



NCN



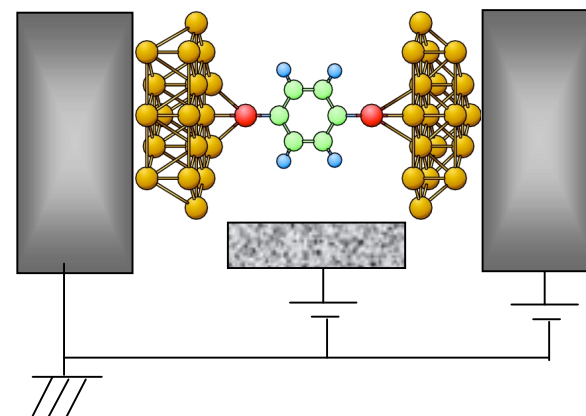
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NEGF Method: Capabilities and Challenges

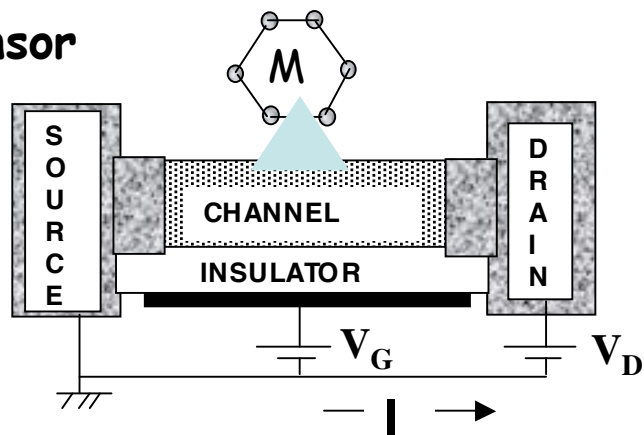
Supriyo Datta

School of Electrical &
Computer Engineering
Purdue University

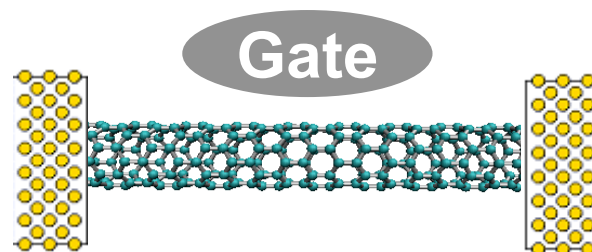
Molecular Electronics



Molecular Sensor



CNT Electronics





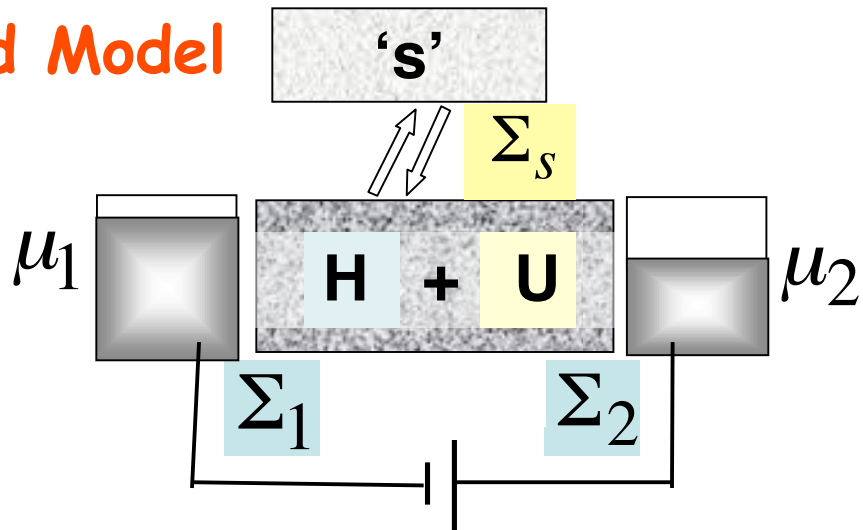
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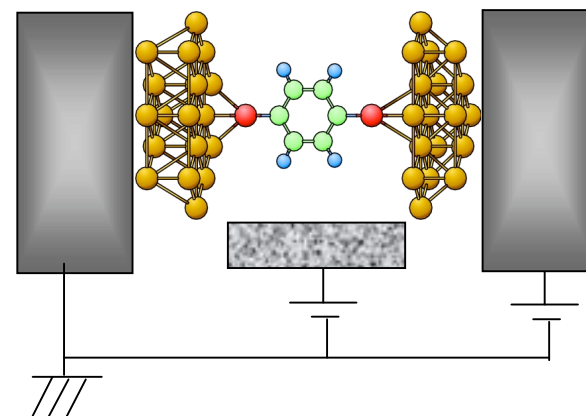
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Nanodevices: A Unified View

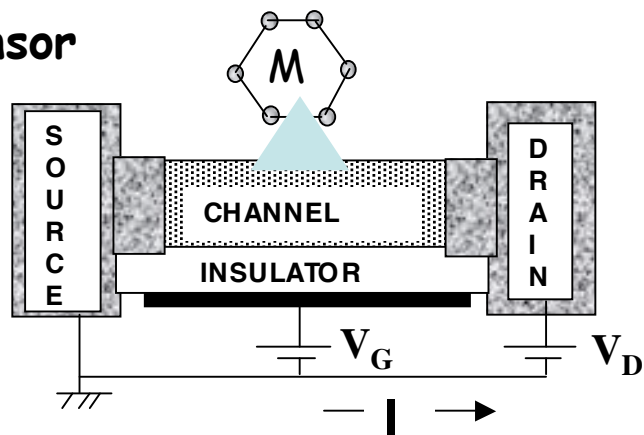
Unified Model



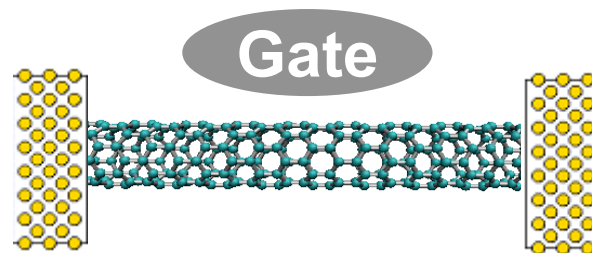
Molecular Electronics



Molecular Sensor



CNT Electronics



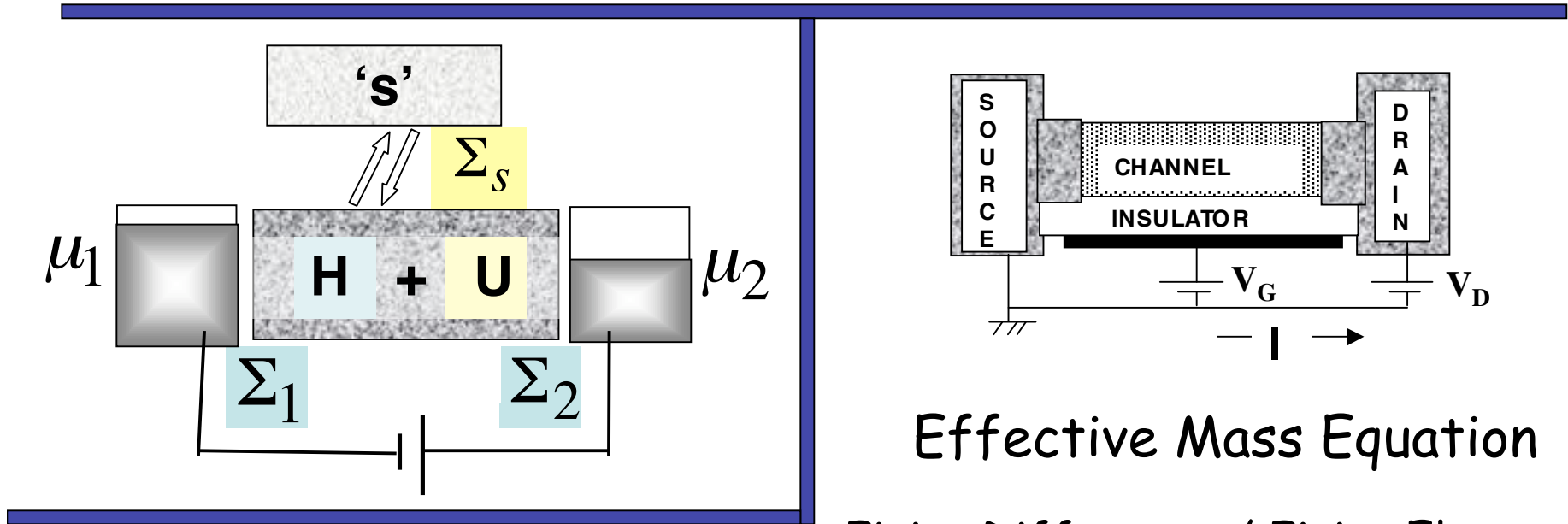


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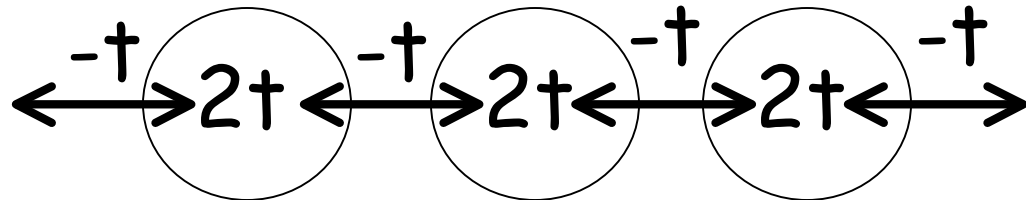
Hamiltonian, [H]



Effective Mass Equation

Finite Difference / Finite Element

$$t \equiv \hbar^2 / 2ma^2$$



Damle, Ren, Venugopal, Lundstrom ---> nanoMOS

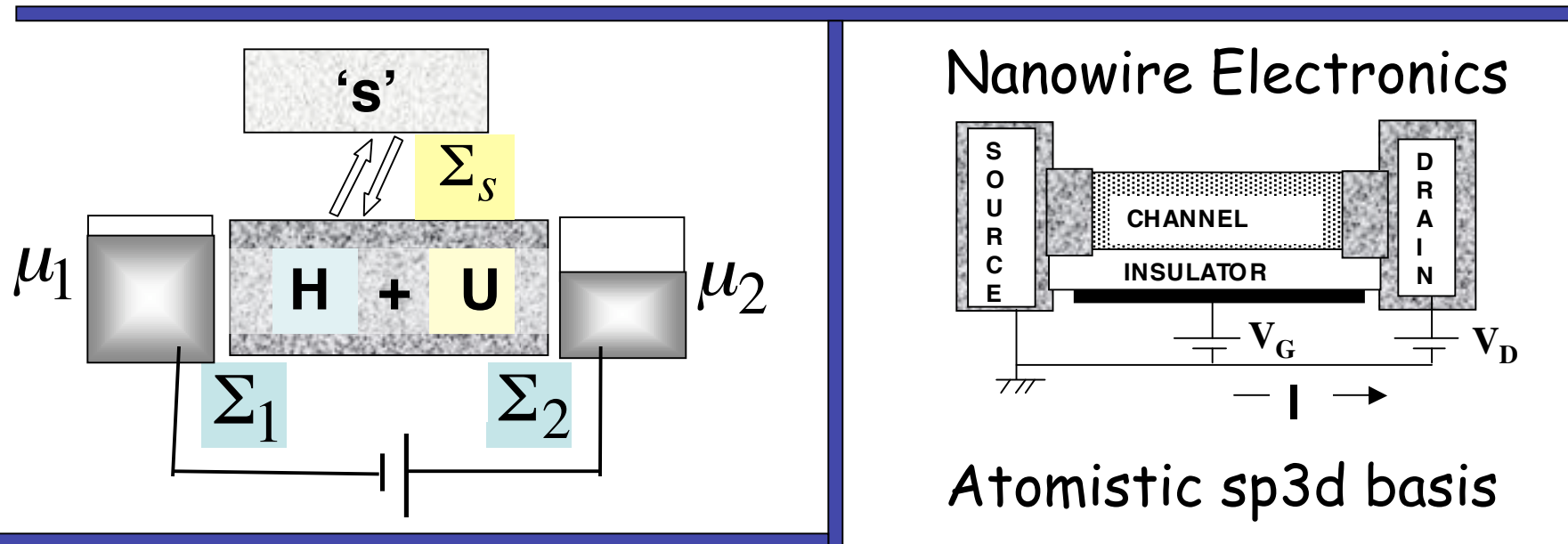


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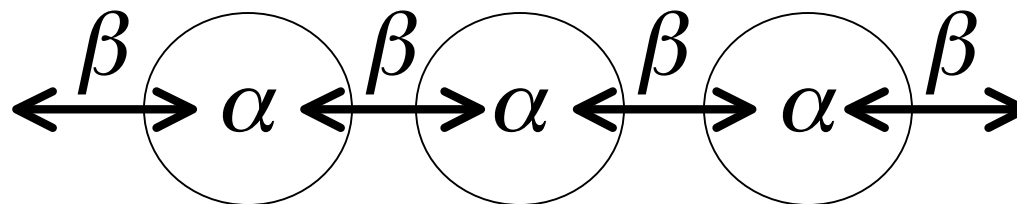


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Hamiltonian, [H]



α, β are matrices



Rahman, Wang, Ghosh, Klimeck, Lundstrom

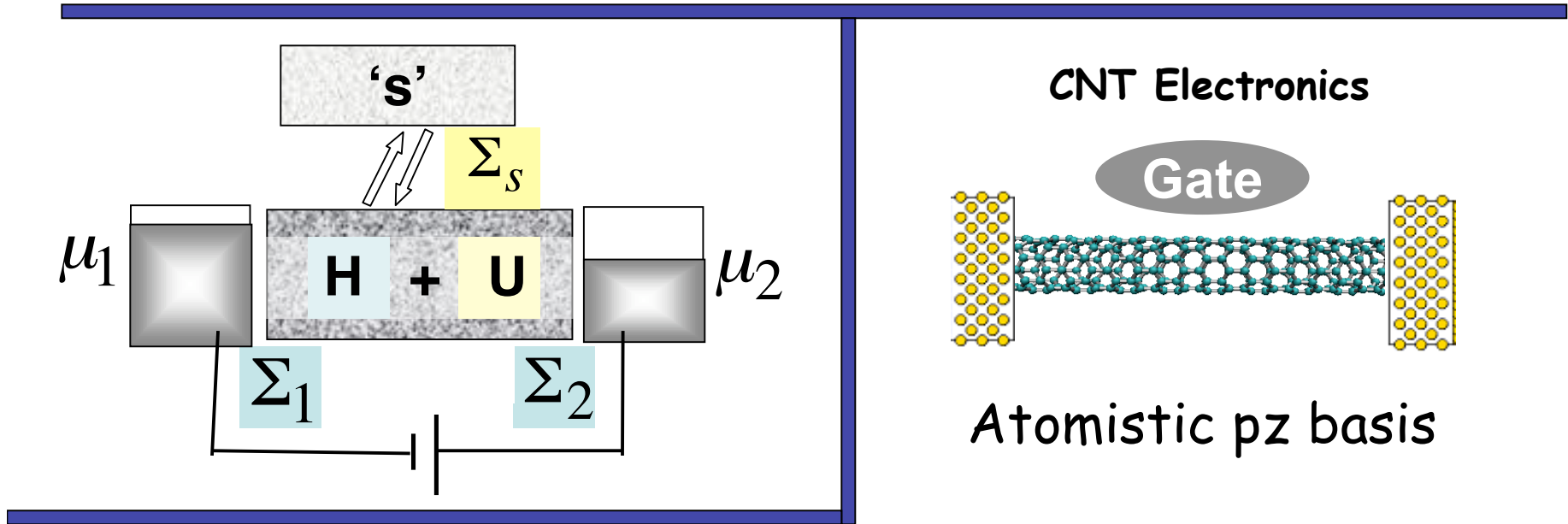


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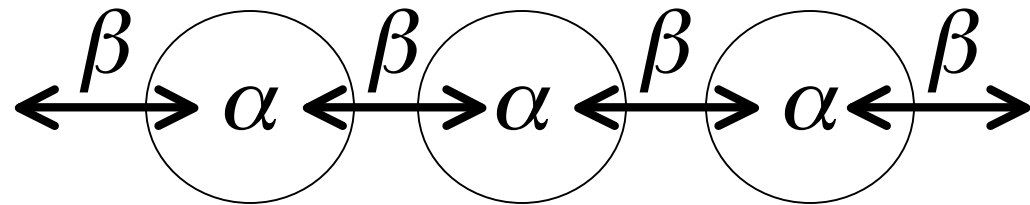


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Hamiltonian, [H]



α, β are (2x2) matrices



Guo, Lundstrom

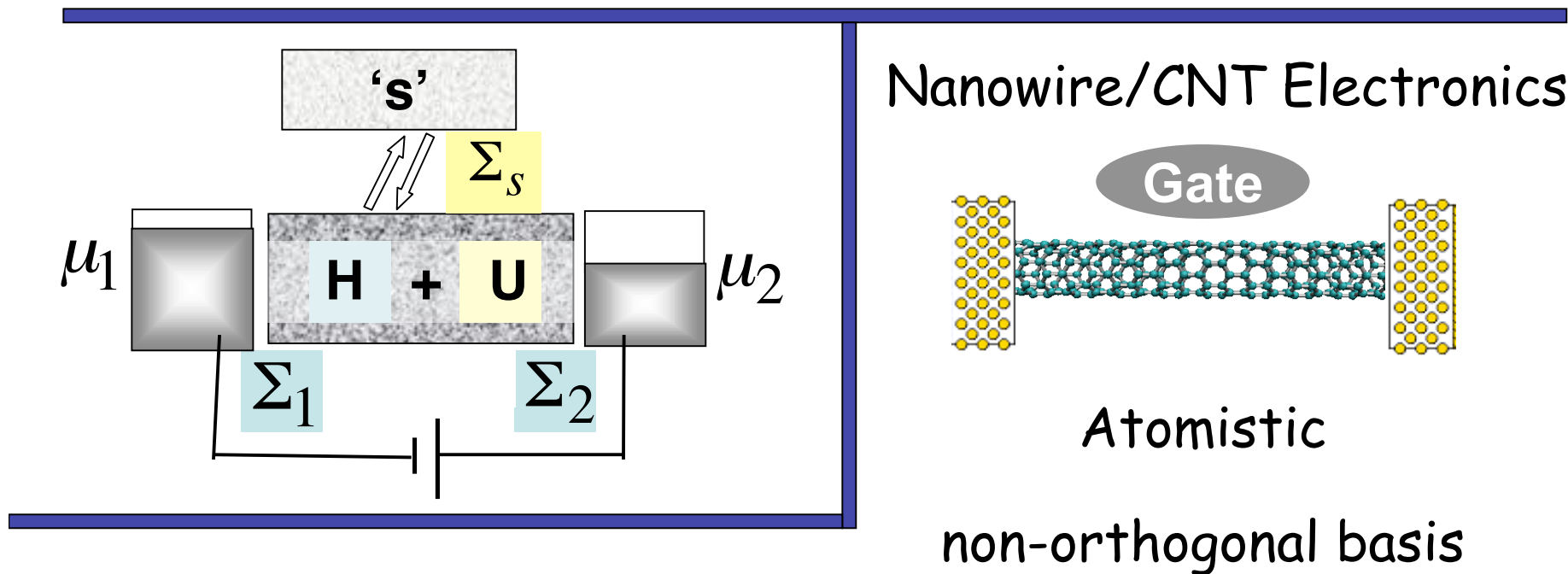


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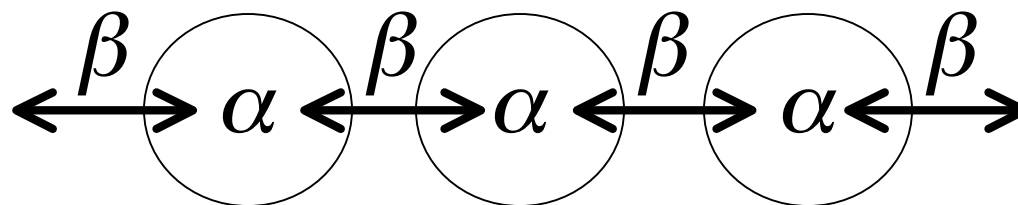


