

Nanoelectronics in the NCN

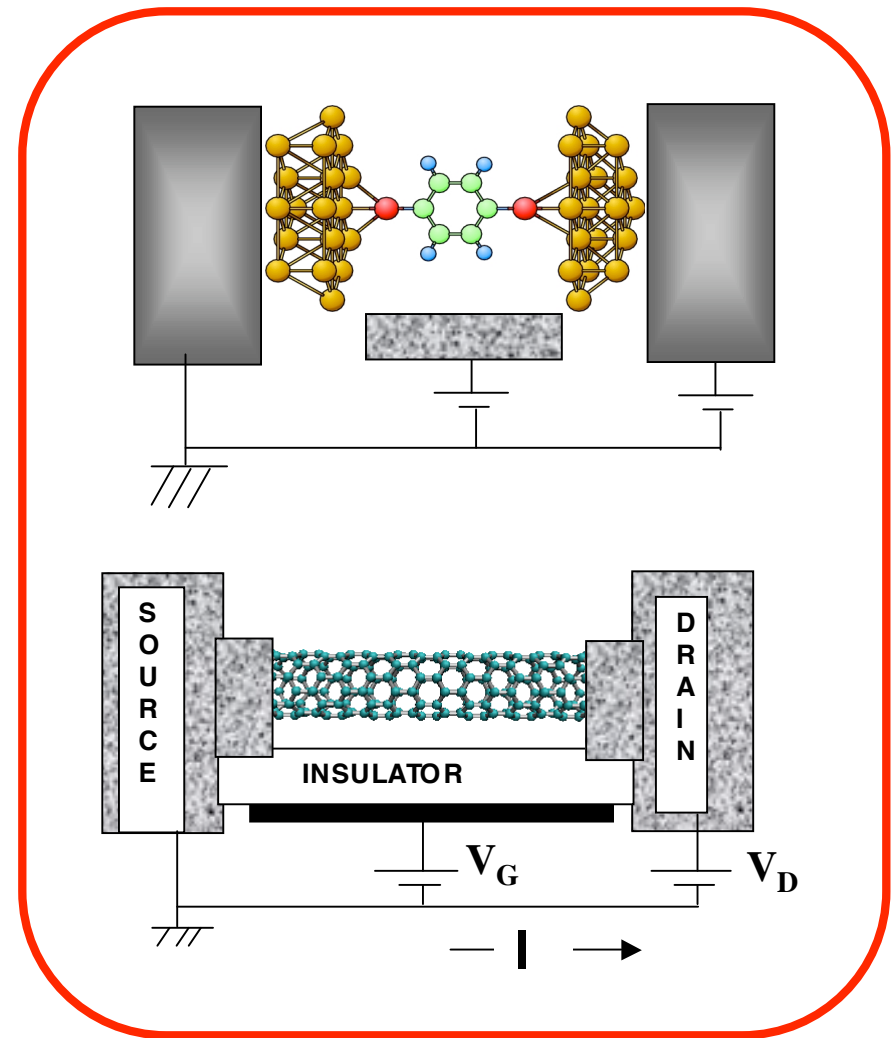
Supriyo Datta
Purdue University

to develop a general
framework for relating
atomic structure to device
and circuit level
performance.

- **Conceptual Understanding**
- **Practical Approaches**
- **Educational Resources**
- **Simulation Tools**
- **Professional Leadership**

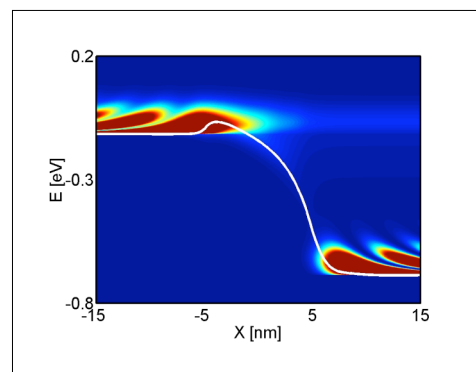
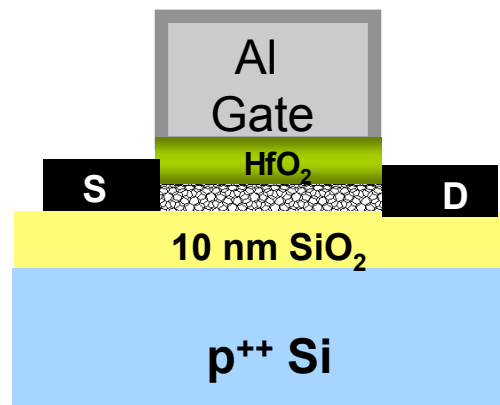
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- **Simulation Tools**
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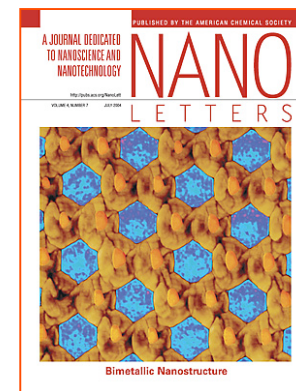


