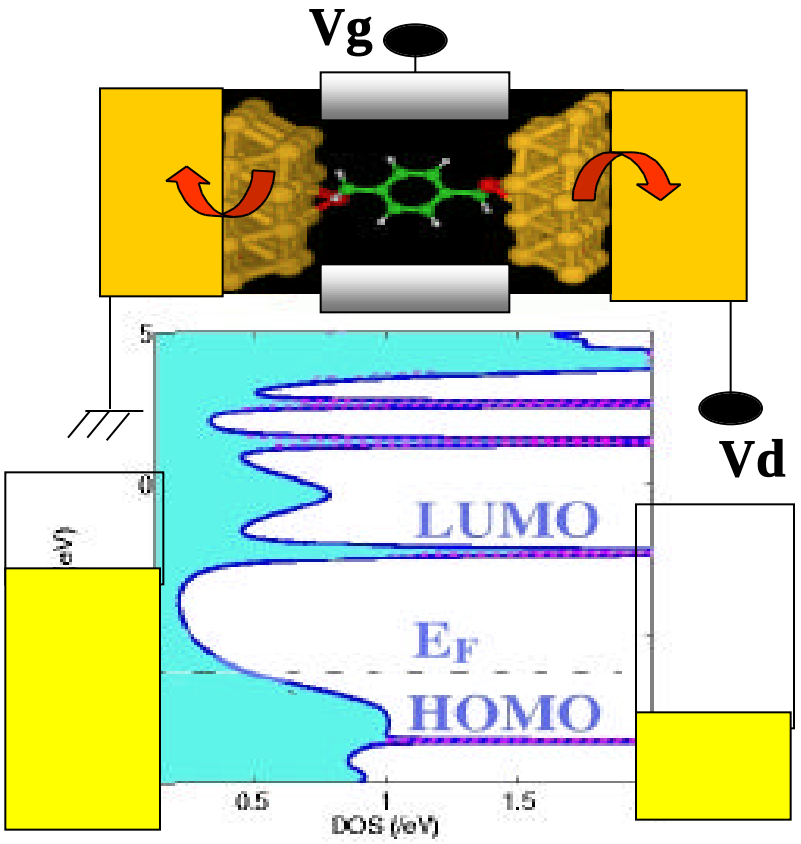
“Schrodinger” vs. “Poisson”







Minimal Physics: Broadening + Charging



"Poisson"

N --> U

Self-consistent

U --> N

"Schrodinger"

$(\{\varepsilon\}, \mu, \gamma_1, \gamma_2)$

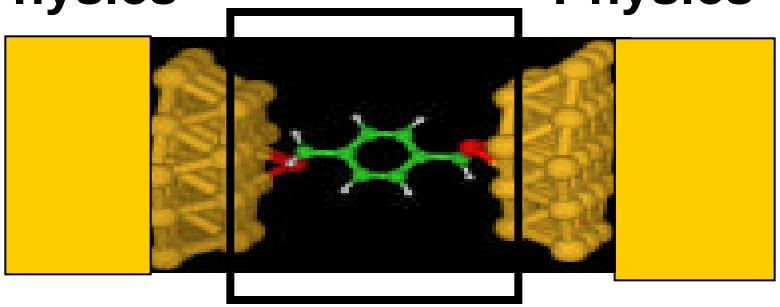
U --> I

Nanoscale MOS:

Rahman, Guo, Lundstrom

Numbers --> Matrices

Surface Physics | Quantum Chemistry | Surface Physics



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

DFT- based model

Modified Gaussian

Hybrid models

Under development

Ghosh,Liang,Rakshit,Damle

$$\varepsilon \rightarrow [H]$$

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

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

$$U \rightarrow [U]$$

$$N \rightarrow [\rho]$$

Toy model

EHT- based model

www.nanohub.purdue.edu

Paulsson, Zahid, Goasguen

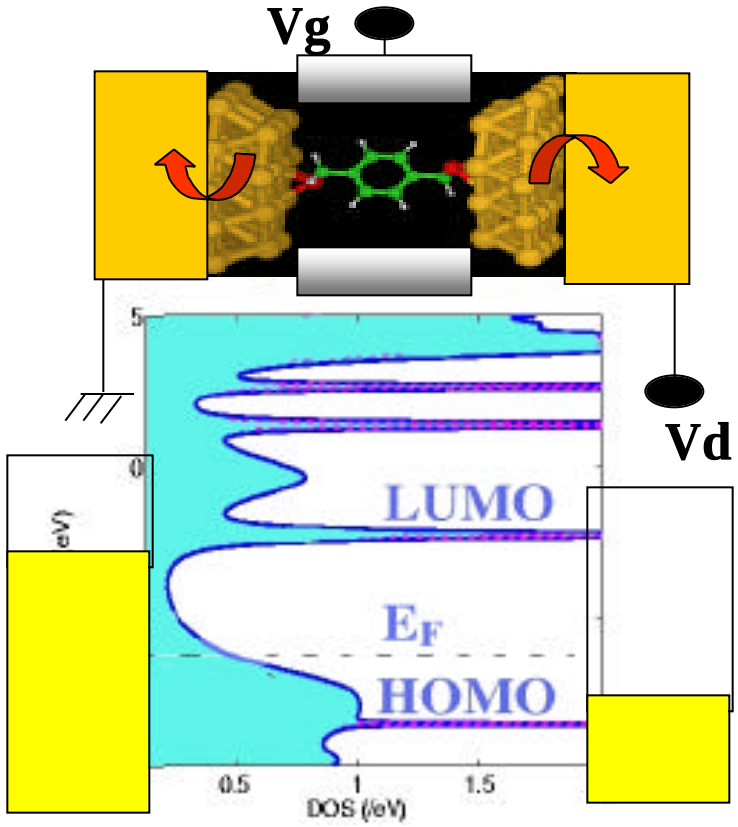
Inflow / Outflow

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

Out In

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

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

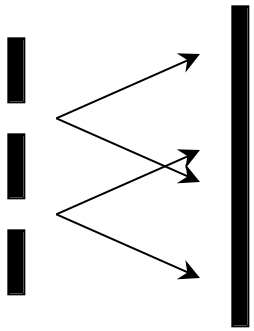


Inflow / Outflow

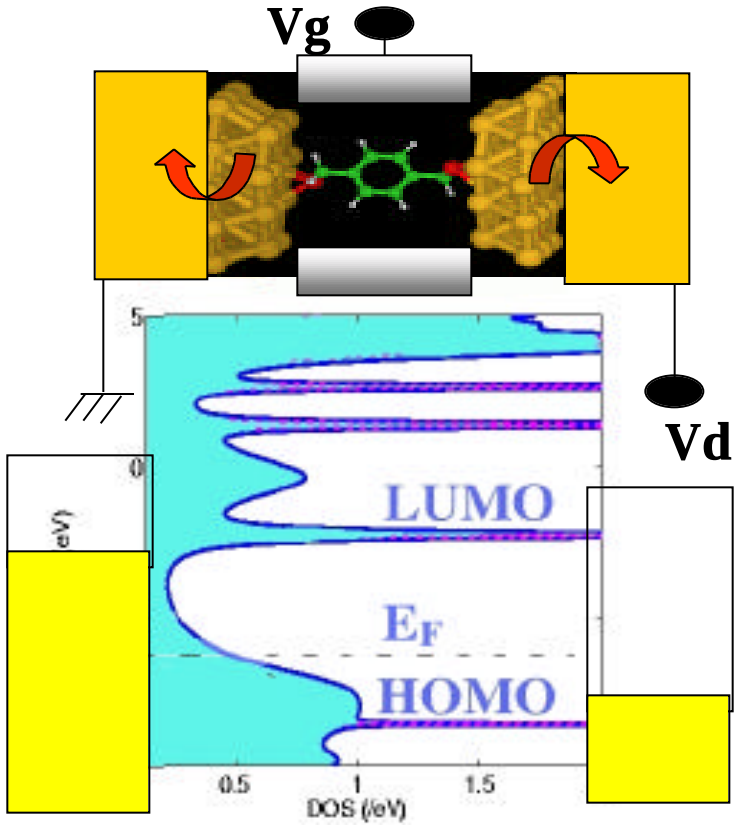
$$\hbar \frac{d}{dt} N + \gamma_1 N = \gamma_1 f_1$$

Out In

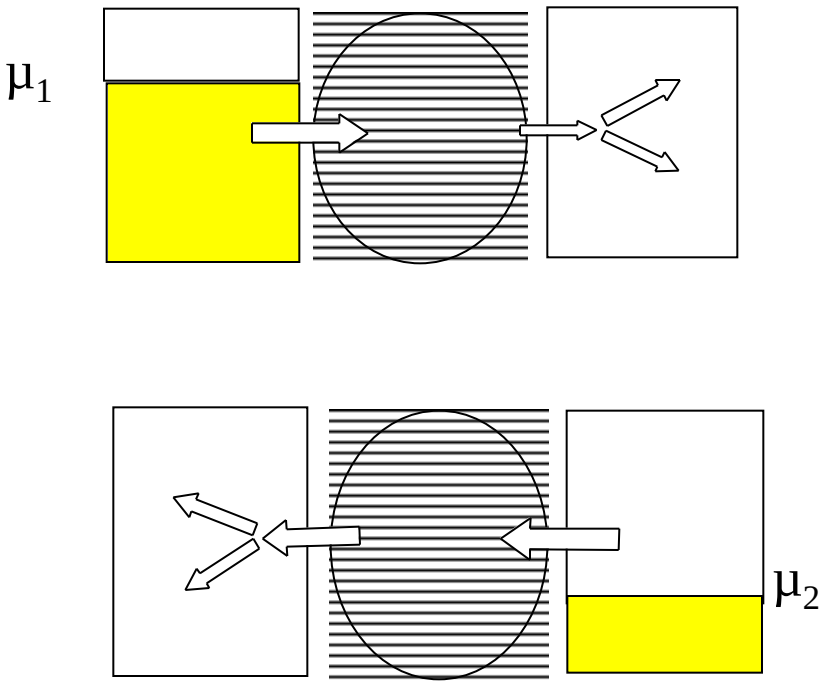
$$i\hbar \frac{d}{dt} \psi - H\psi - \Sigma_1 \psi = S_1$$



Each contact eigenstate
"illuminates" the channel
like an independent "slit"



Pauli blocking?