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Hamiltonian, [H]



EHT



Siddiqui, Kienle, Ghosh, Klimeck

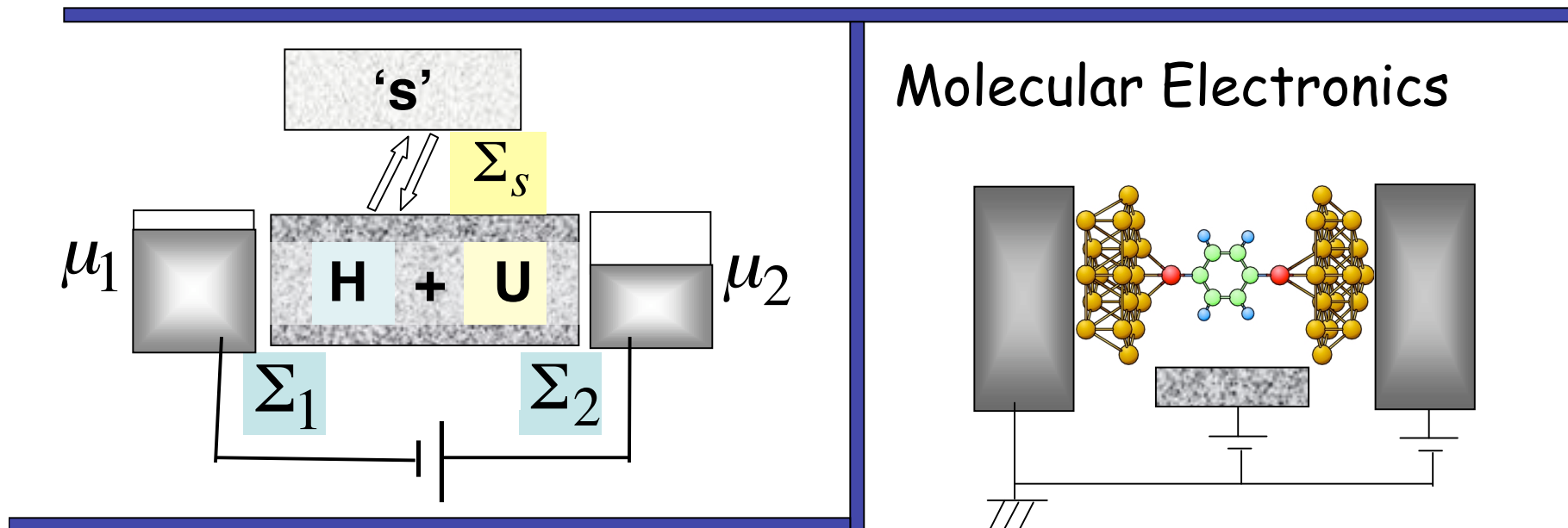


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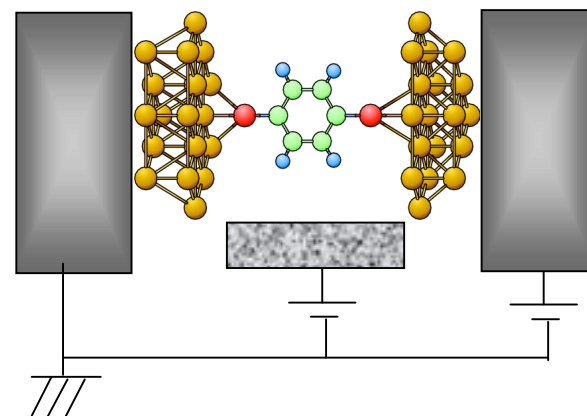


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Hamiltonian, [H]



Molecular Electronics



Atomistic basis:

Huckel / EHT / Gaussian

Ghosh, Rakshit, Liang, Zahid,
Siddiqui, Golizadeh, Bevan, Kazmi

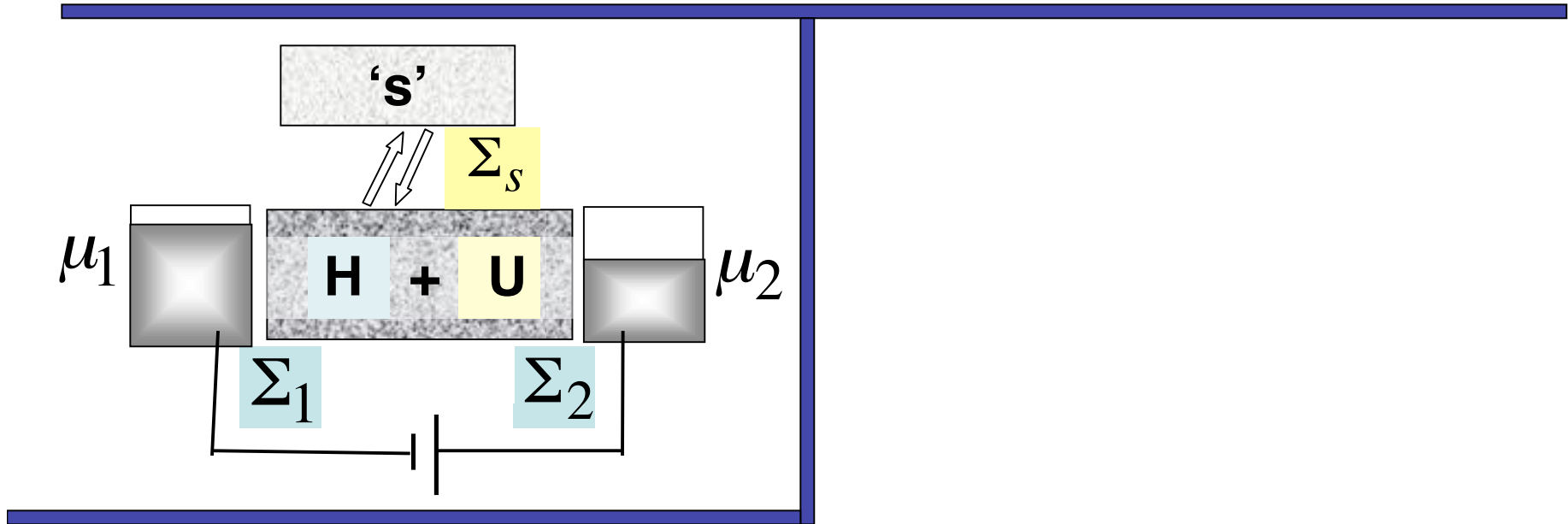


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"Self-energy", Σ



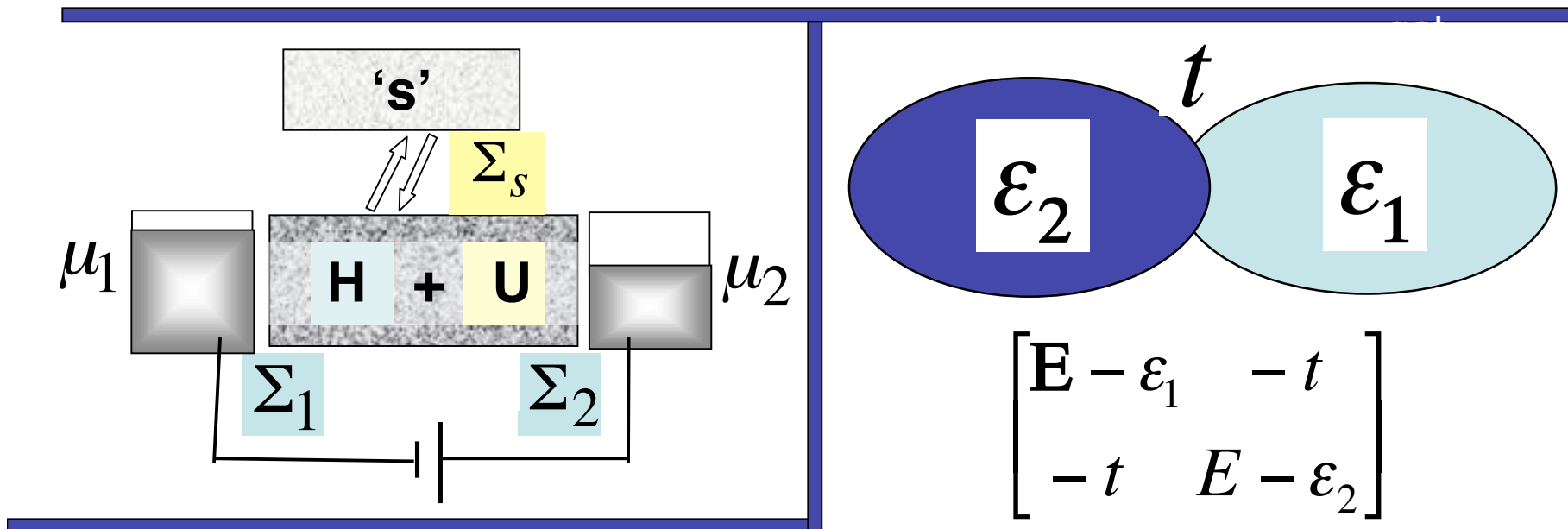


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"Self-energy", Σ



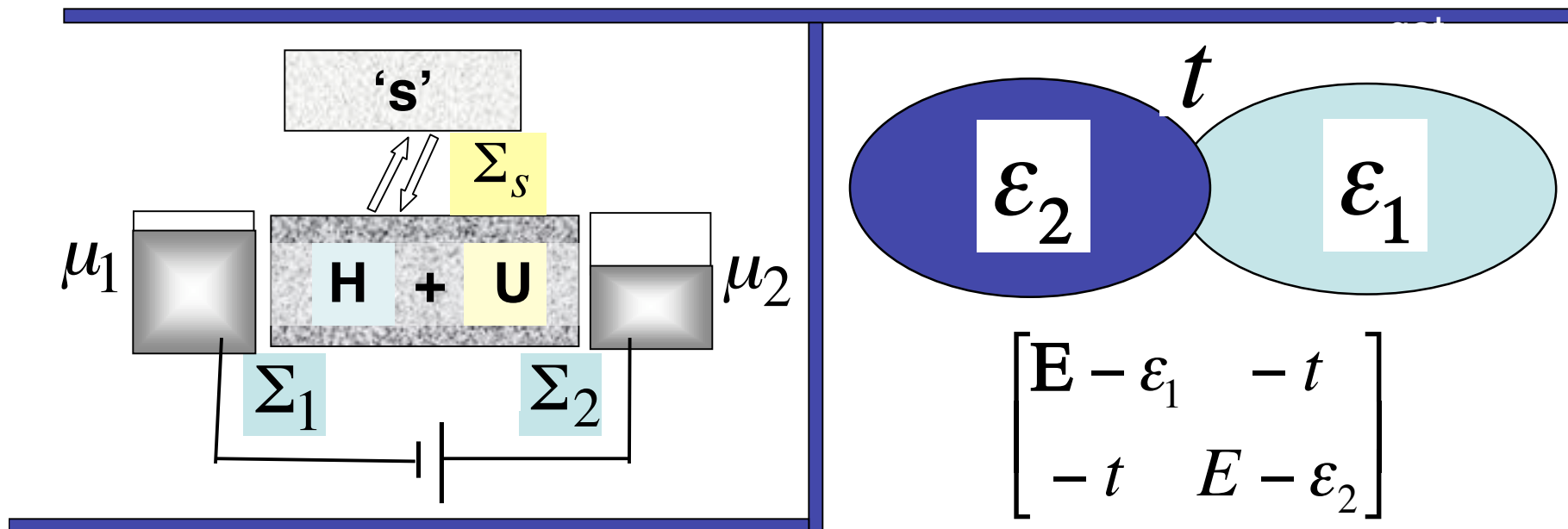


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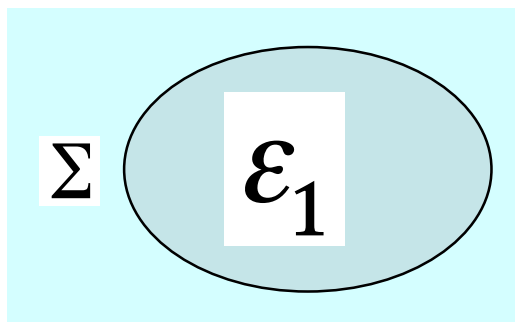
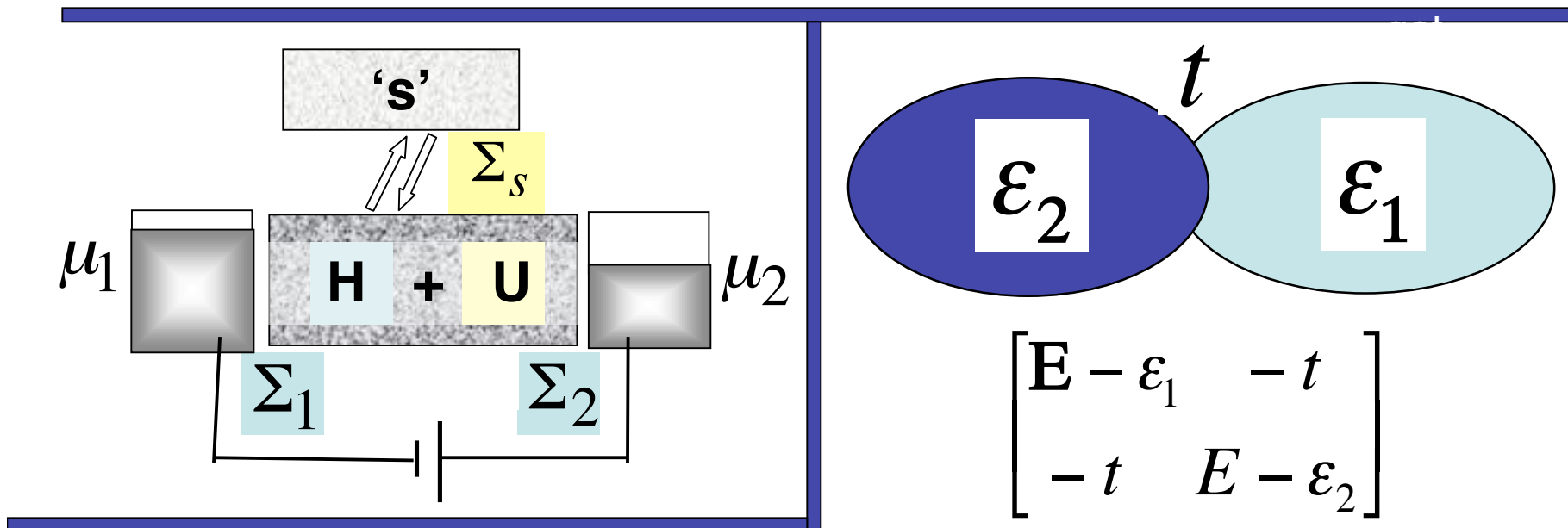
"Self-energy", Σ