- Cho (contacts)
- Datta (basic theory)
- Lundstrom (devices)
- Leburton (phonons)
- Klimeck (software)
- Roy (circuits)
- Dai (experiments)

Carbon nanotube electronics



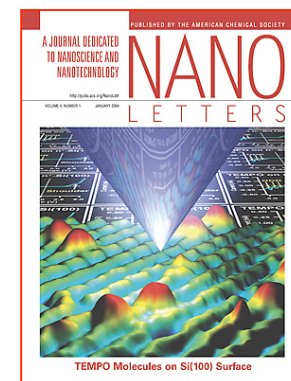
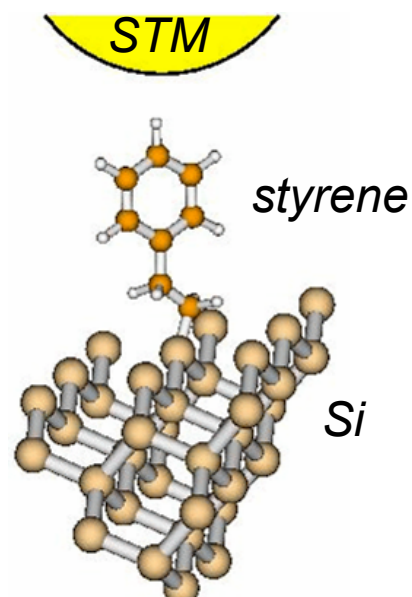
Dai / Lundstrom
Javey / Guo



July 2004

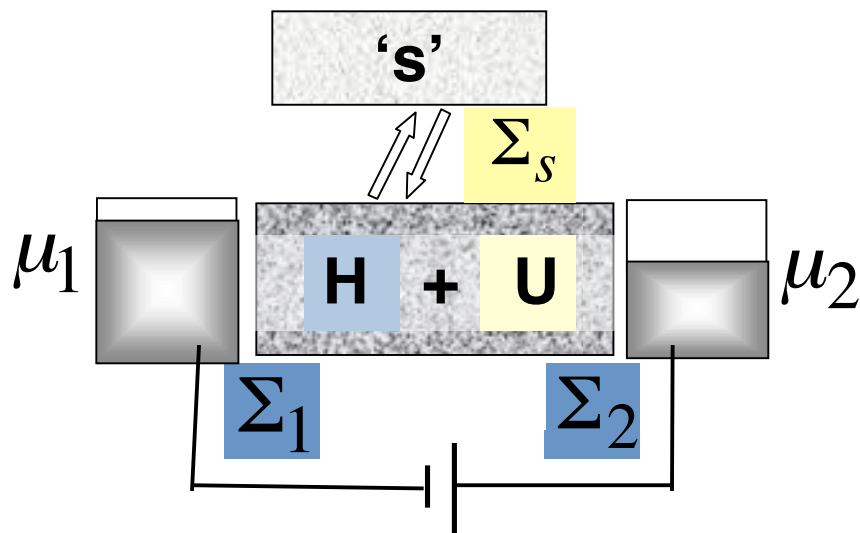
- Ratner (chemistry)
- Datta (basic theory)
- Klimeck (software)
- Roy/Lundstrom (circuits)
- Hersam (experiments)