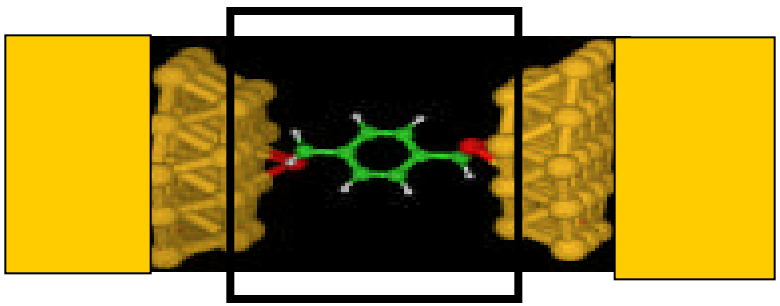
$$|1'\rangle = \exp\left[-iHt/\hbar\right]|1\rangle$$

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

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

NOT applicable to phase-breaking processes

Phase-breaking

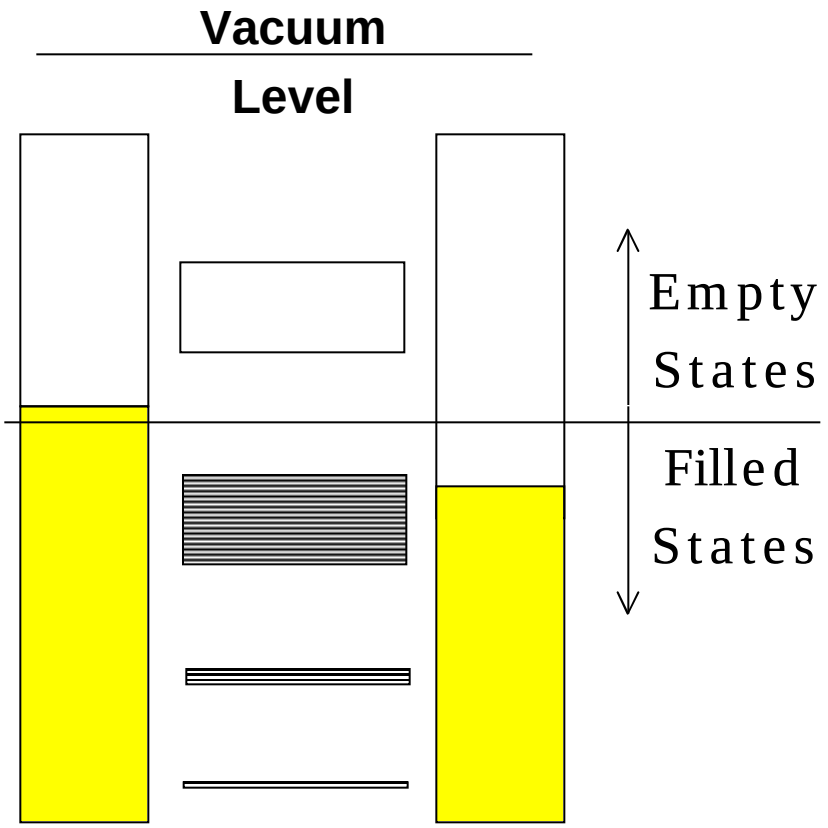


$$i\hbar \frac{d}{dt}\psi - H\psi - \Sigma_P \psi = S_P$$