$$\left[E - \epsilon_1 - \frac{t^2}{E - \epsilon_2} \right]$$



"Self-energy", Σ



$$\left[E - \epsilon_1 - \frac{t^2}{E - \epsilon_2} \right]_{\Sigma}$$

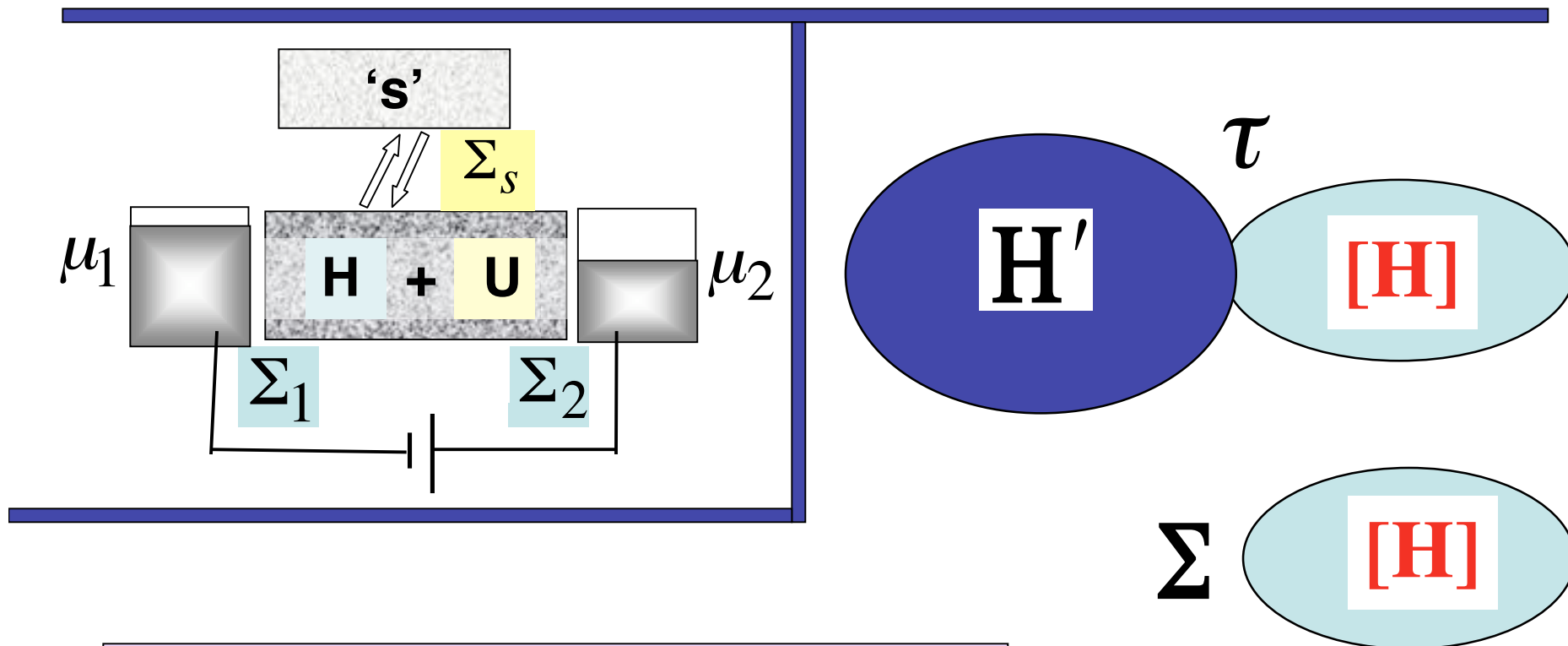


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"Self-energy", Σ



$$\Sigma = \tau [ES - H']^{-1} \tau^+$$

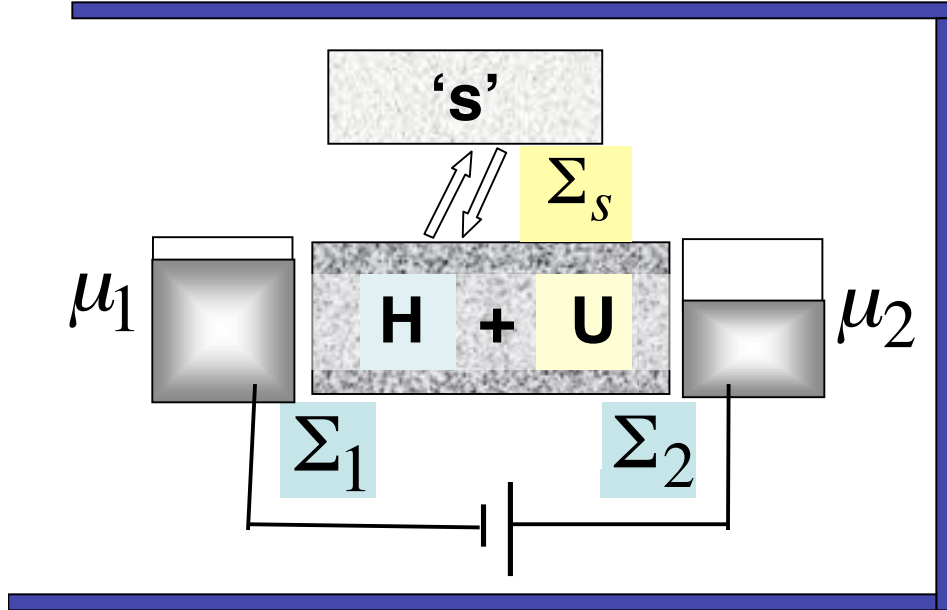


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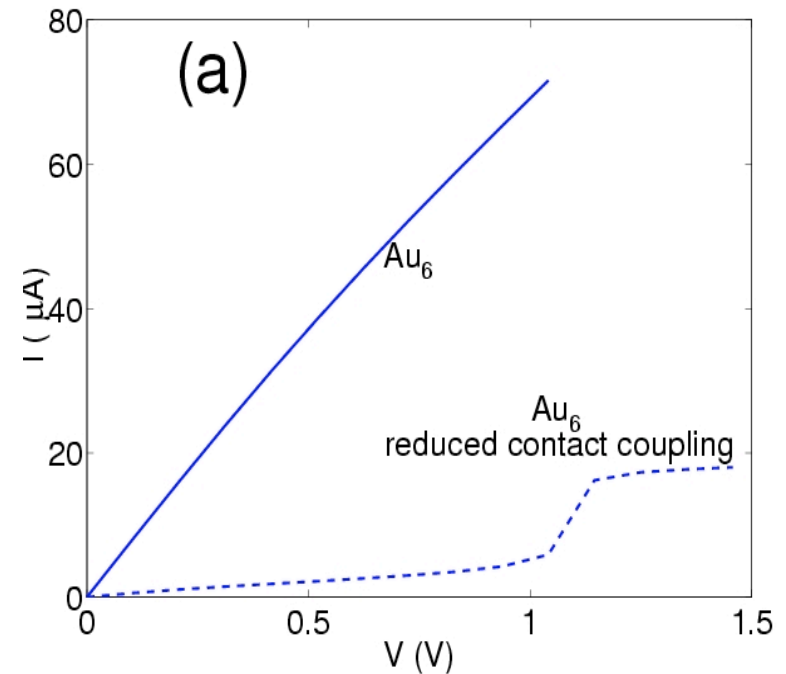
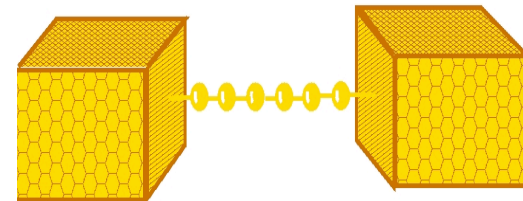


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From molecule to QPC



Au_6 "molecule"



$$\Sigma = \tau [ES - H']^{-1} \tau^+$$

Damle, Ghosh PRB (2001)

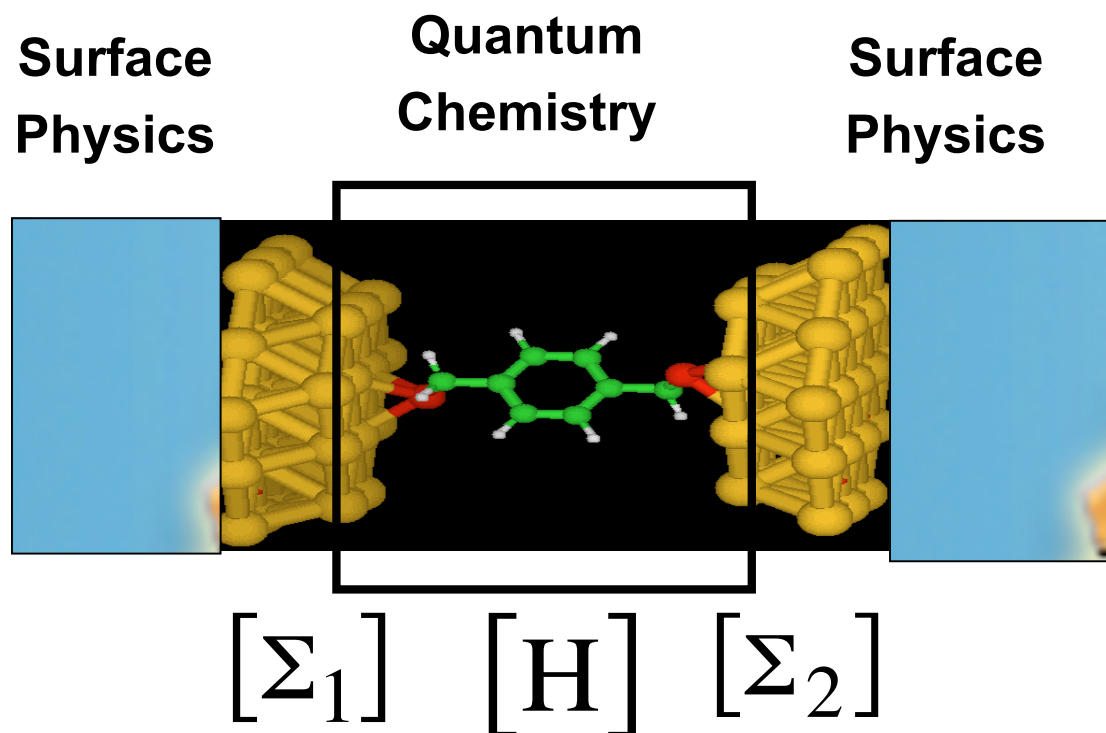


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Bridging Disciplines



Basis mixing: Ghosh, Liang, Kienle, Polizzi

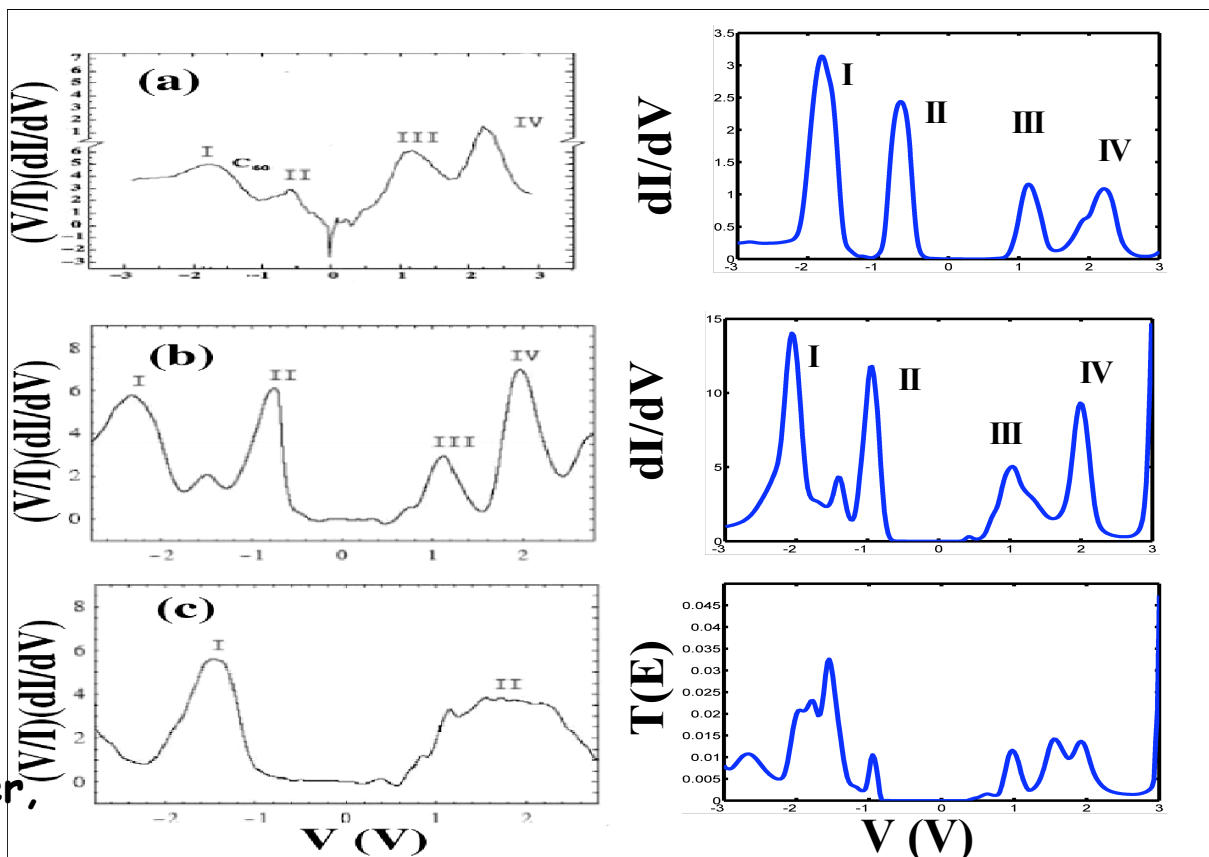
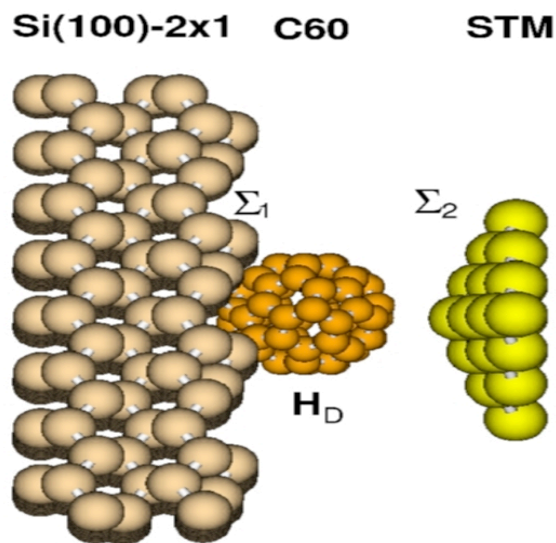


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C60 on Silicon



STS measurements: (a) Dekker, et al., surface science 2002.
 (b)& (c) Yao, et al, surface science 1996

Theory: Liang, Ghosh



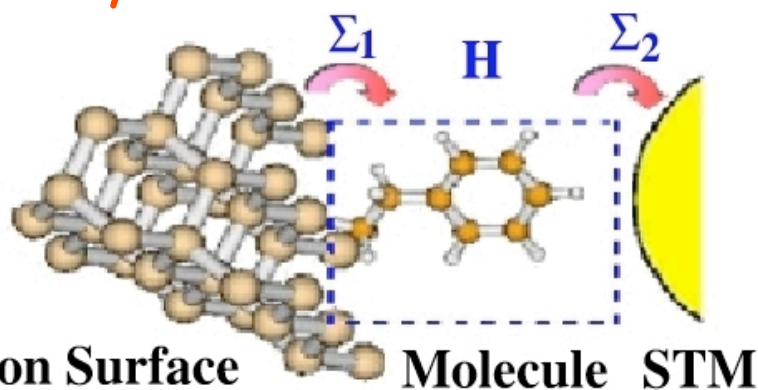
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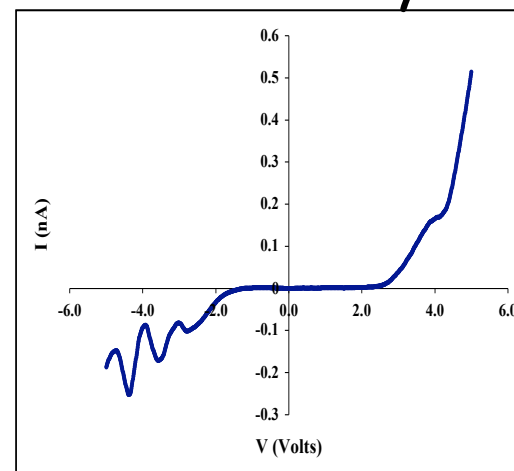
Molecule on silicon

Surface Quantum
Physics chemistry

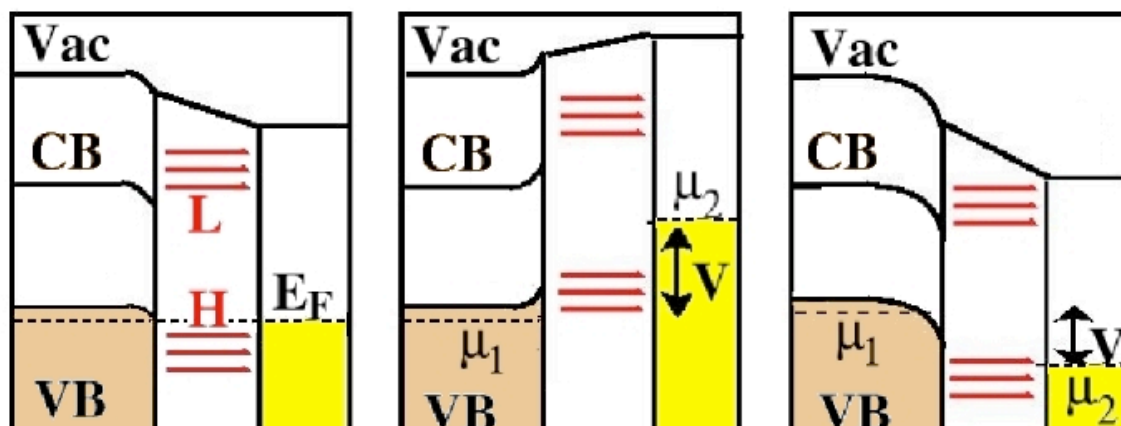


Expt: Mark Hersam
Nanoletters, 01/04

Cover story



Room temperature



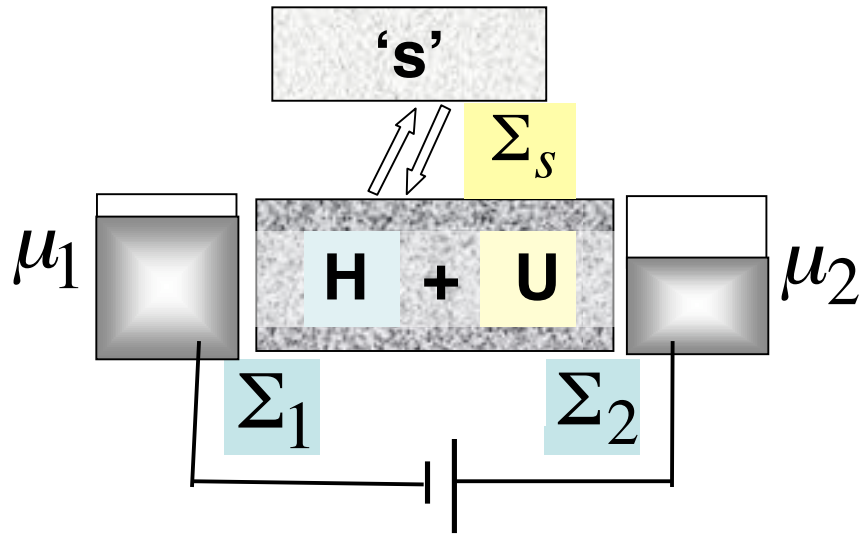


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NEGF equations



$$G = (ES - H - \Sigma)^{-1}$$

$$A = i [G - G^+]$$

$$\Gamma = i [\Sigma - \Sigma^+]$$

$$[G^n] = [G\Gamma_1G^+] f_1 + [G\Gamma_2G^+] f_2$$

$$\begin{aligned} \tilde{I} &= \frac{q}{h} \text{Trace} \Gamma_1 [f_1 [A(E)] - [G^n(E)]] \\ &= \frac{q}{h} \text{Trace} \Gamma_2 [f_2 [A(E)] - [G^n(E)]] \end{aligned}$$

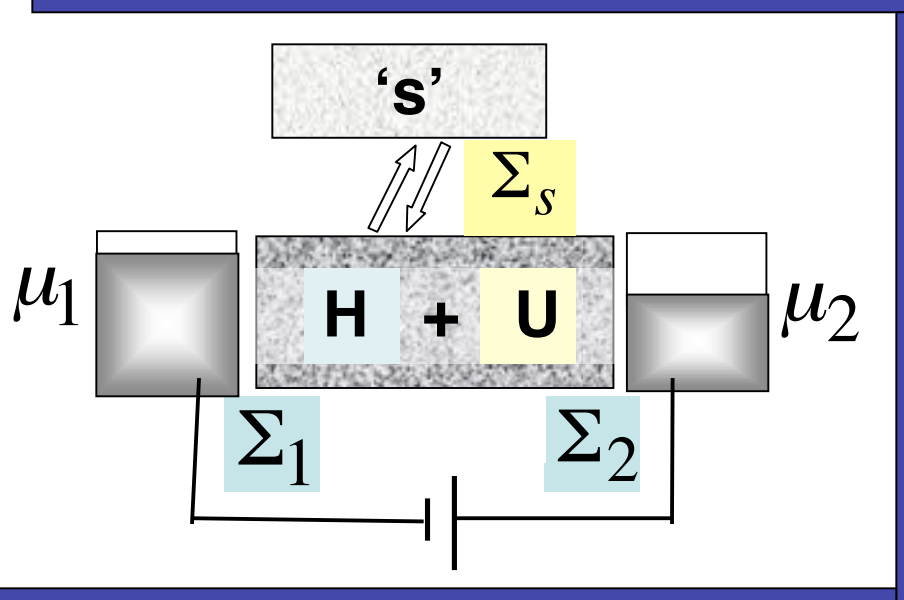


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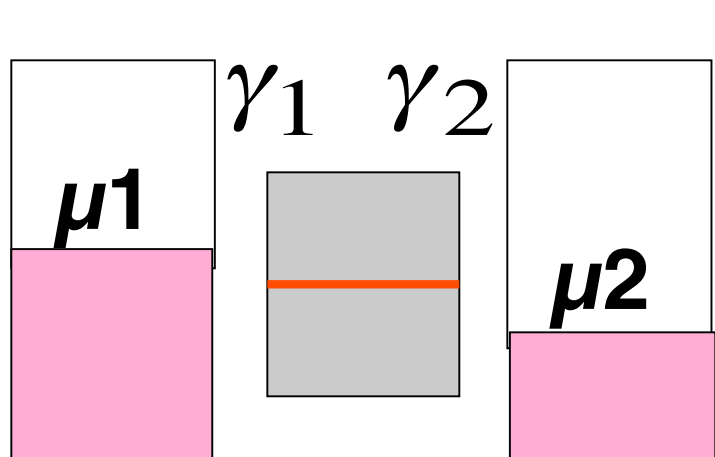
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Matrices \leftrightarrow Numbers



$$\varepsilon \leftrightarrow [H]$$

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



$$n(E) \leftrightarrow [G^n(E)] = -i [G^<(E)]$$

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

$$N \leftrightarrow [\rho]$$

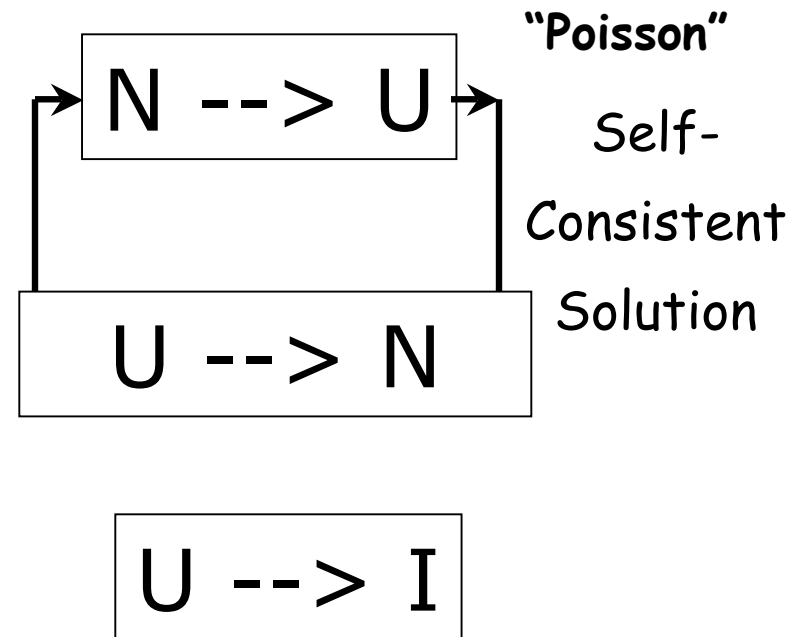
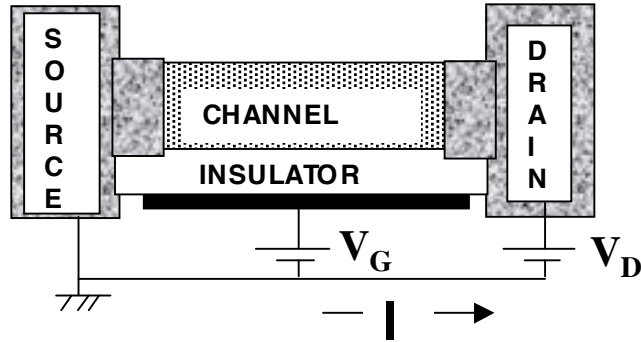