Molecular electronics on Si

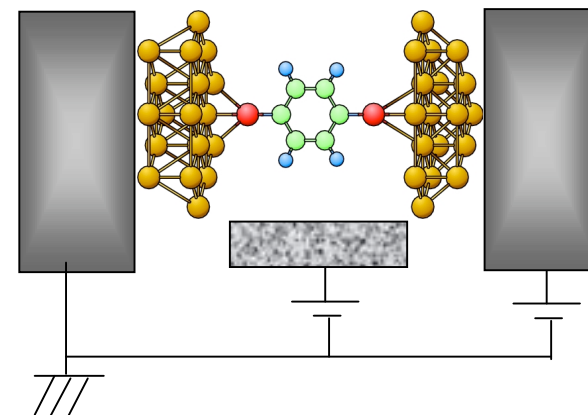


January 2004

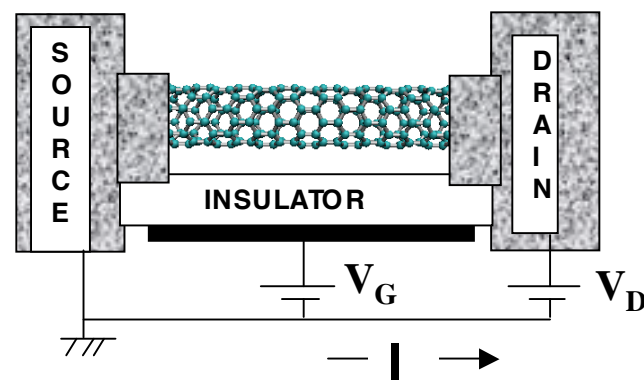
Unified Model



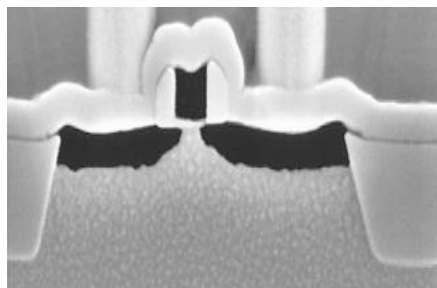
Molecular Electronics



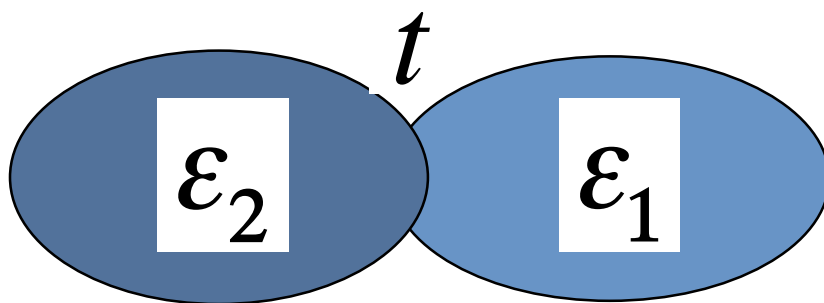
CNT Electronics



MOSFET's

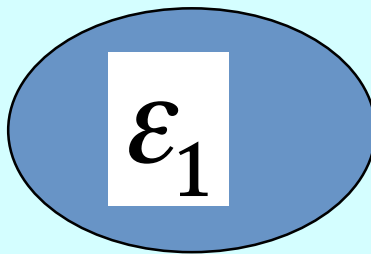


Σ : A toy example

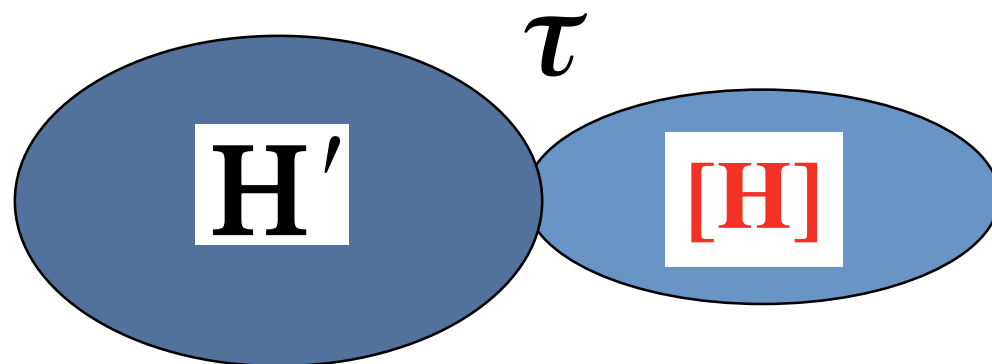


$$\begin{bmatrix} E - \epsilon_1 & -t \\ -t & E - \epsilon_2 \end{bmatrix}$$

$$\frac{t^2}{E - \epsilon_2} = \Sigma$$

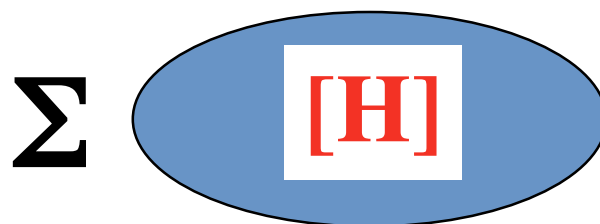


$$\Sigma \leftarrow \begin{bmatrix} E - \epsilon_1 - \frac{t^2}{E - \epsilon_2} \end{bmatrix}$$