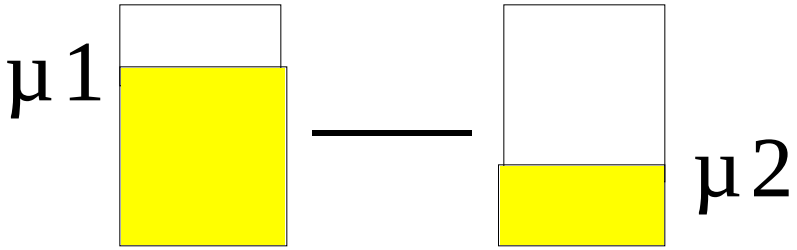
In

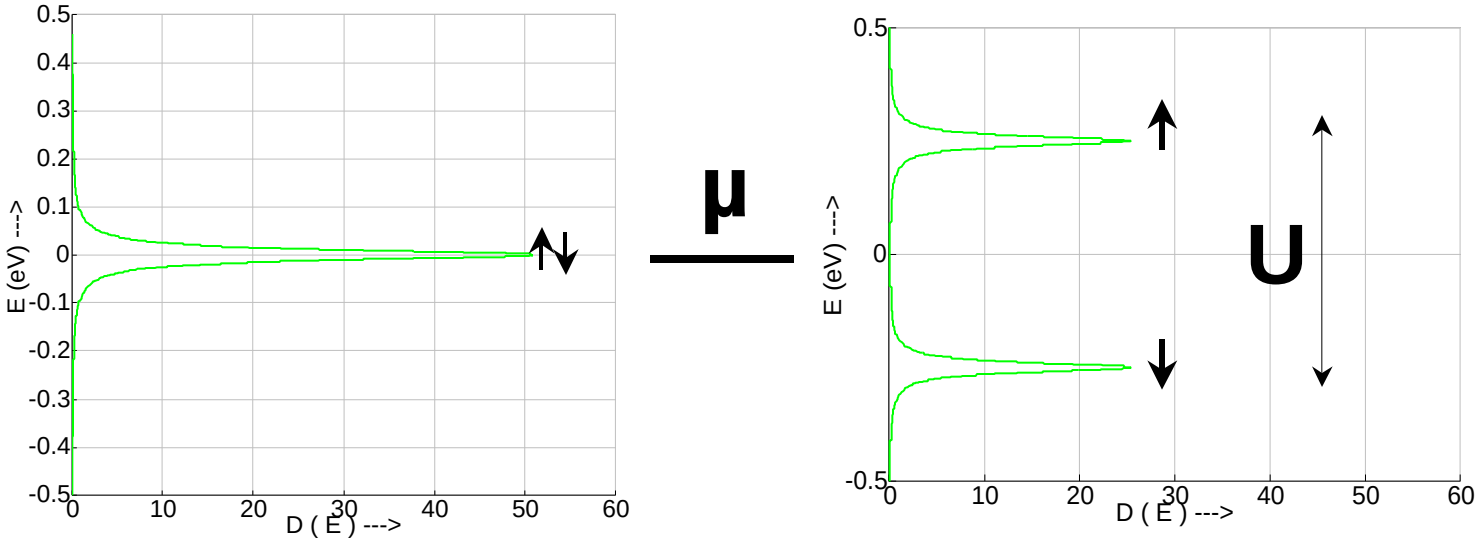
Out

Σ_P , S_P **depend on 'f'**



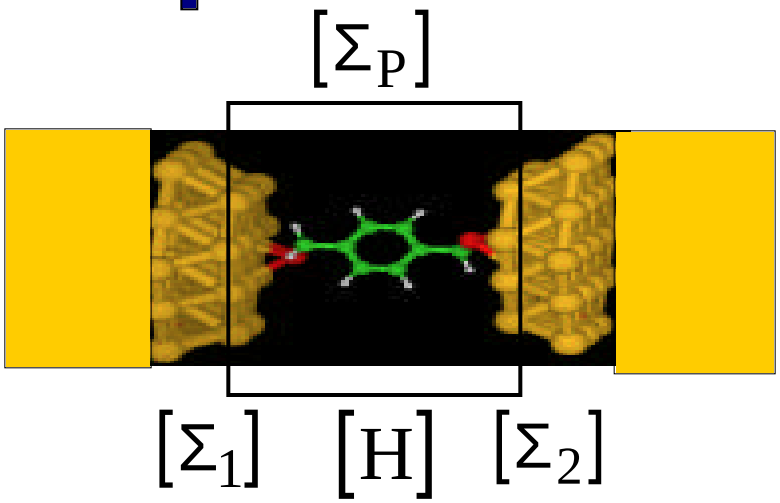
Coulomb blockade ($\Gamma << U$)

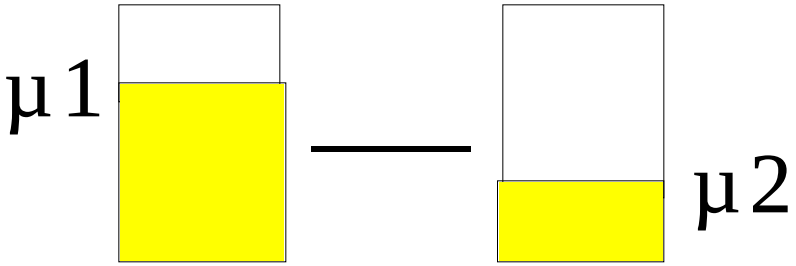




$$\Gamma \ << \ U \ \sim \ q^2 / 4\pi\varepsilon R$$

Kondo Resonance (Γ ~ U)