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Minimal Model



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

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

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

Nanowires / Nanotubes / Molecules



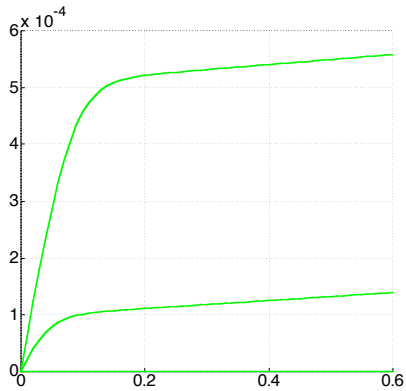
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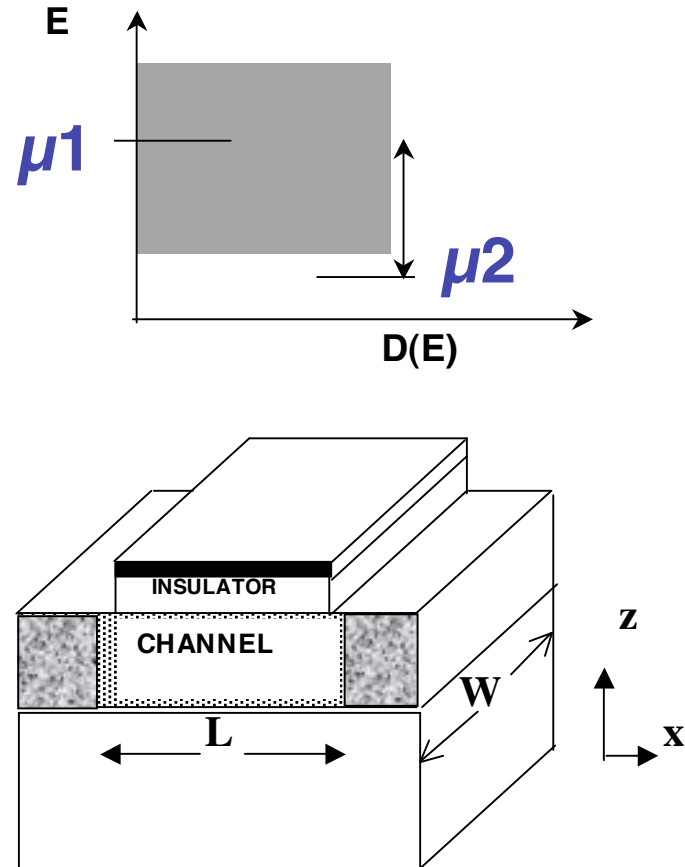
FET: Why current "saturates" ?

Drain current



Drain voltage

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



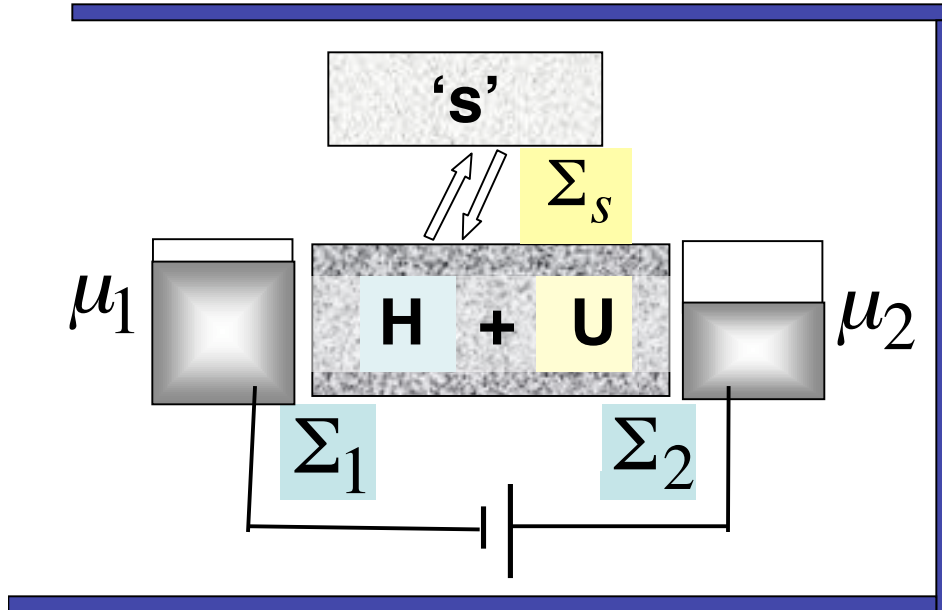


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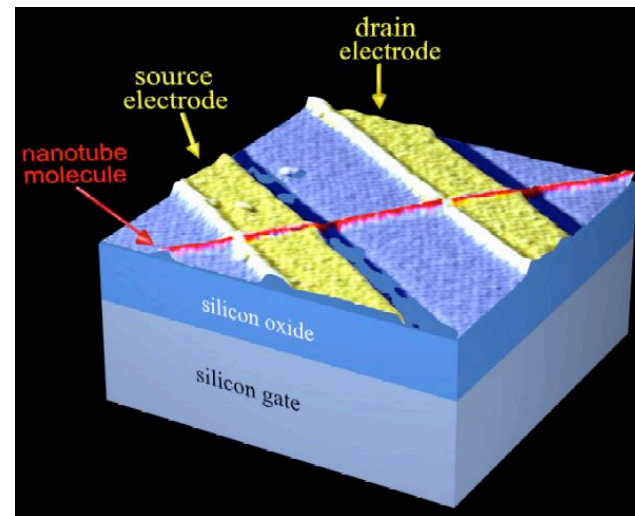
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Self-consistent field, U



Method of moments:

Jing Guo



3D Poisson solver:

Eric Polizzi

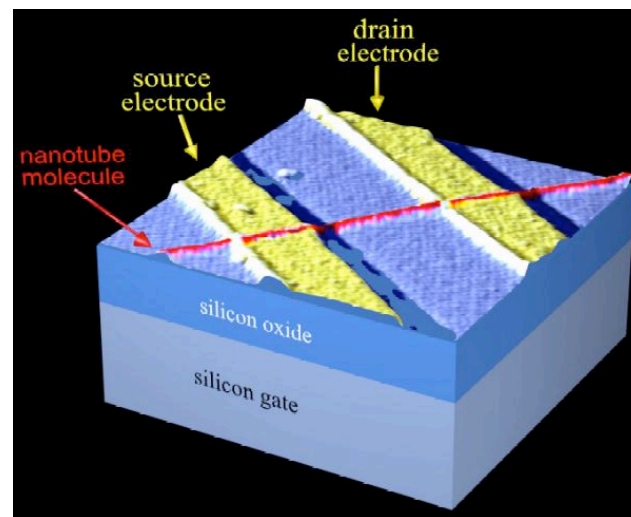
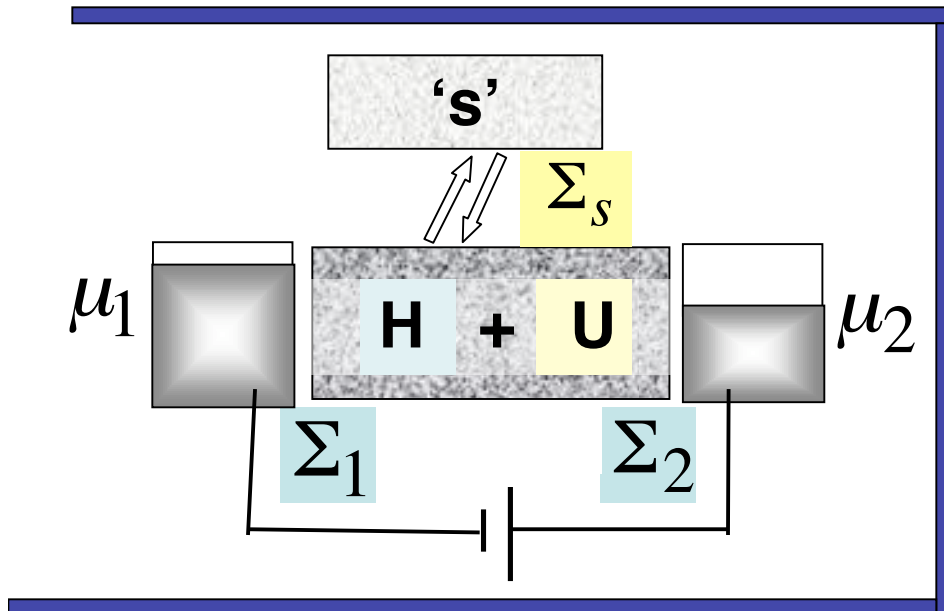


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Self-consistent field, U



Method of moments:

Jing Guo

3D Poisson solver:

Eric Polizzi

Correlations

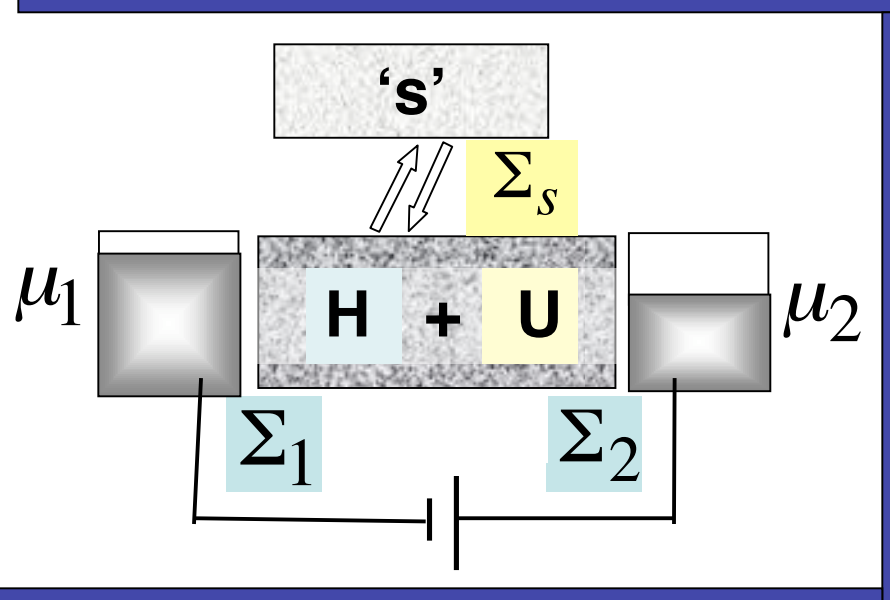


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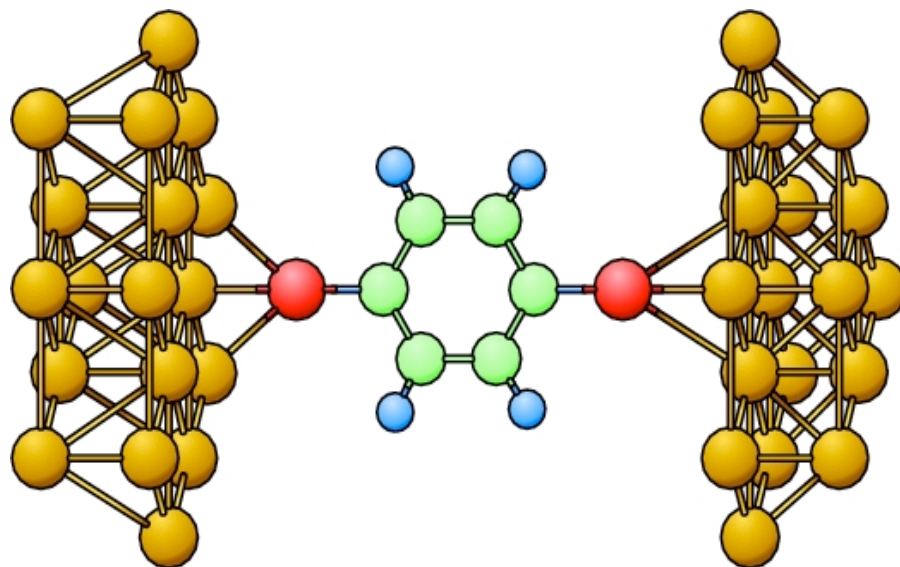
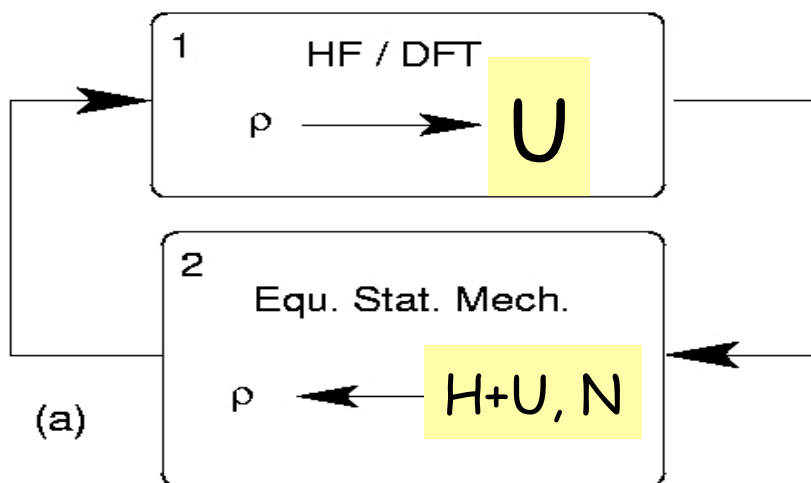


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Self-consistent field, U



Quantum Chemistry:
Closed System
in Equilibrium



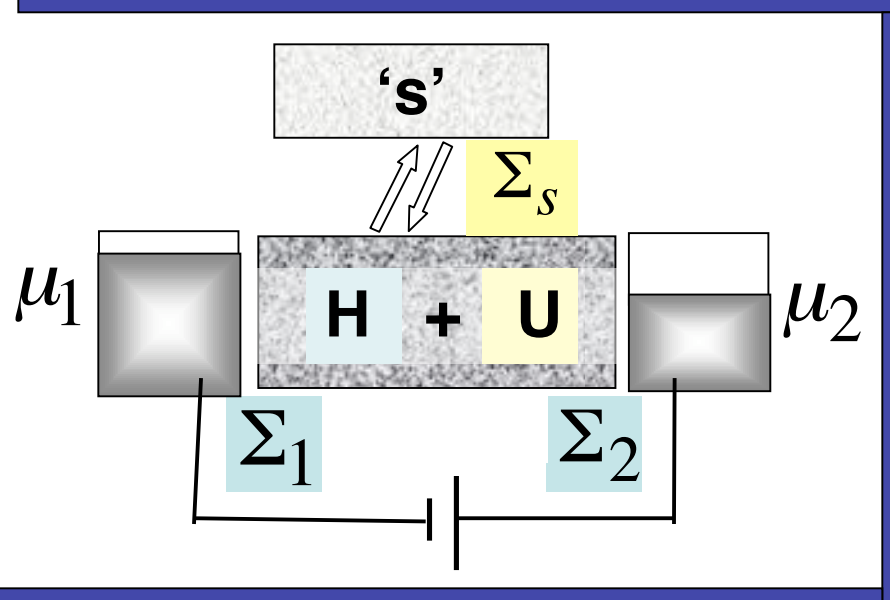


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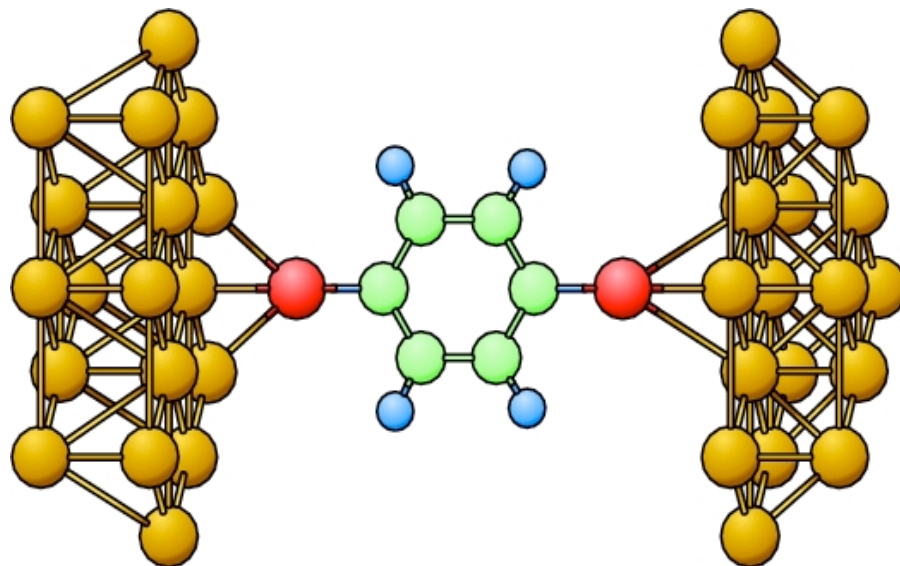
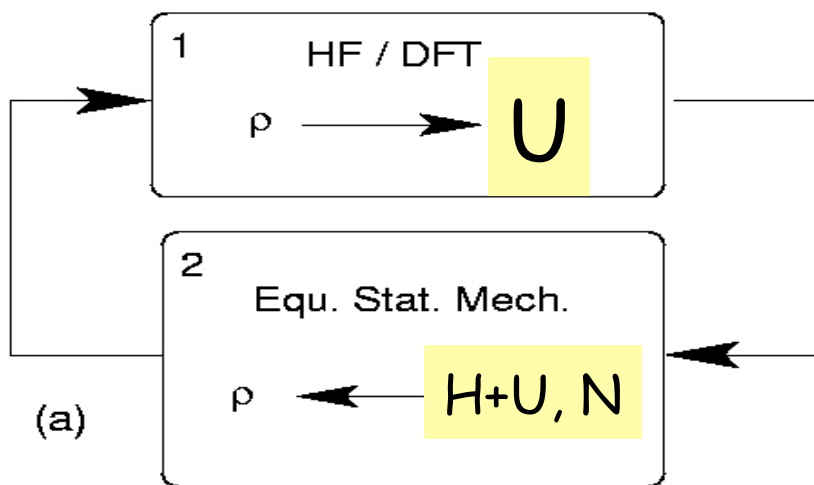