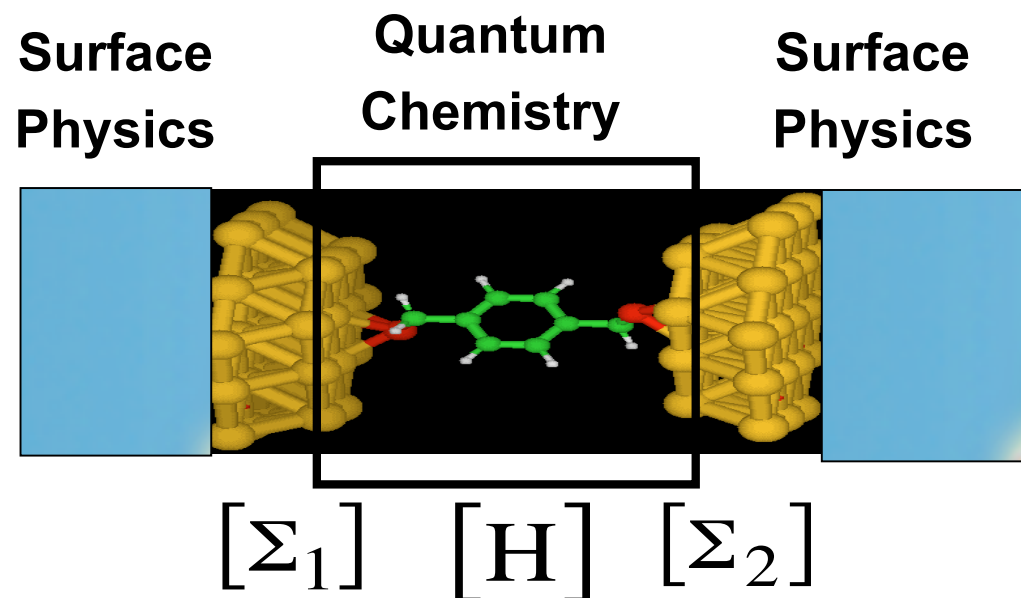


$$\begin{bmatrix} H & \tau \\ \tau^+ & H' \end{bmatrix}$$

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



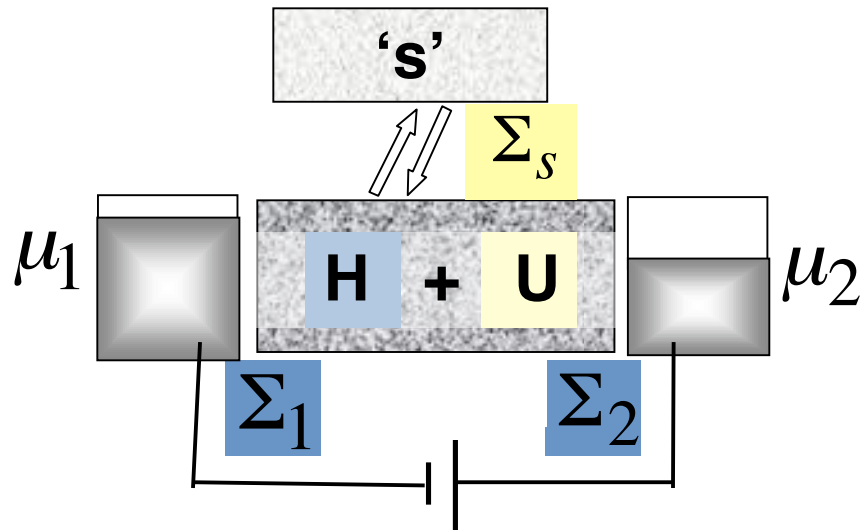
$$[H + \Sigma]$$



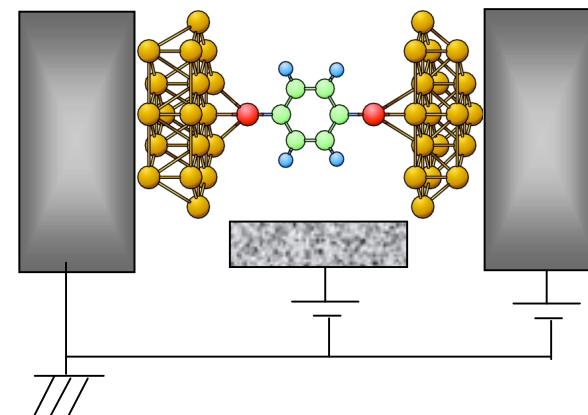
$$\Sigma(\mathbf{c}, \mathbf{c}) = \tau(\mathbf{c}, \mathbf{p}) \, g(\mathbf{p}, \mathbf{p}) \, \tau^+(\mathbf{p}, \mathbf{c})$$