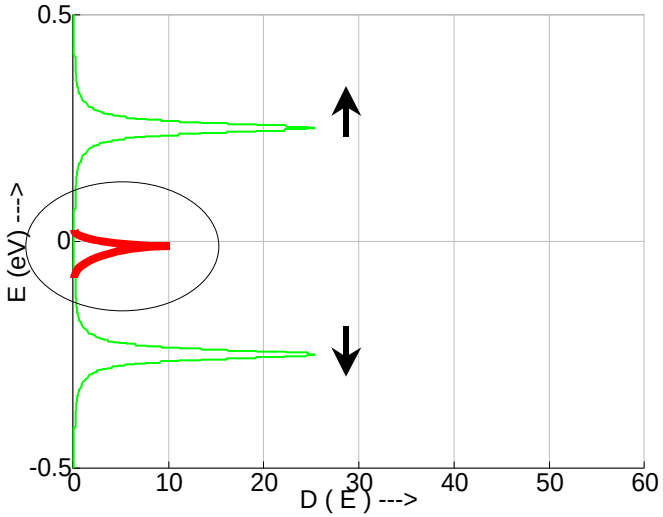




In

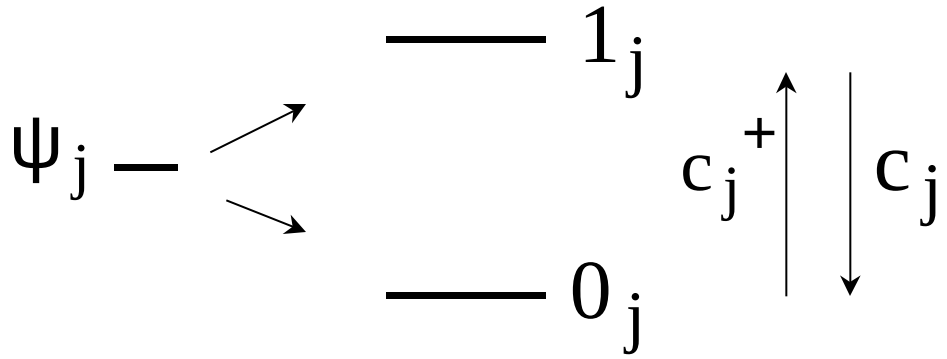
$$i\hbar \frac{d}{dt}\psi - H\psi - \Sigma\psi = S$$

Out



Σ, S **depend on 'f'**

Second quantization

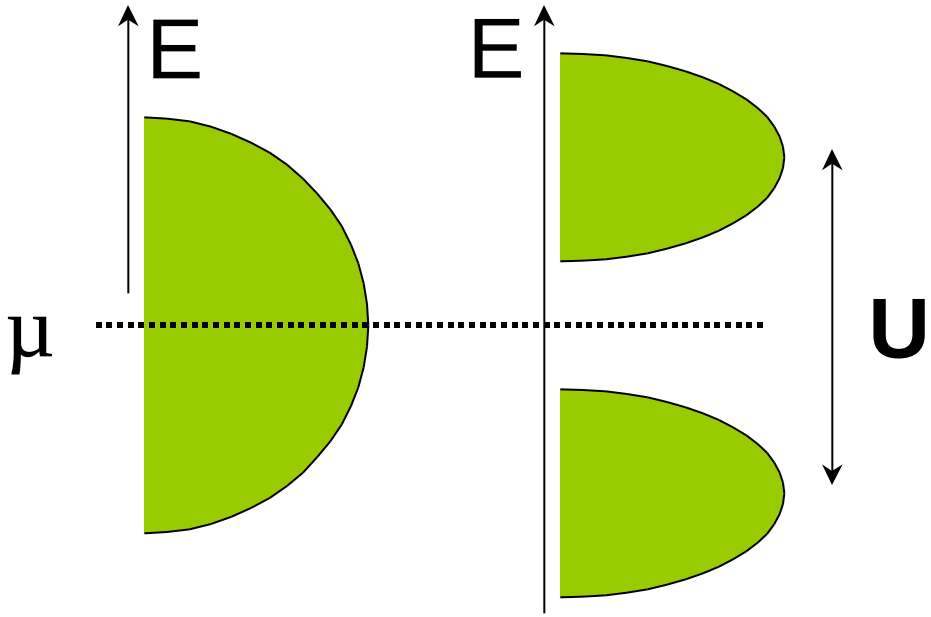


$$i\hbar \frac{d}{dt} \begin{pmatrix} c_L \\ c \\ c_R \end{pmatrix} = \begin{pmatrix} H_L & \tau^+ & 0 \\ \tau & H & \tau \\ 0 & \tau^+ & H_R \end{pmatrix} \begin{pmatrix} c_L \\ c \\ c_R \end{pmatrix}$$

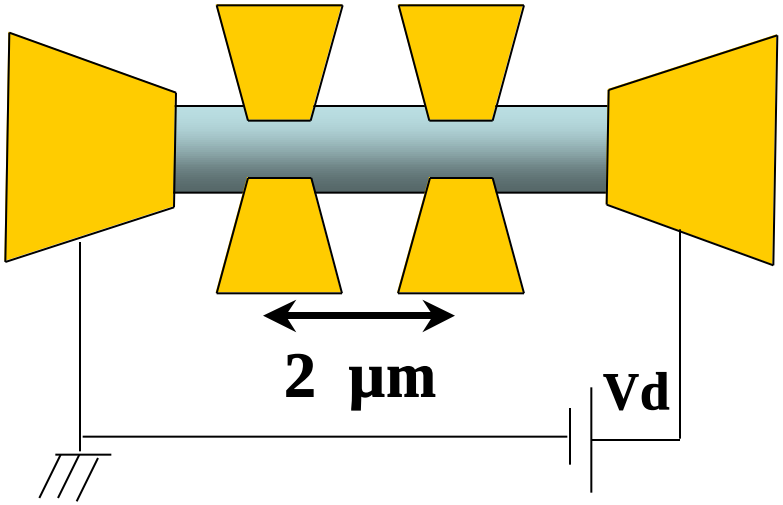
$$i\hbar \frac{d}{dt} c - Hc - \Sigma c = S + U d^+ d c$$