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Self-consistent field, U



~~Quantum Chemistry:
Closed System
in Equilibrium~~



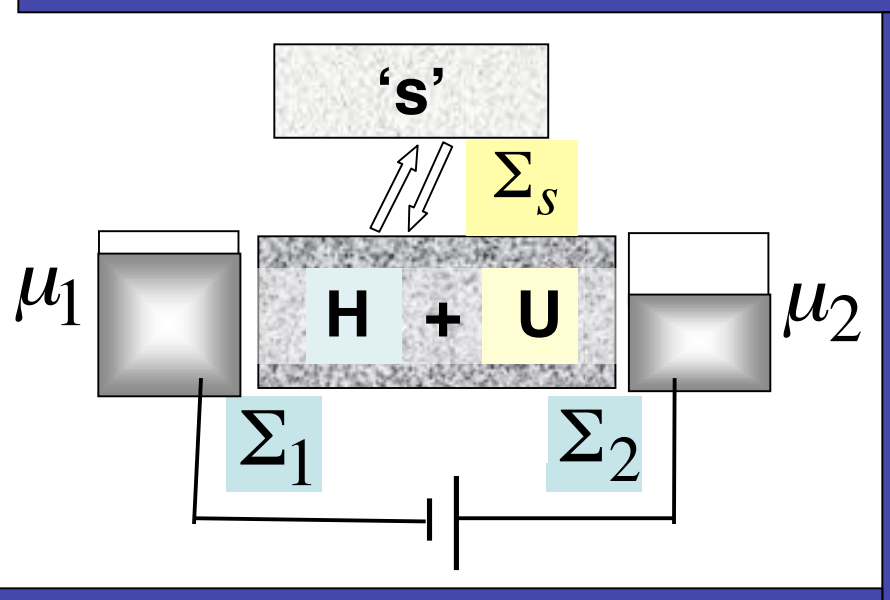


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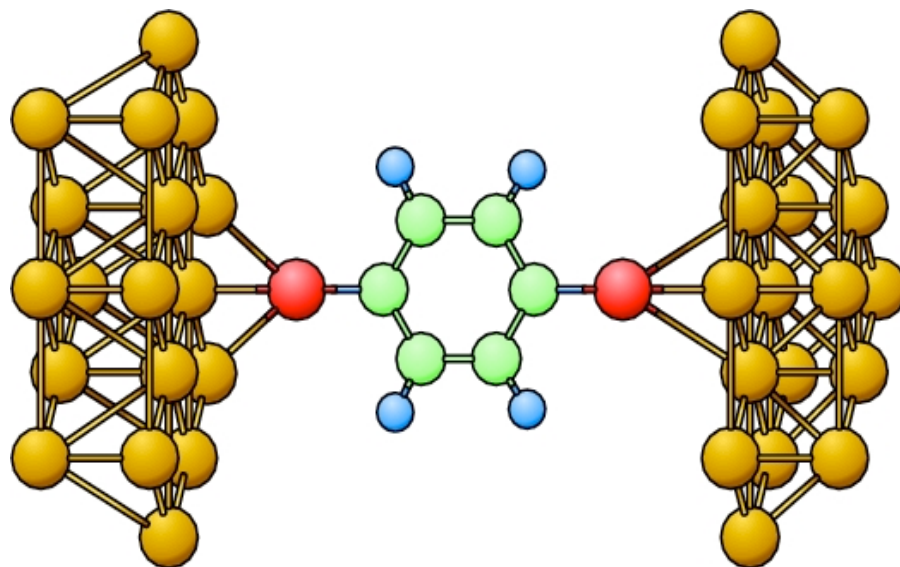
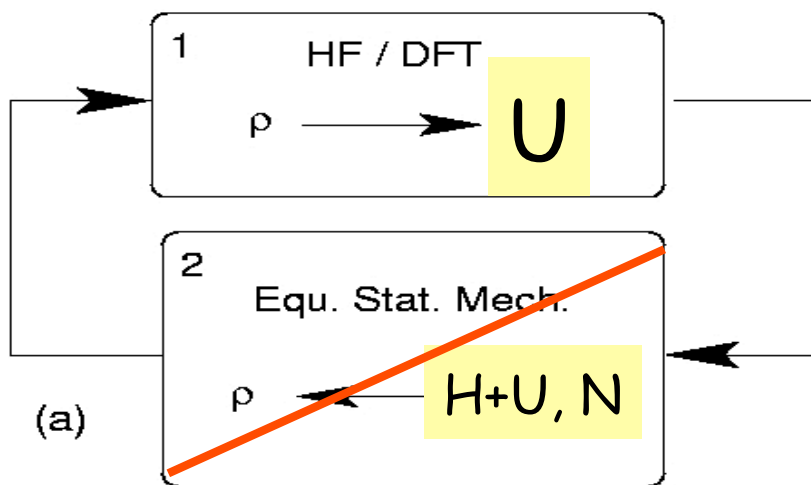


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Self-consistent field, U

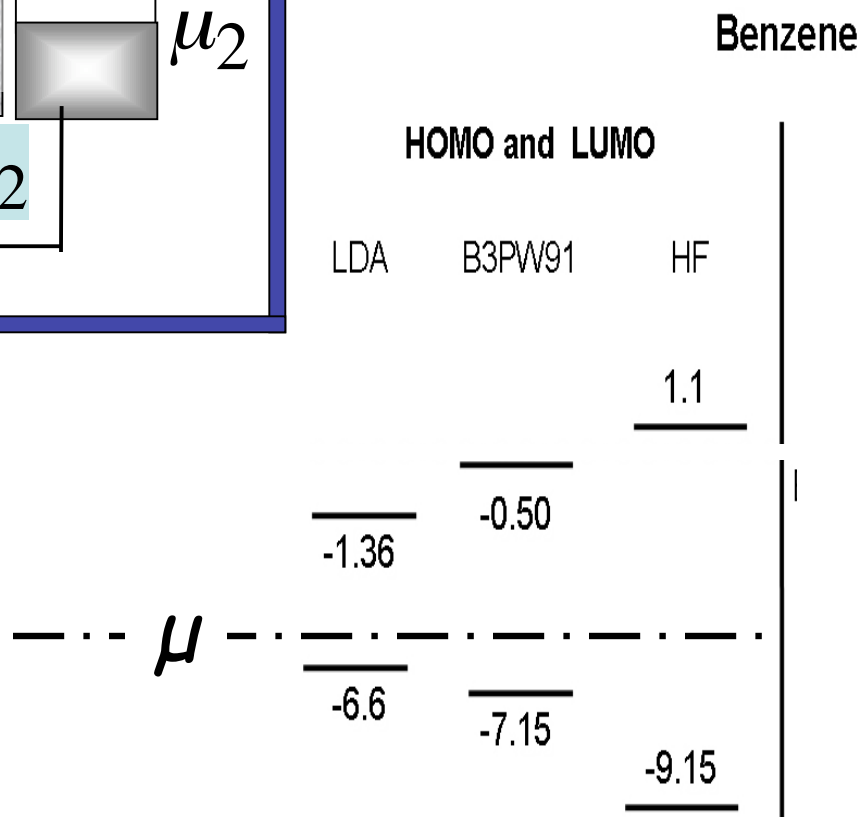
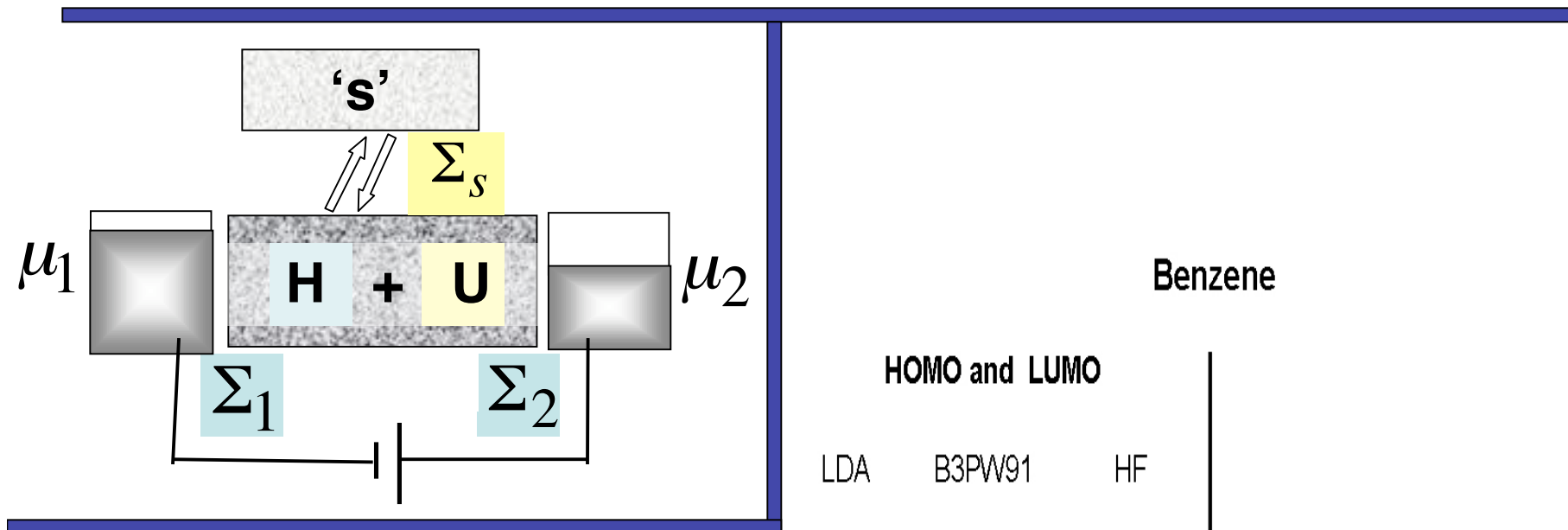


~~Quantum Chemistry:
Closed System
in Equilibrium~~



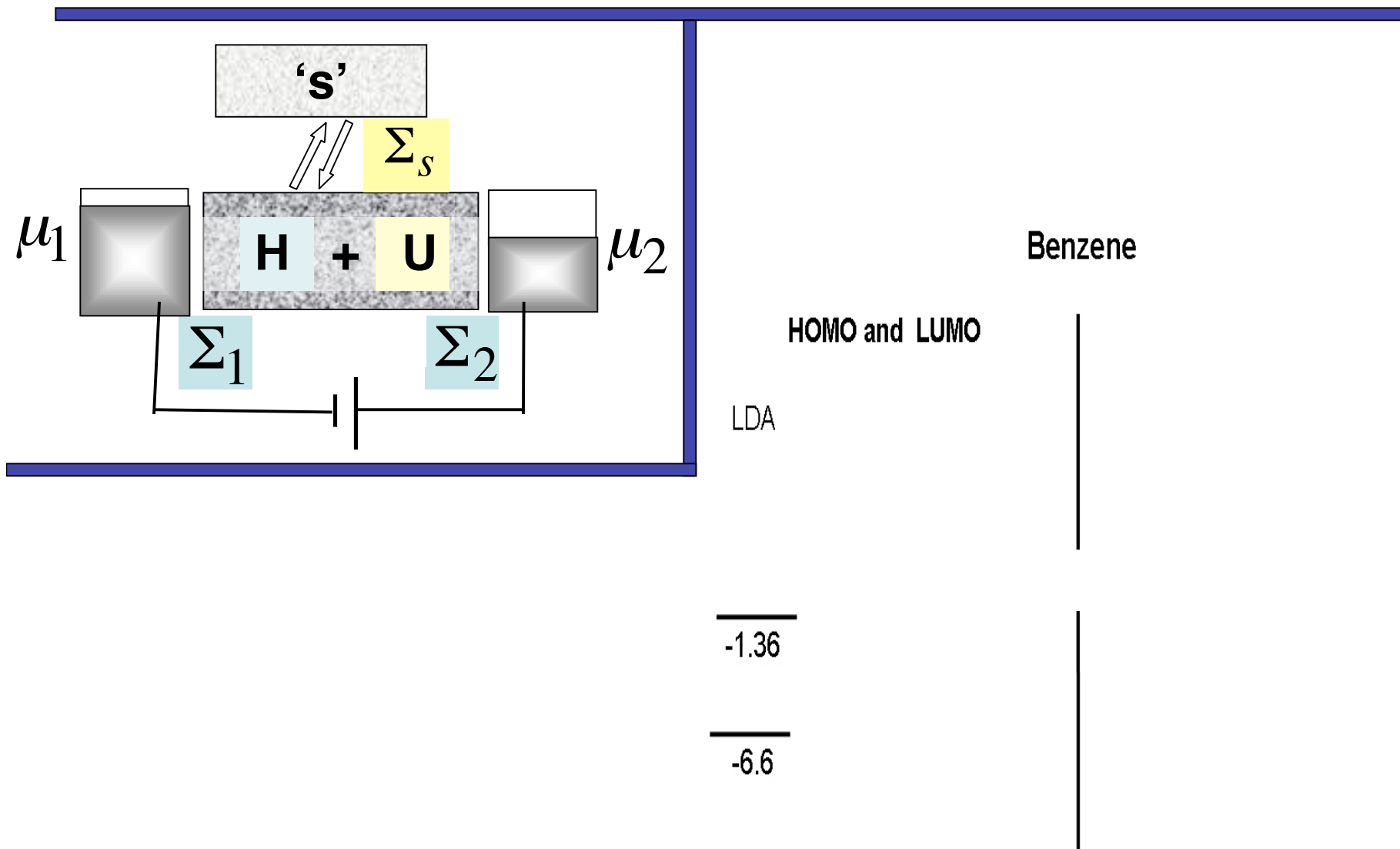


Which self-consistent field ?



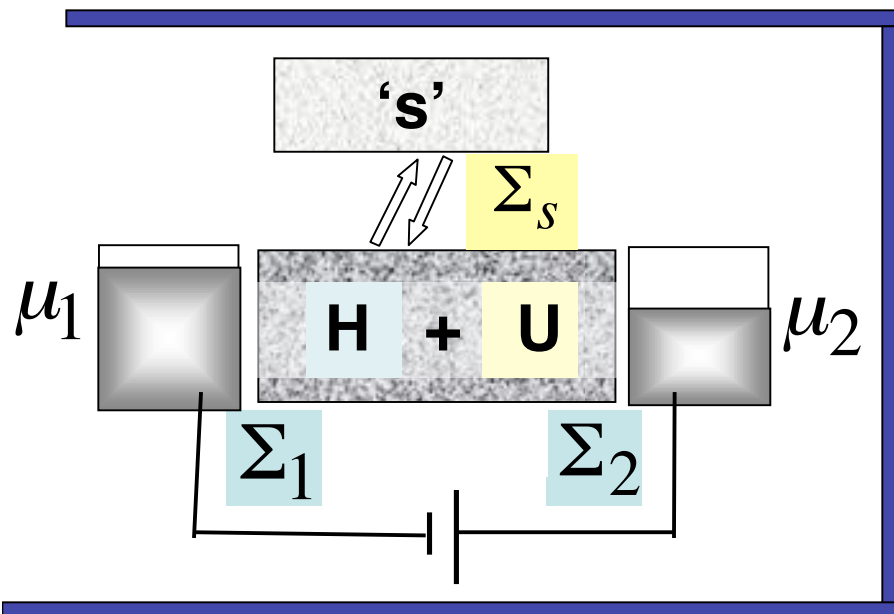


Which LDA ?





Which LDA ?