Avik Ghosh, Albert Liang, Diego Kienle, Eric Polizzi

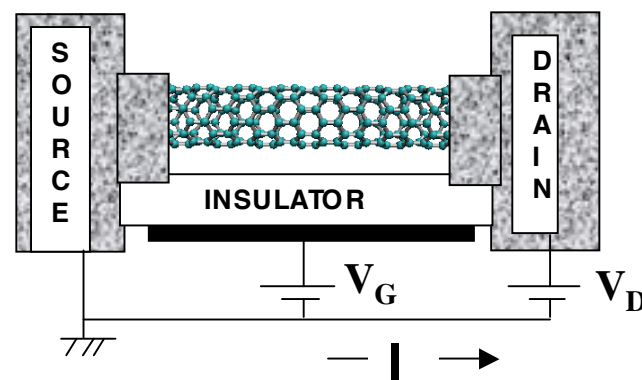
Unified Model



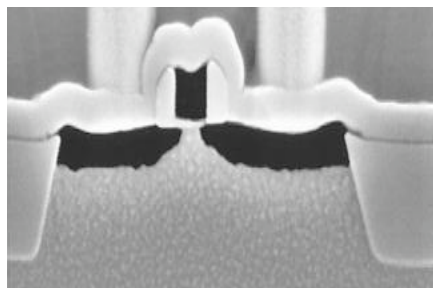
Molecular Electronics



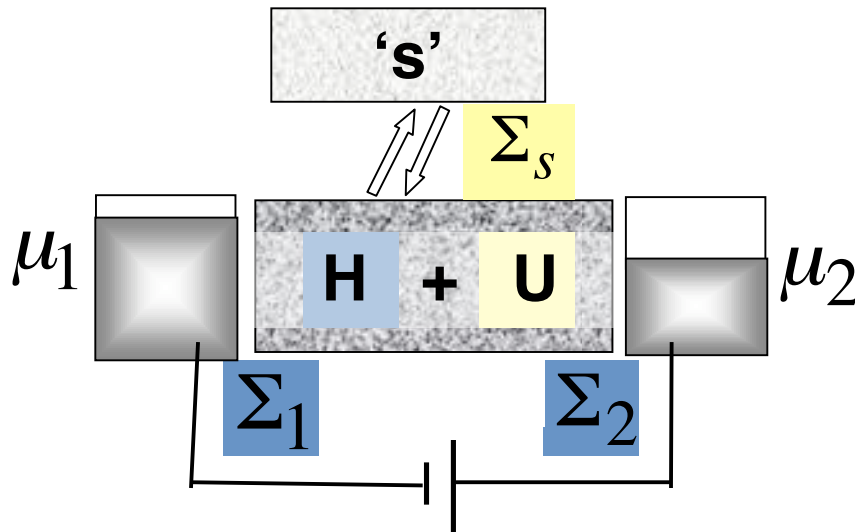
CNT Electronics



MOSFET's



Unified Model



to develop a general framework for relating atomic structure to device and circuit level performance.