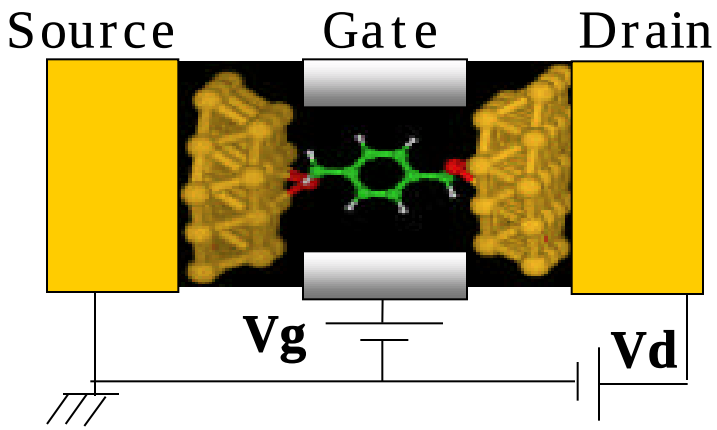
Solid state version

Mott transition



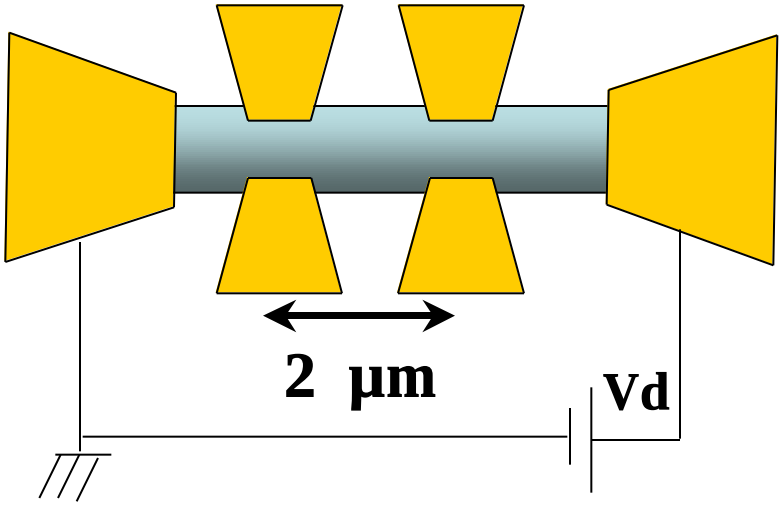
Electrical Resistance: Bottom-up view

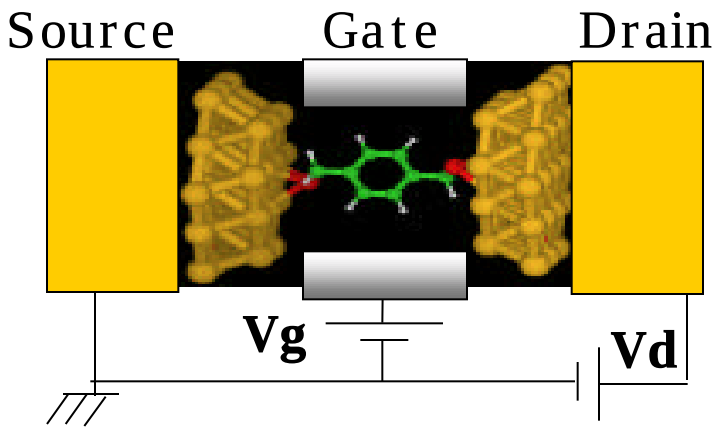




- Energy levels
- Electrochemical Potential
- Broadening
- Charging

Electrical Resistance: Bottom-up view





Phase- breaking processes

Conformational changes

Strong correlations