$$IP = E(N) - E(N-1)$$

$$EA = E(N+1) - E(N)$$

Benzene

HOMO and LUMO

LDA

LDA

1.64

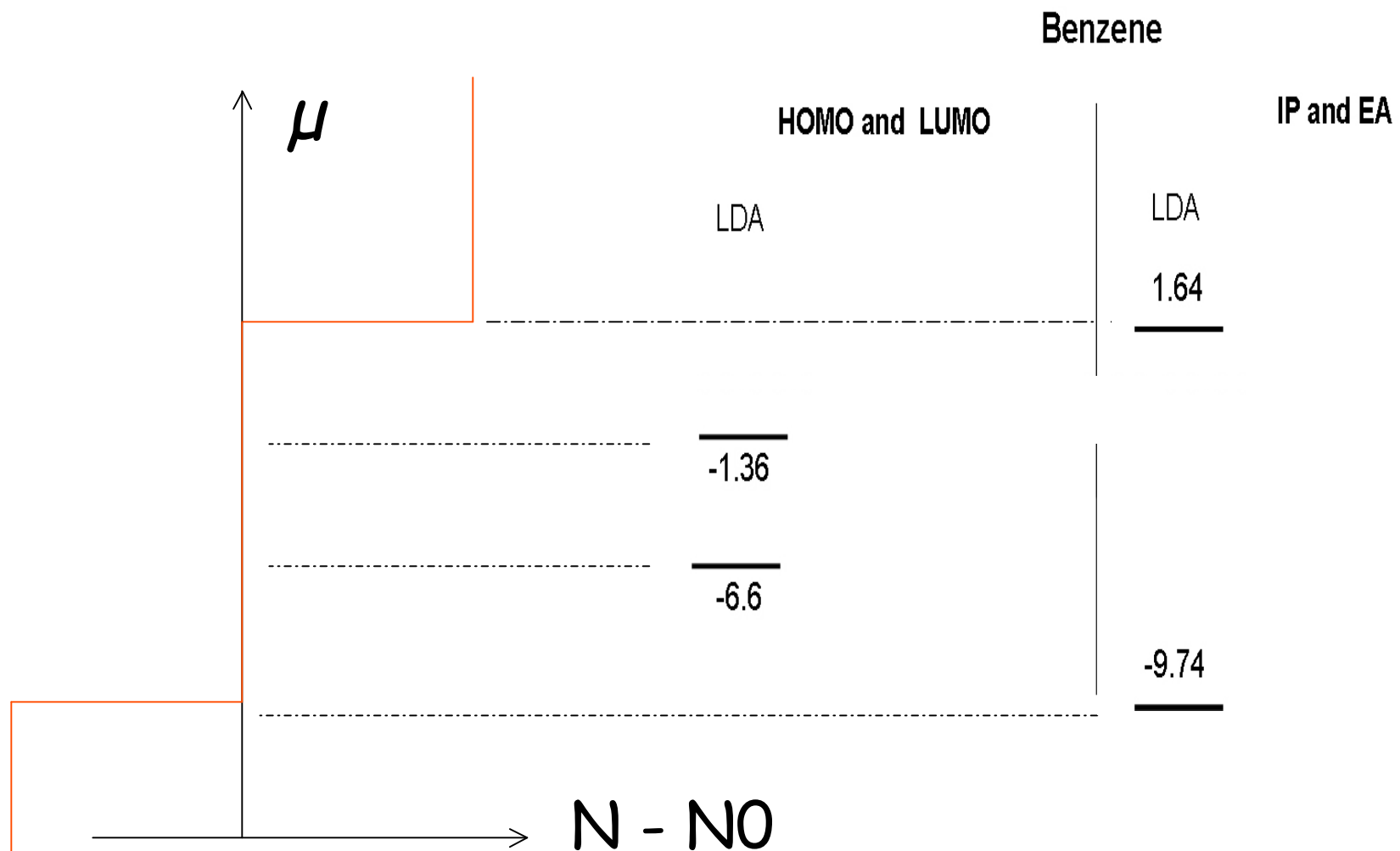
-1.36

-6.6

-9.74



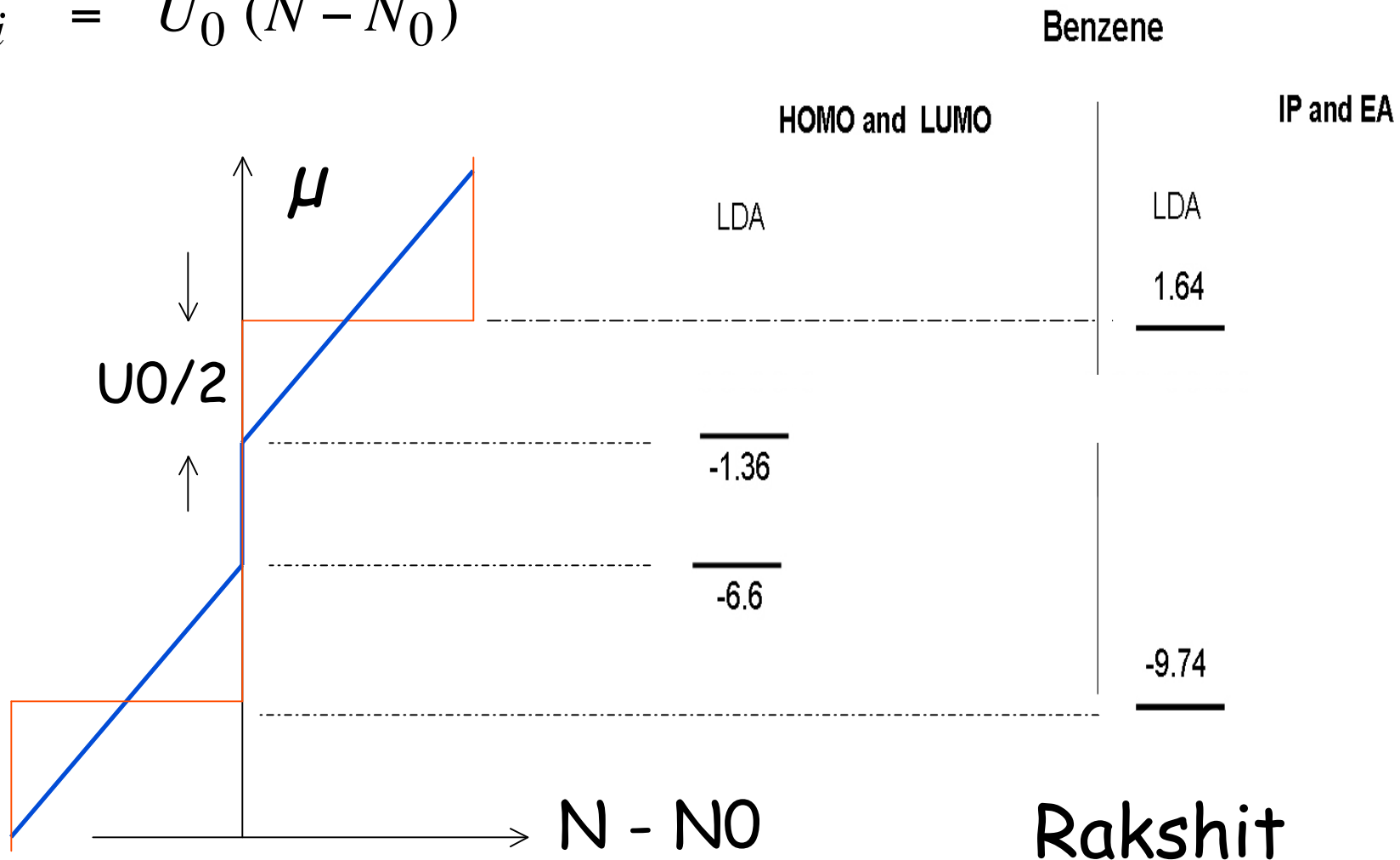
N vs. μ





N vs. μ : SCF Theory

$$U_i = U_0 (N - N_0)$$





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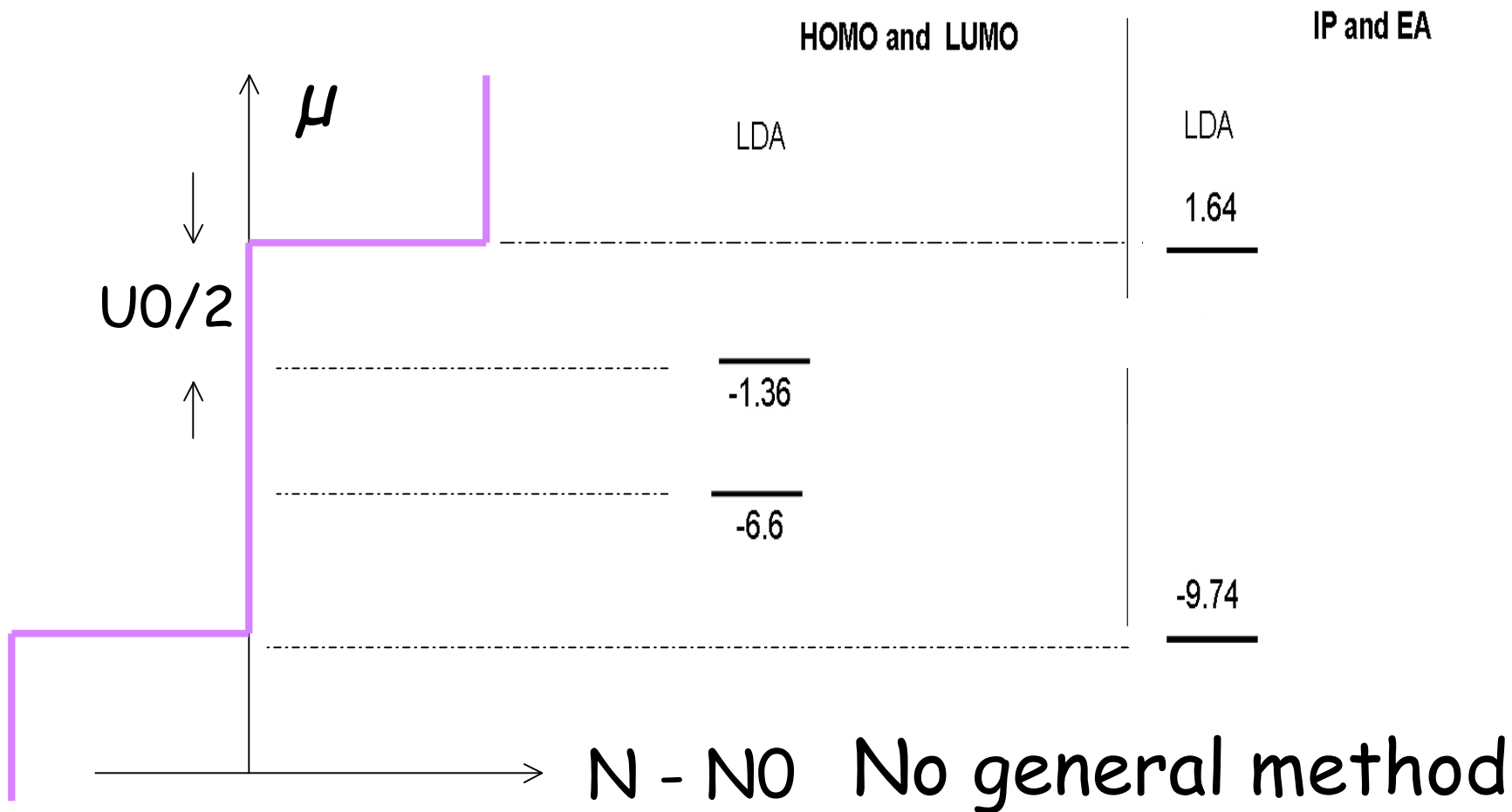


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Self-interaction Correction

$$U_i = U_0 (N - N_0 + 0.5 - n_i)$$

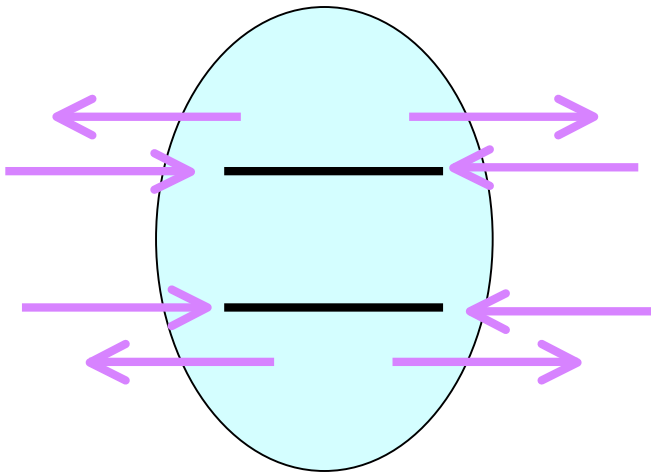
Benzene



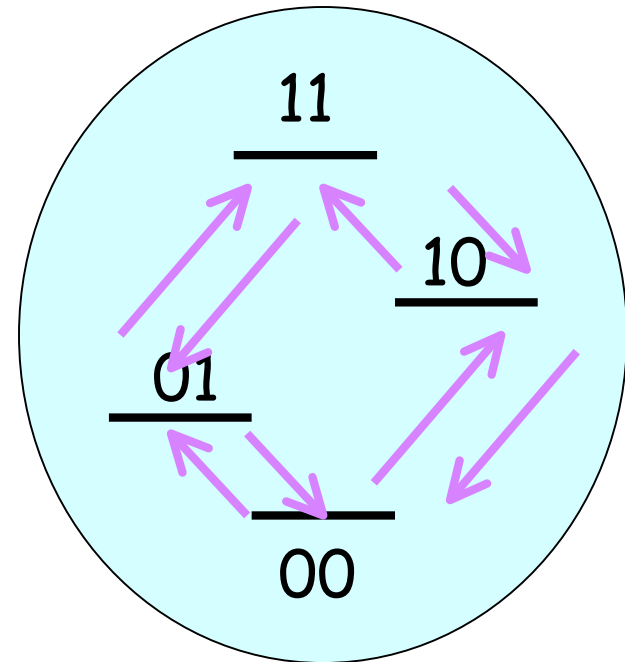


One-electron vs. Many-electron

N one-electron levels



2^N many electron levels



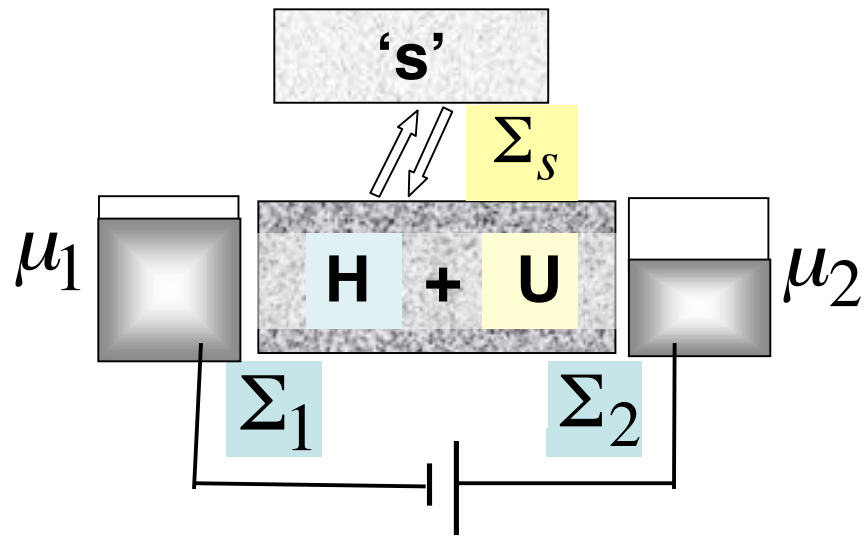


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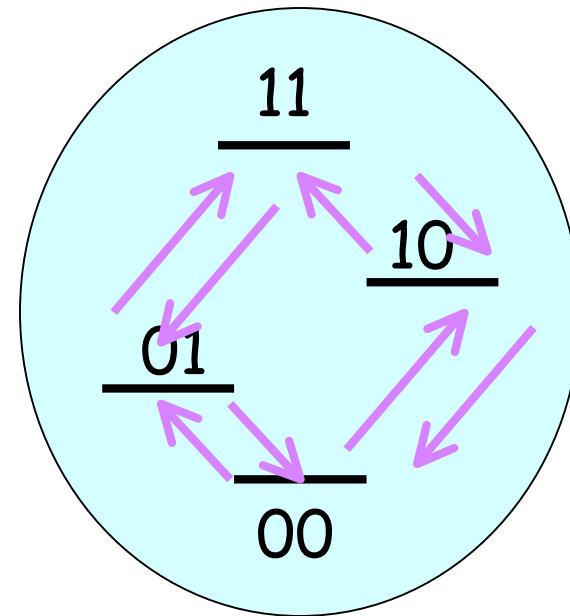
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Two choices



Works for $\Gamma \geq U$

2^N many electron levels



Works for $\Gamma \ll U$

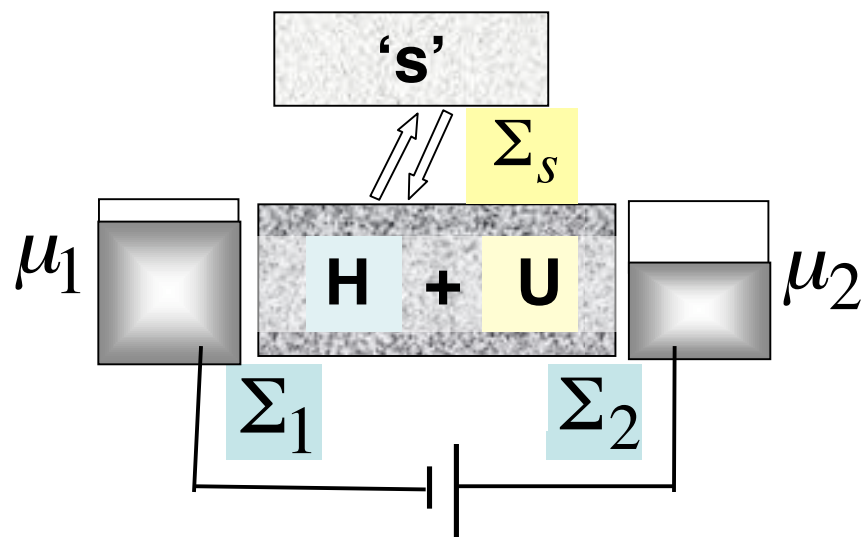


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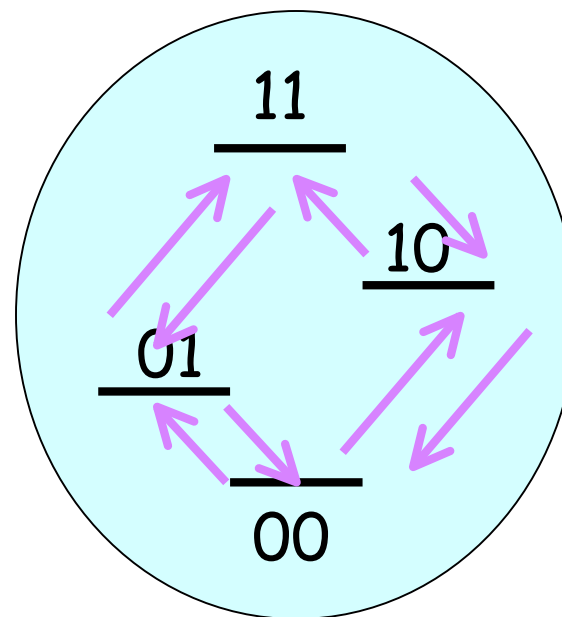
Two choices



Works for $\Gamma \geq U$

Band theory

2^N many electron levels



Works for $\Gamma \ll U$

Mott insulator



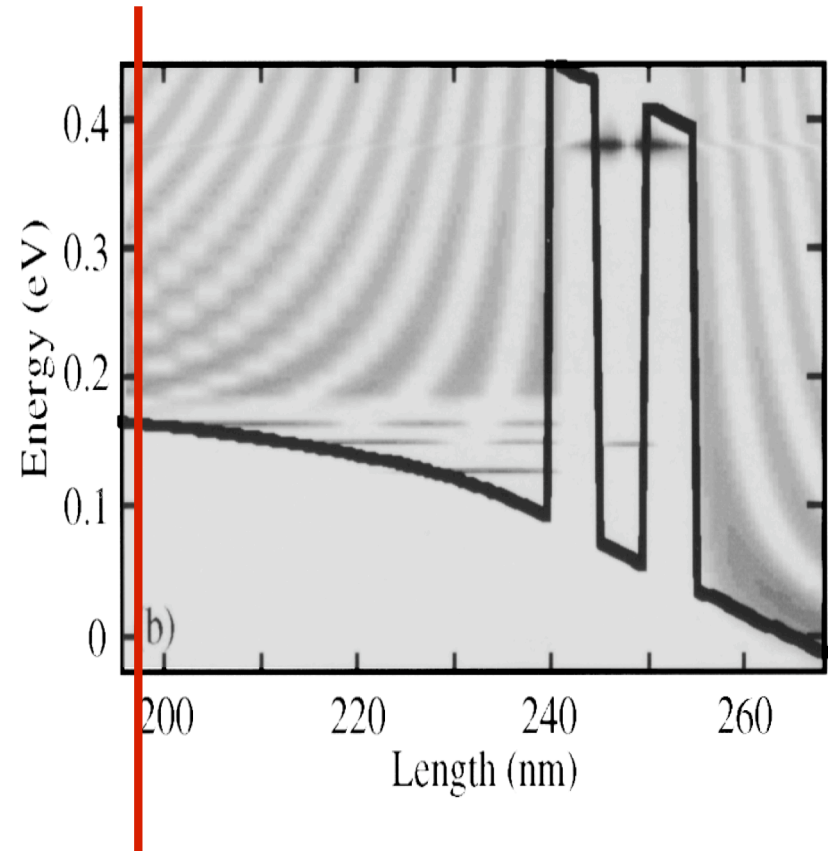
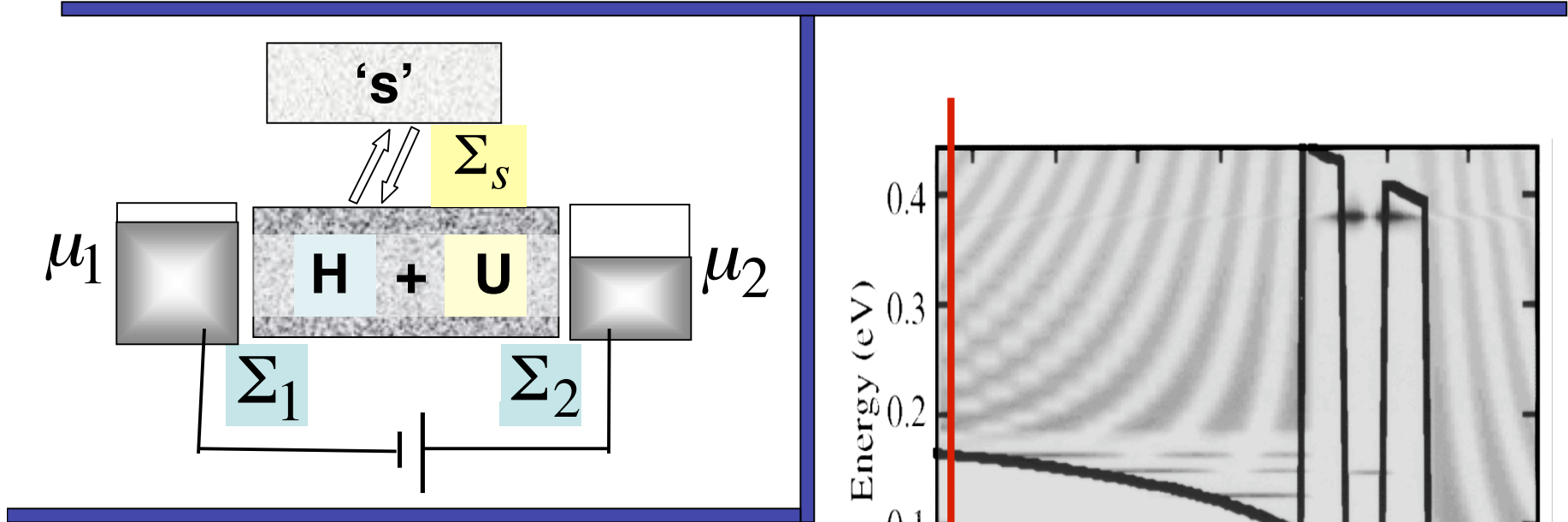


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What is a contact?