Ferdows Zahid

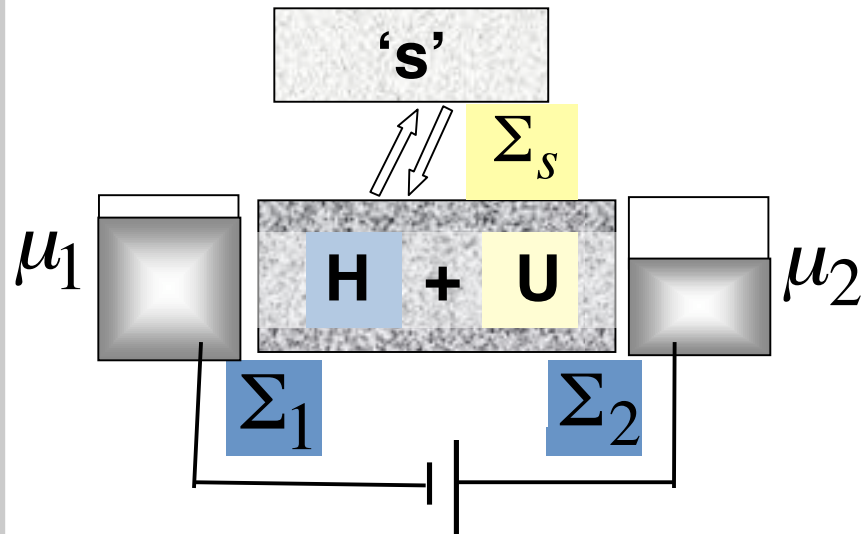
Tehseen Kazmi

Michael McLennan

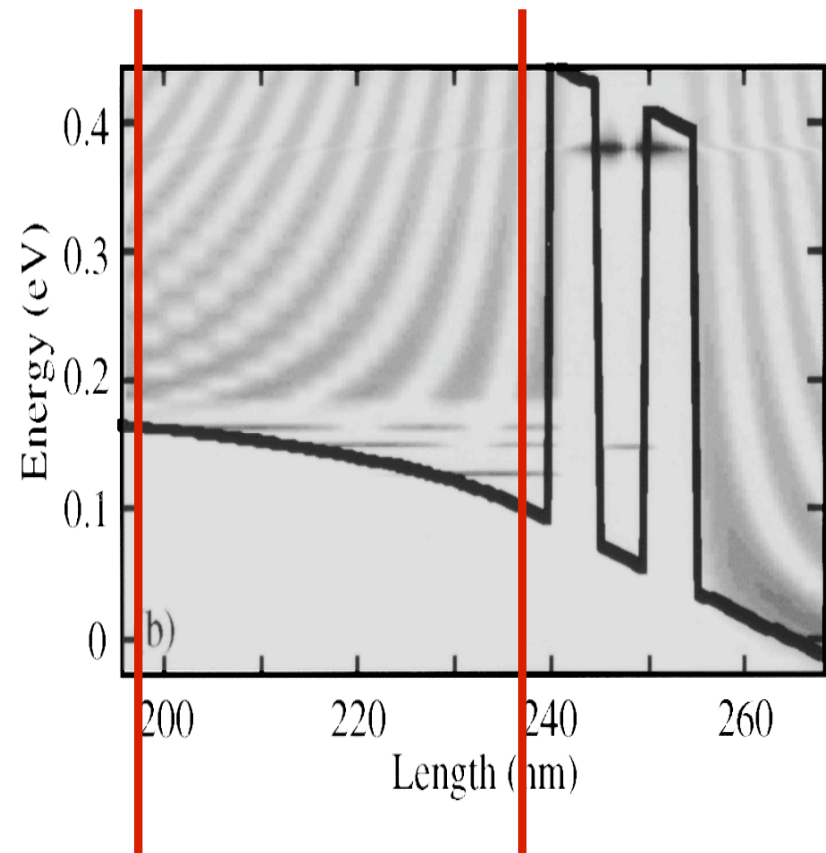
- Conceptual Understanding
- Practical Approaches
- Educational Resources
- Simulation Tools
- Professional Leadership

What is a contact?