Summary

DFT- based model

Hybrid models

Ghosh, Damle, Liang,

Rakshit, Polizzi, Zahid,

Paulsson, Goasguen

Toy model

EHT- based model

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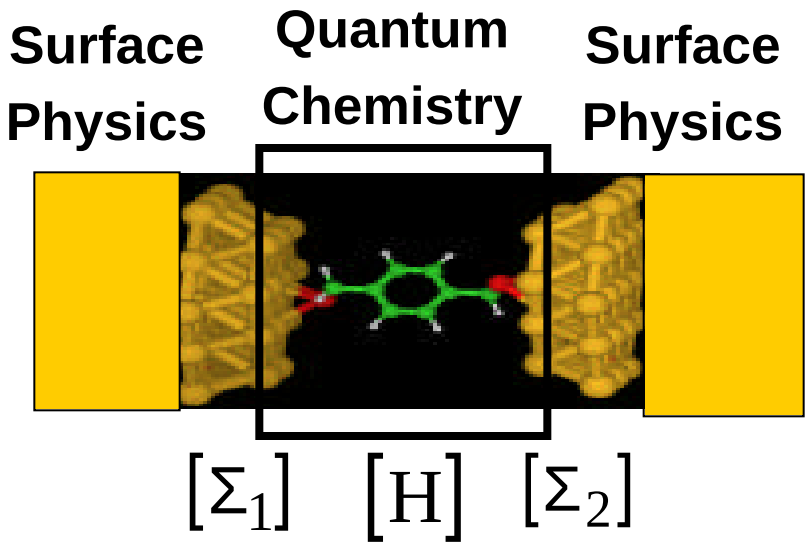
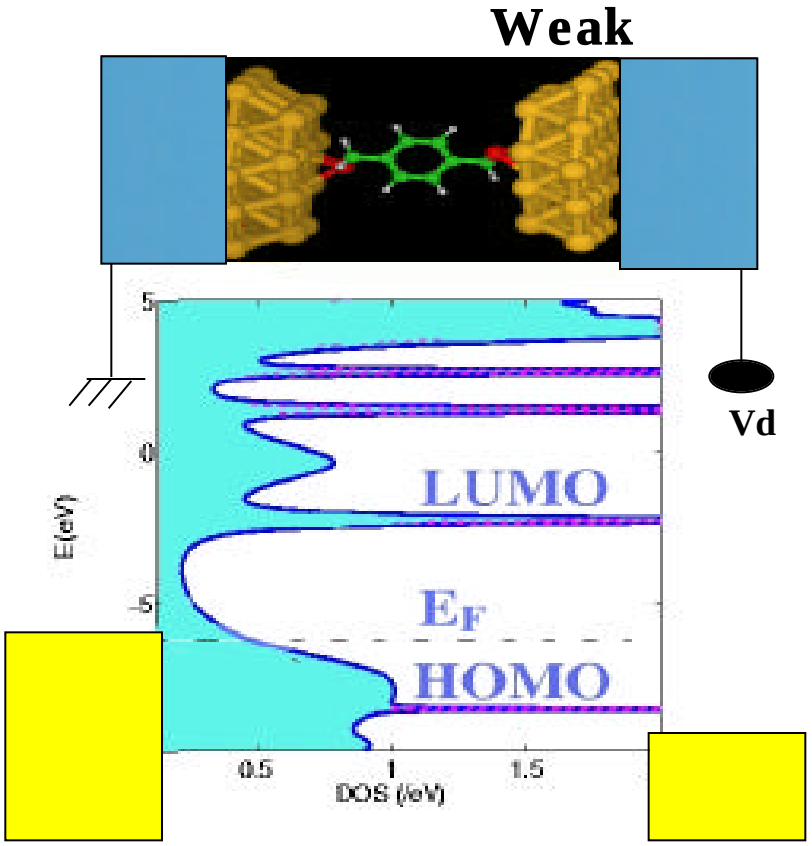
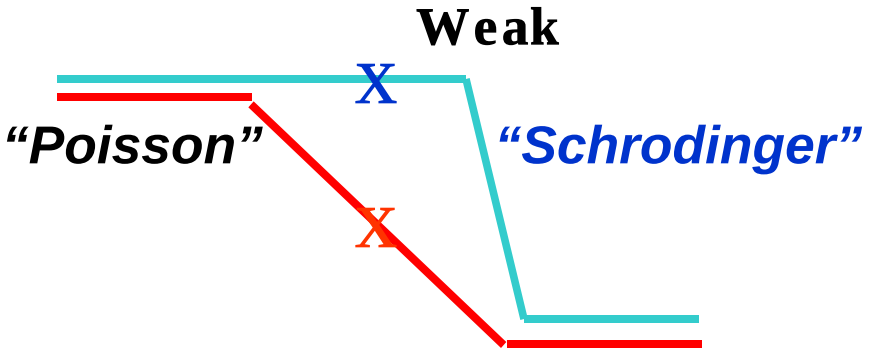


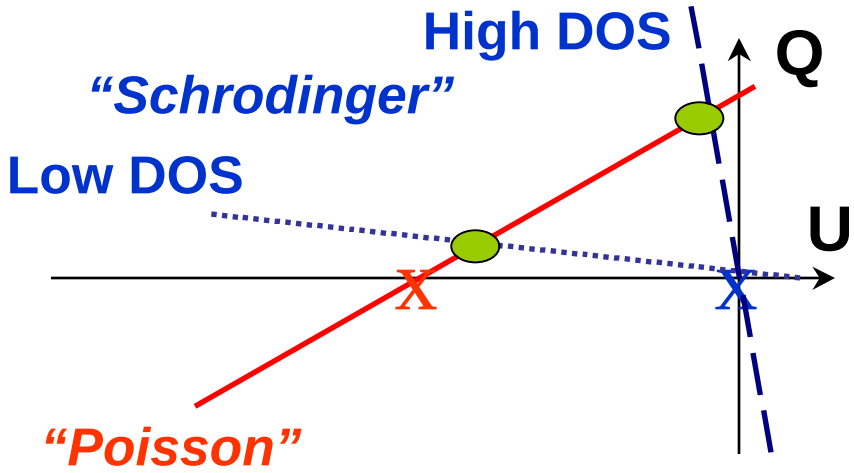
NanoMOS, Nanotubes

(Lundstrom et.al.)