Klimeck, Lake et.al.
APL (1995)

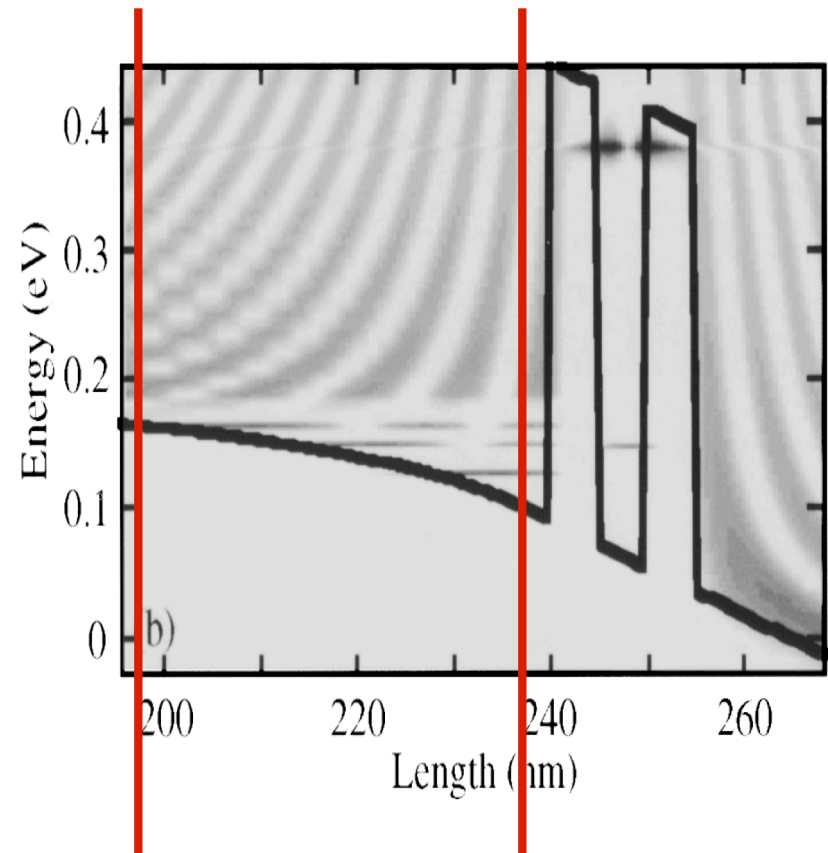
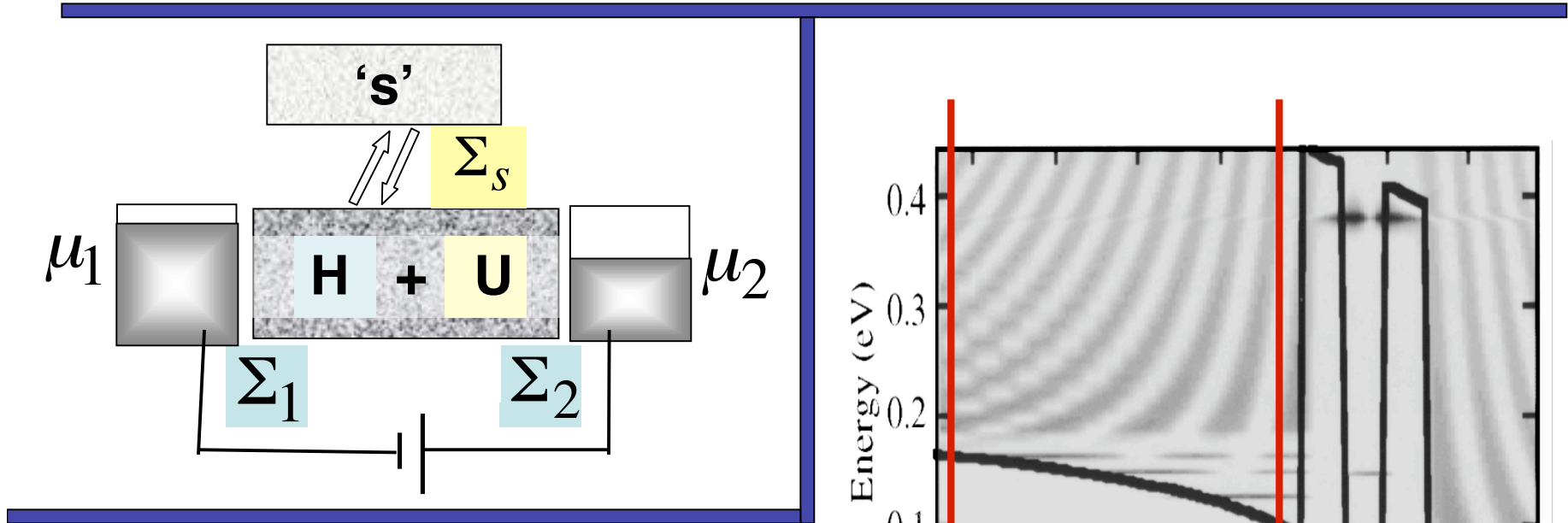


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What is a contact?



Klimeck, Lake et.al.
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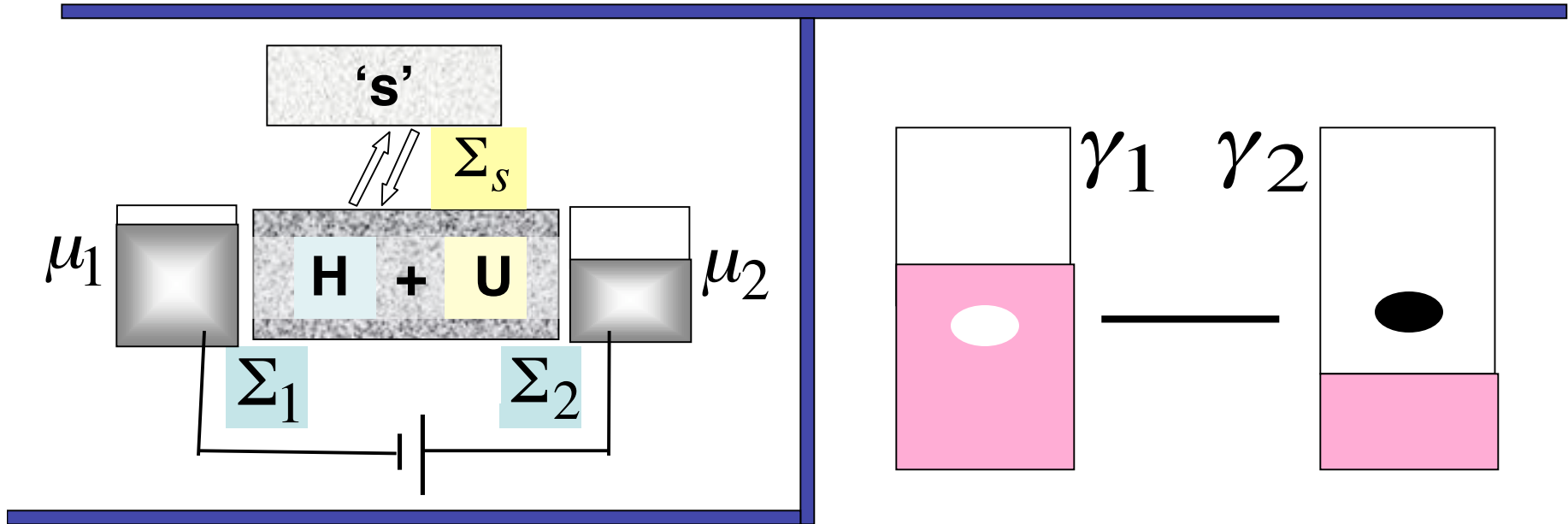


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"Hot" contacts



Energy has to be removed efficiently

from the contacts: otherwise

--> "hot" contacts

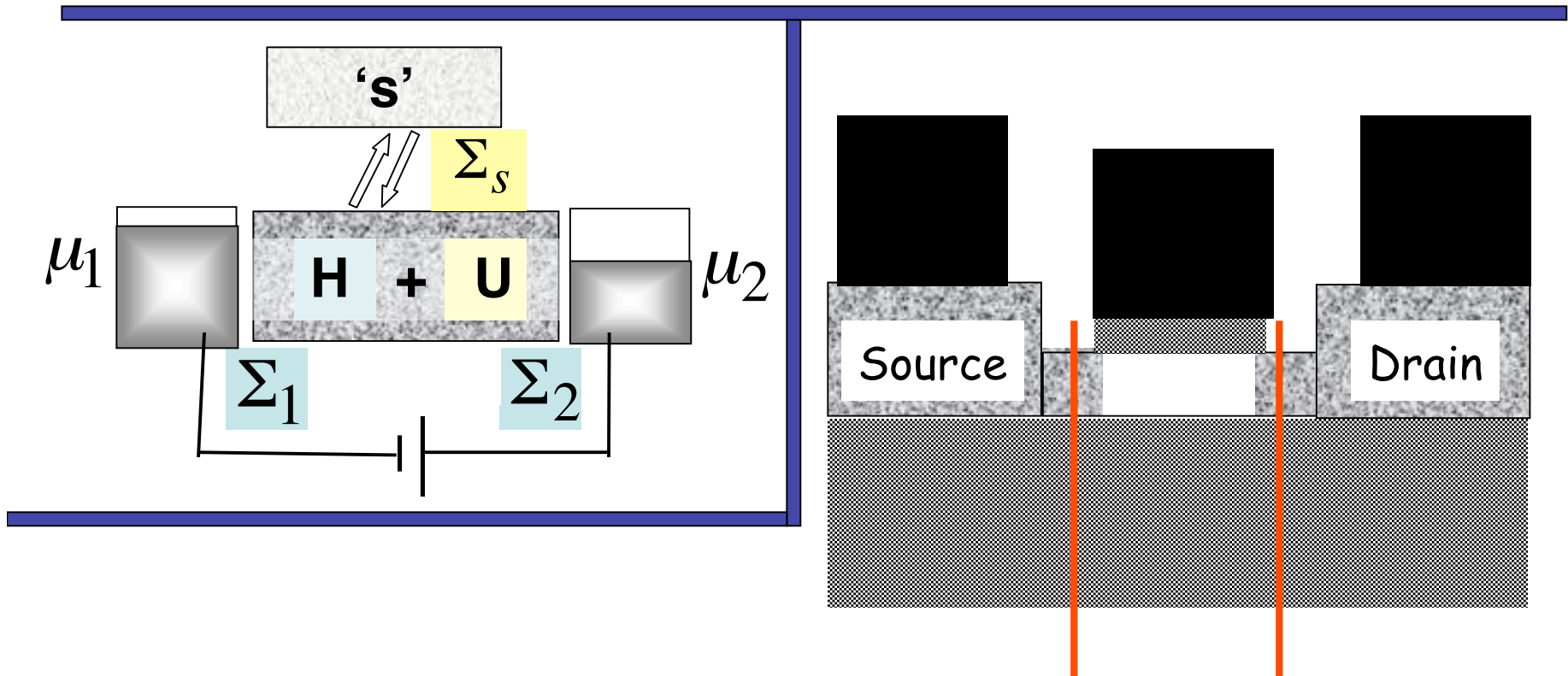


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"Hot" contacts



Venugopal, Lundstrom

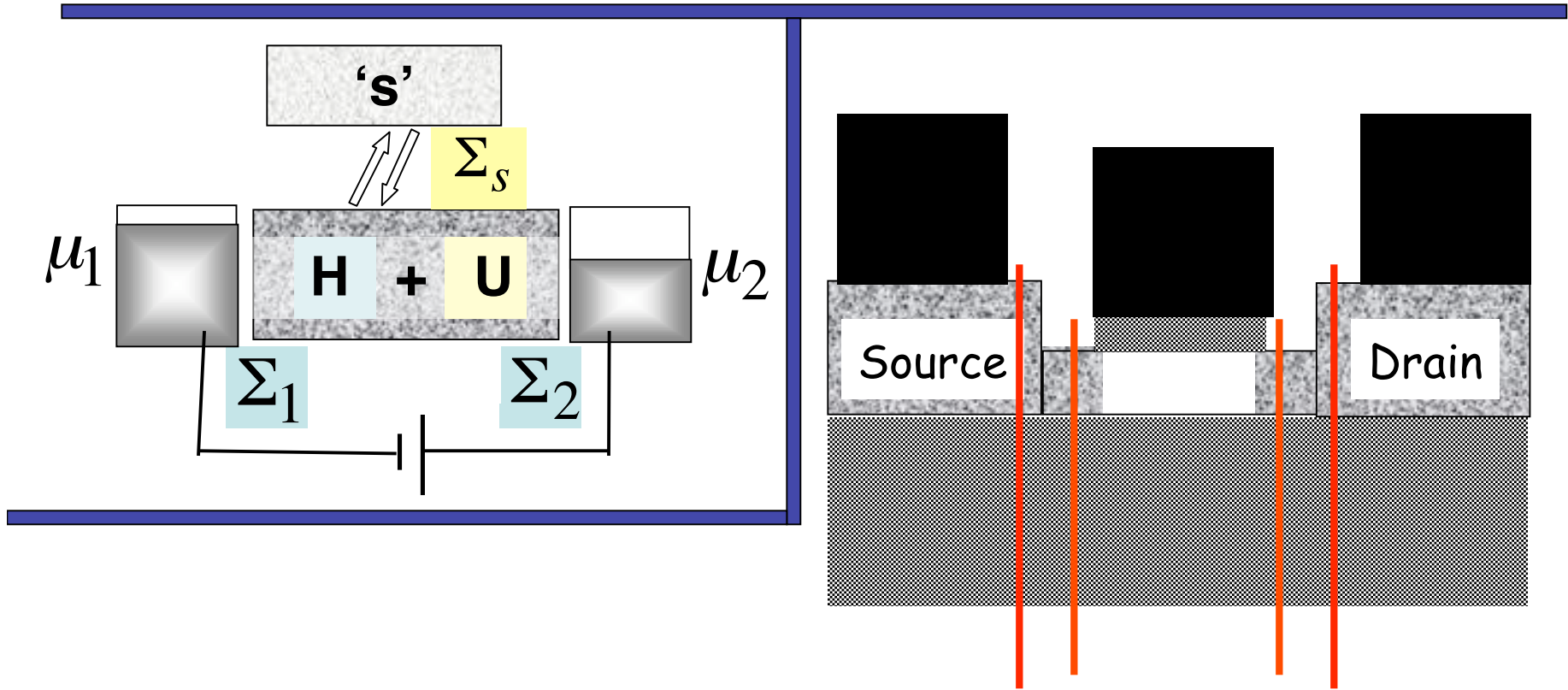


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"Hot" contacts



Venugopal, Lundstrom

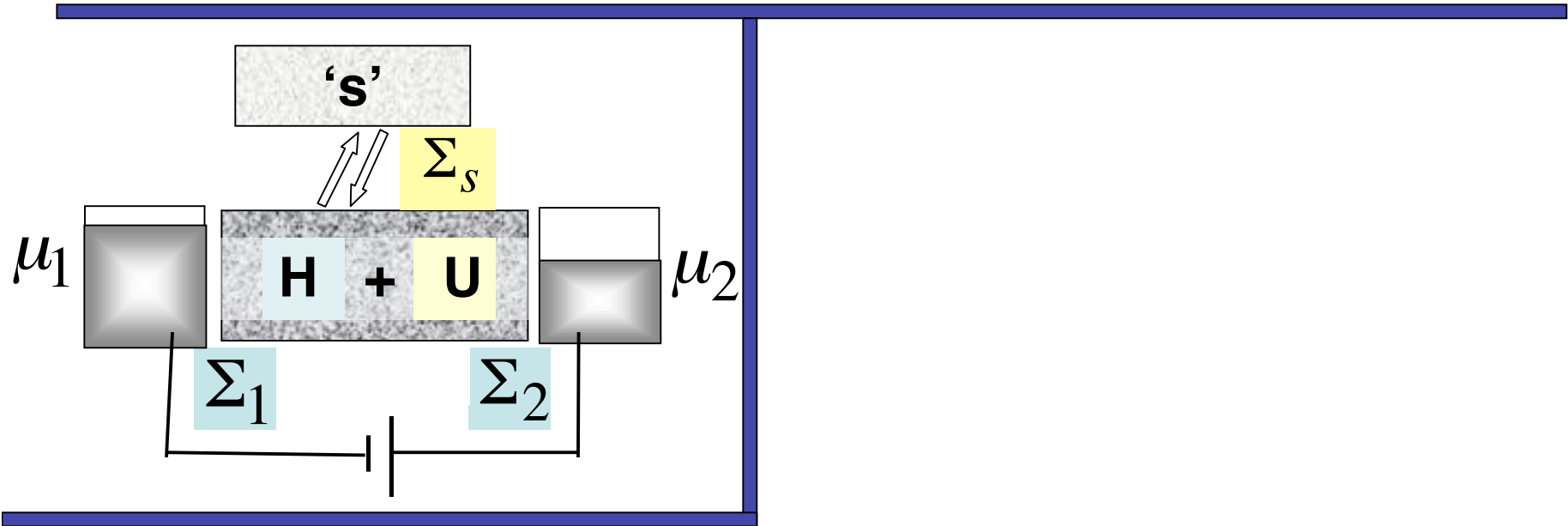


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Other "contacts"



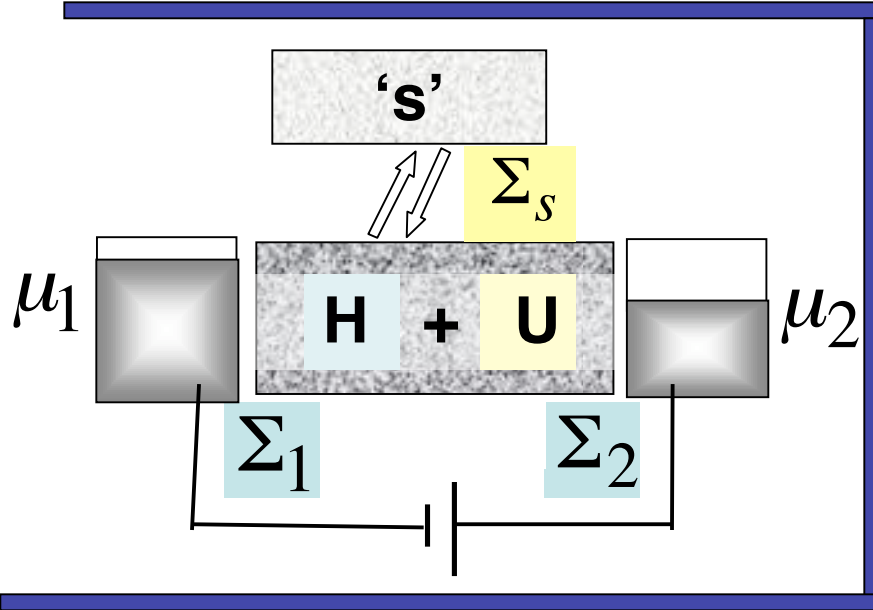


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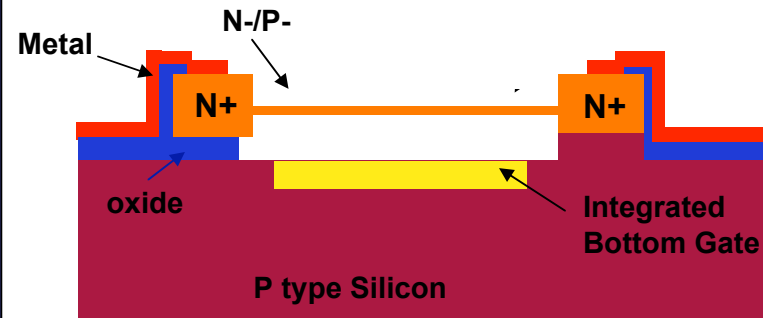


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Other "contacts"



Hot phonons ?