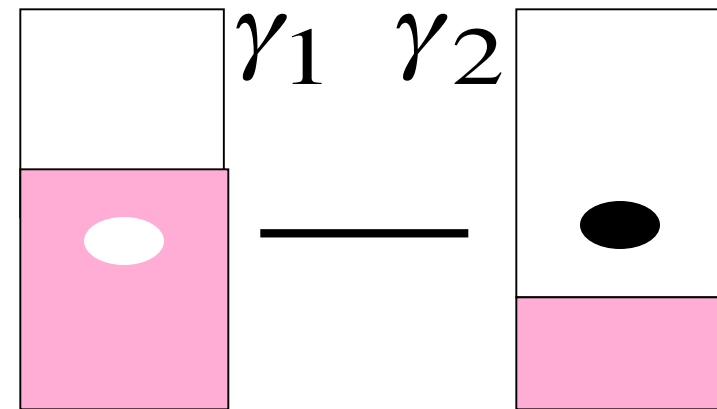
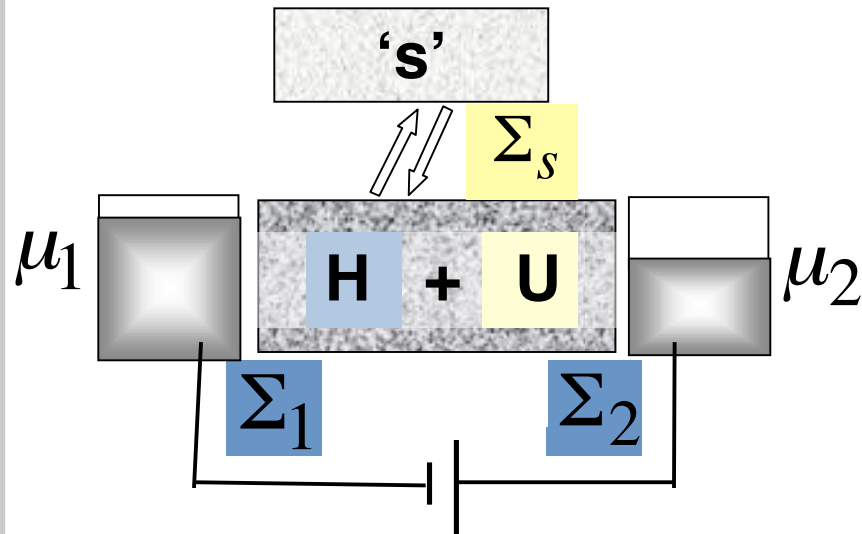
Unified Model



Klimeck, Lake et.al.
APL (1995)

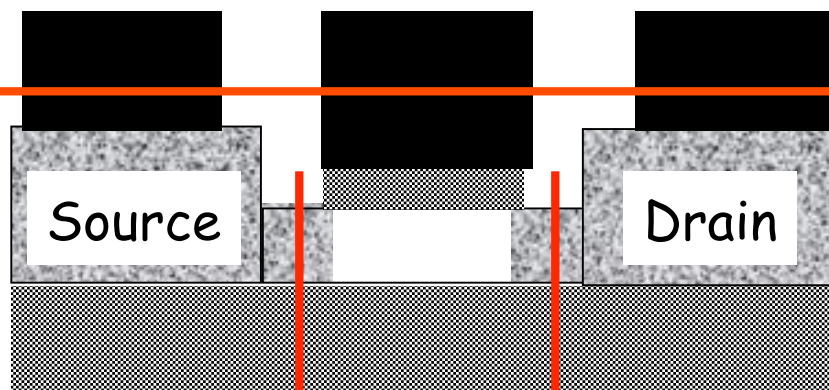
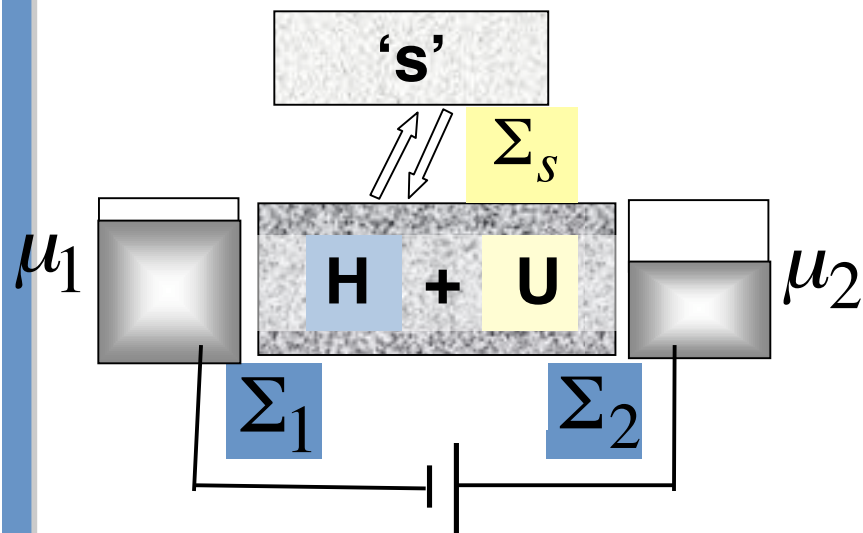