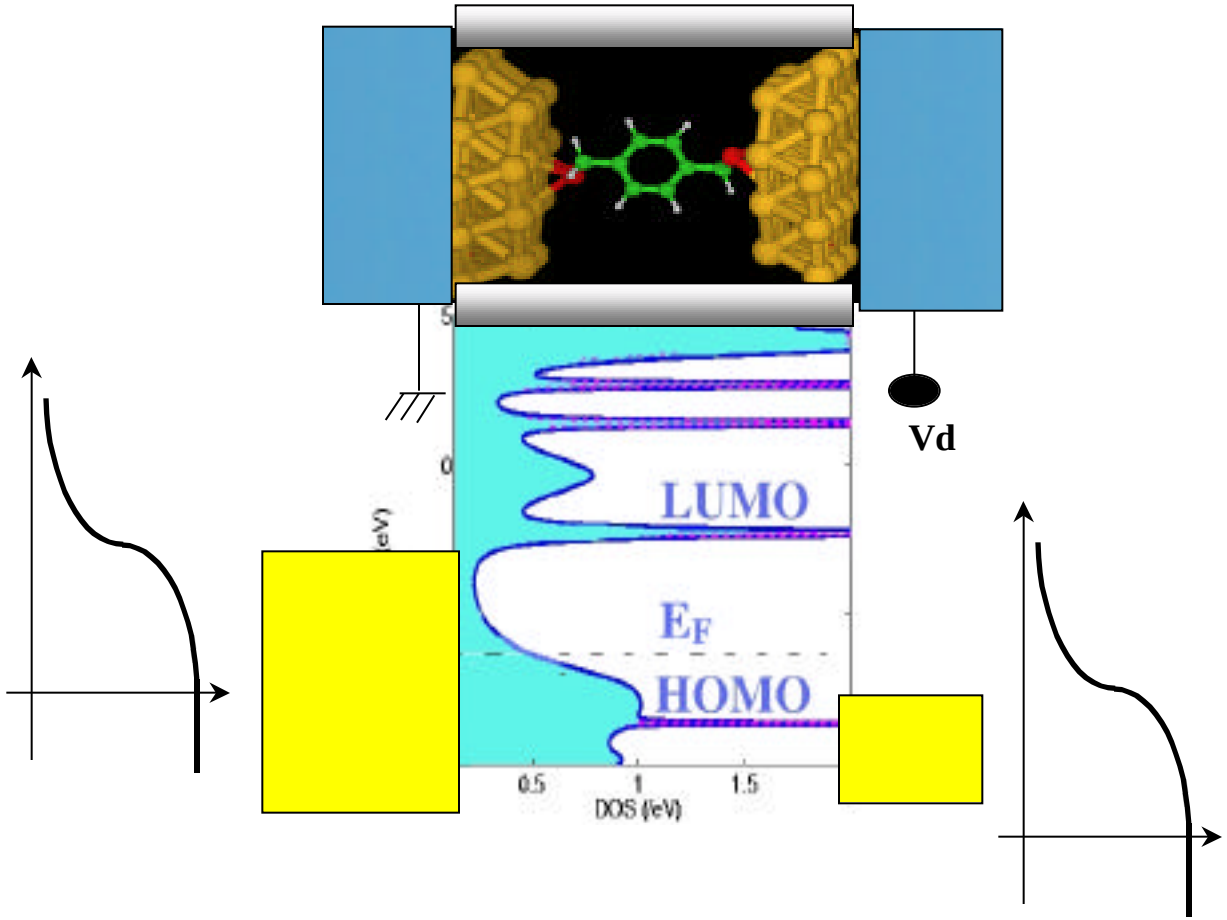
“Schrodinger” vs. “Poisson”





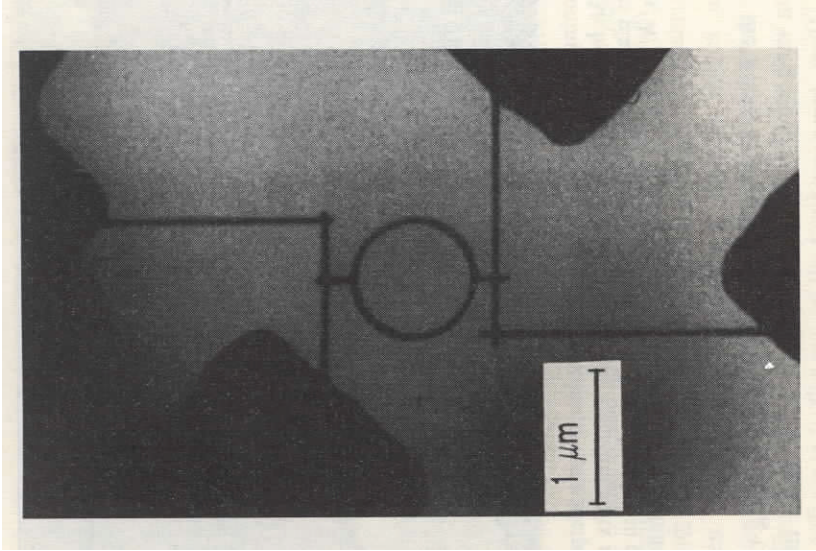


QMech + StatMech



Landauer Approach

Top-down and Bottom-up



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Webb, Washburn, Umbach