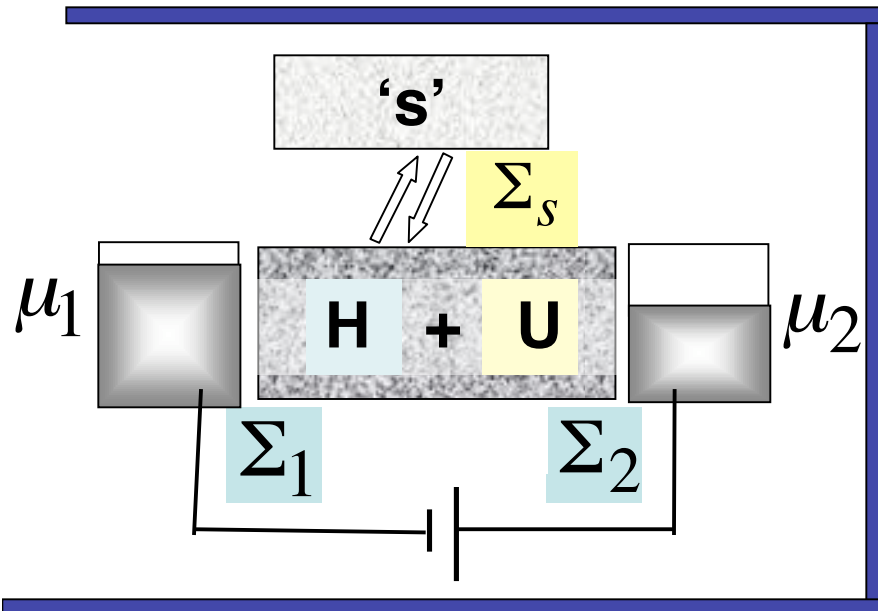


NCN

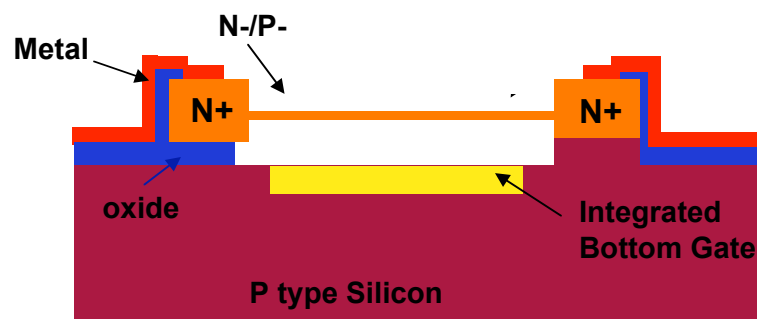


INAC

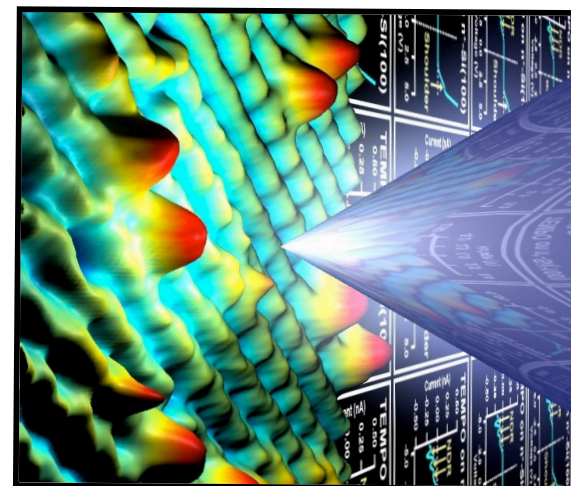
Other "contacts"



Hot phonons ?



Molecular desorption ?



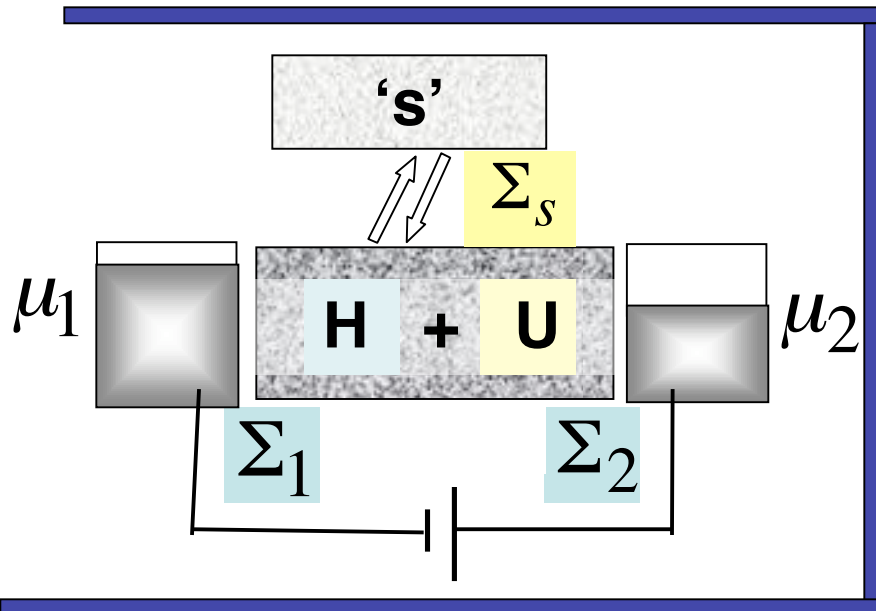


NCN

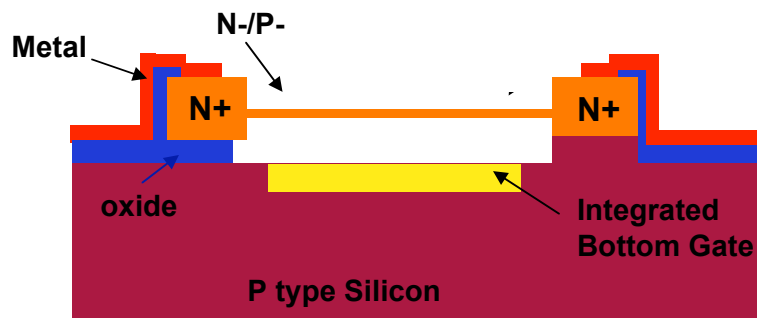


INAC

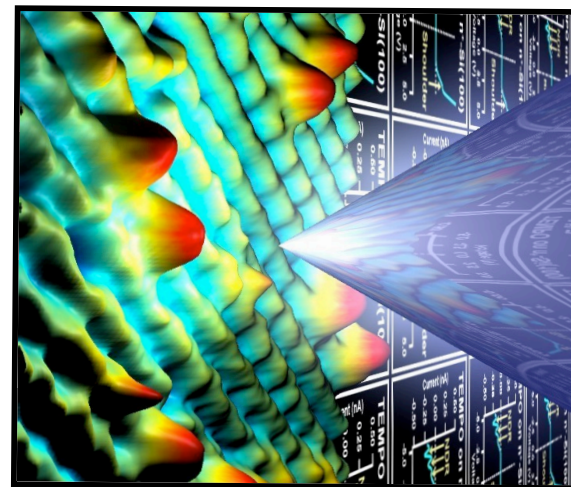
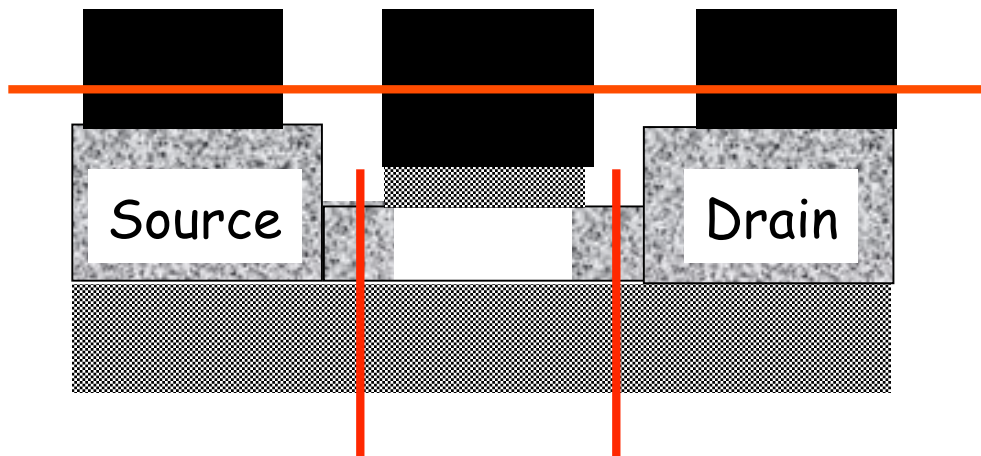
Hot "contacts"



Hot phonons ?



Molecular desorption ?



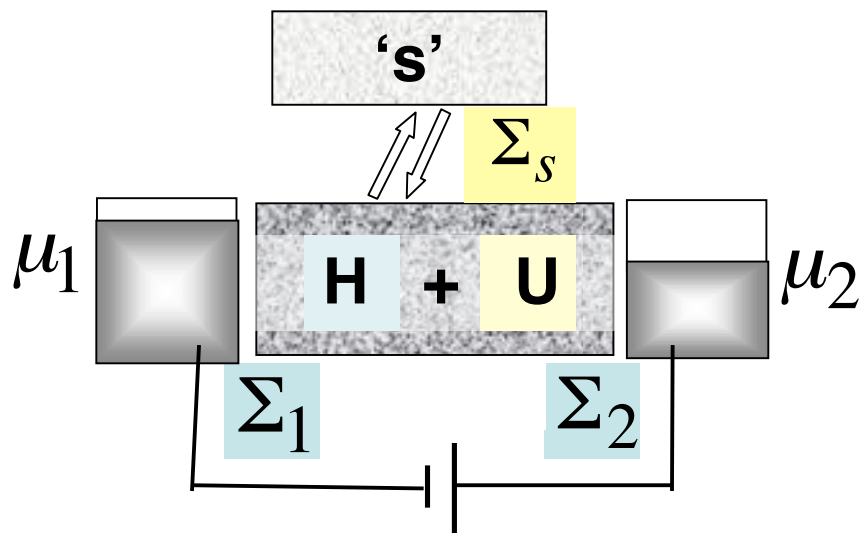


NCN

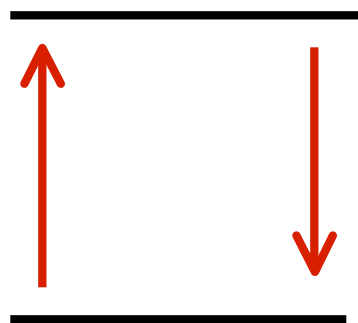


INAC

Two choices

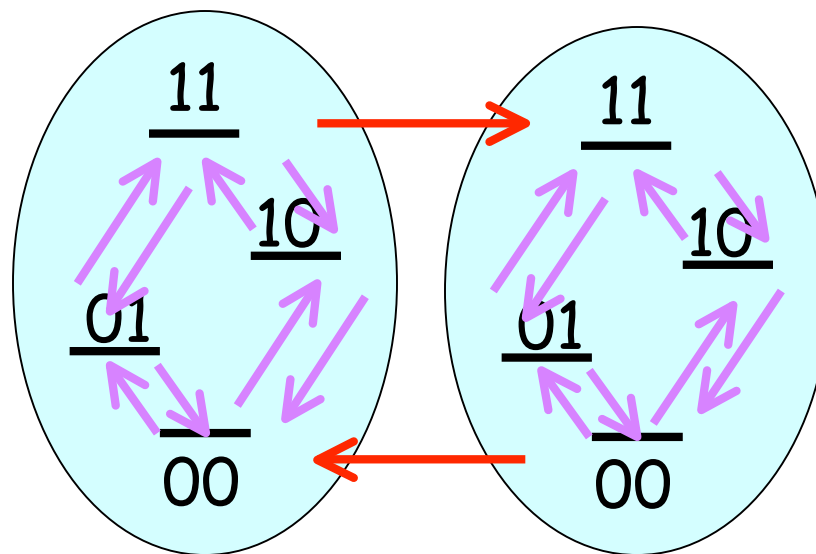


Supplement
NEGF with
*separate rate
 equation*
 for "contact"



"Contact"
 State A

"Contact"
 State B

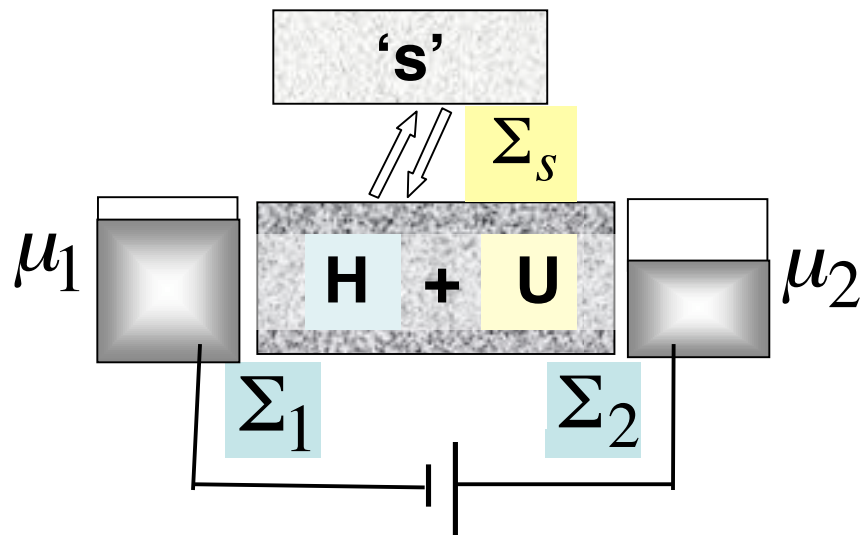


Rate equation for full system

Works for $\Gamma \ll U$

Summary

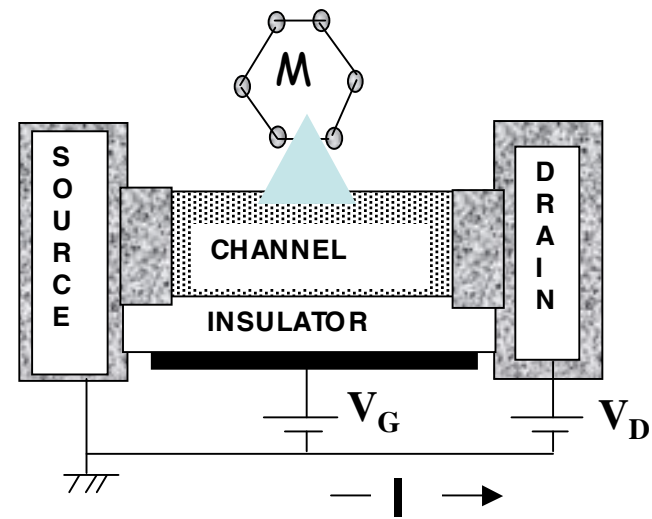
Unified Model



www.nanohub.org

Electrical Resistance: An Atomistic View,
Nanotechnology 15, S433
(2004)

Electronics & Sensing



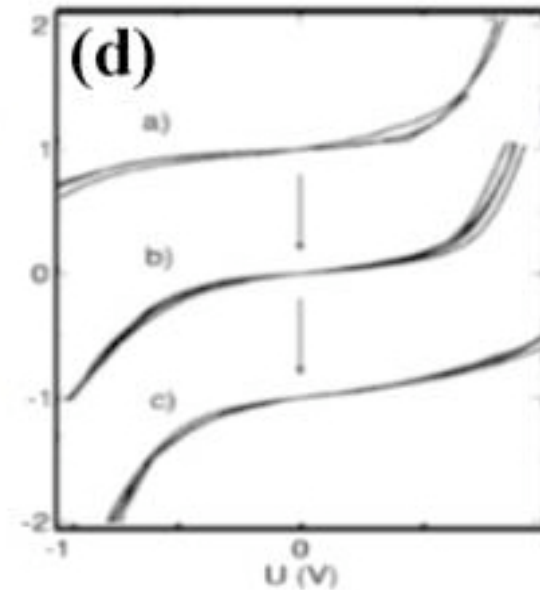
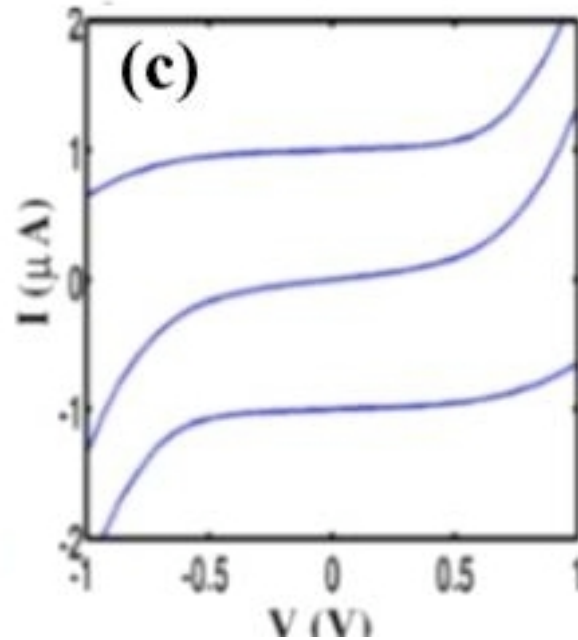
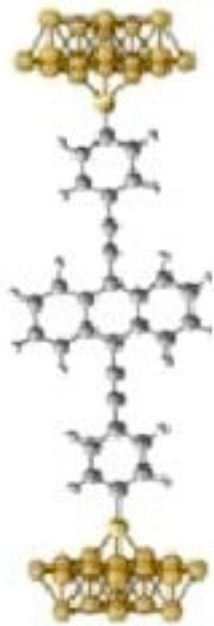
Transients?

Strong correlations?

"Hot contacts"?



Experiment vs. Theory



THEORY:
Purdue Group
(cond-mat/0403401)

EXPT:
Karlsruhe

Zahid, Paulsson, Ghosh