Unified Model



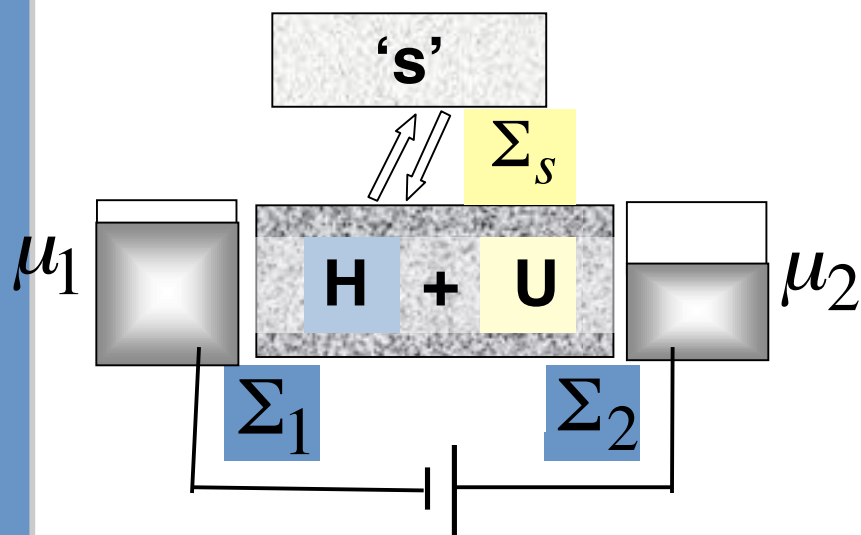
Energy has to be removed efficiently
from the contacts: otherwise
--> "hot" contacts

Unified Model

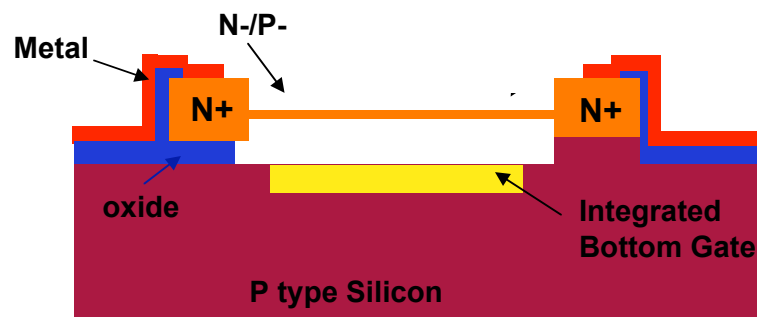


Hot "contacts"

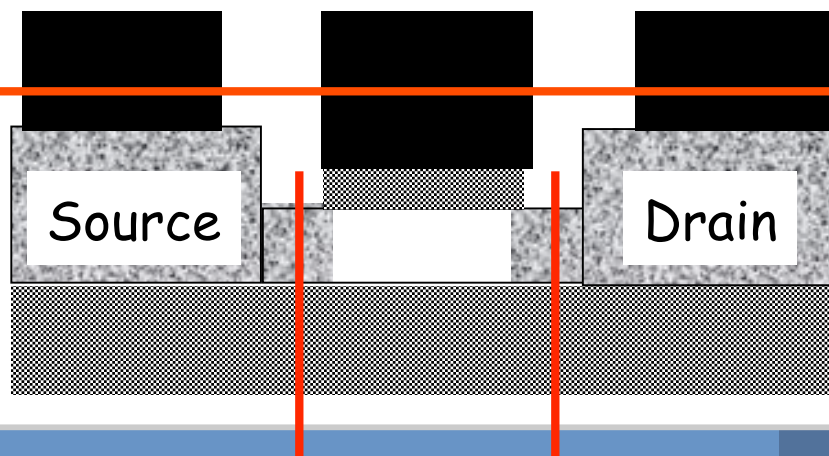
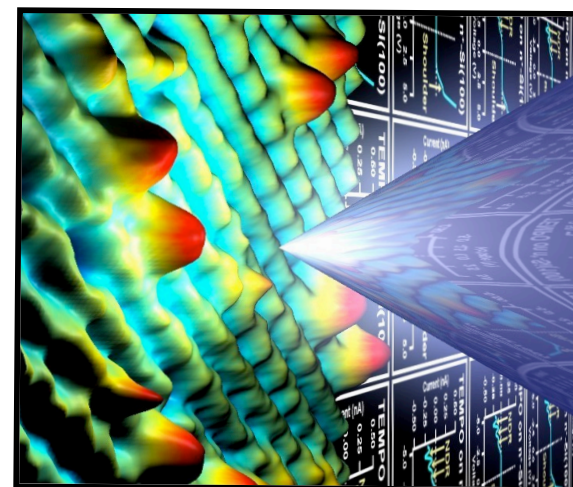
Unified Model



Hot phonons ?

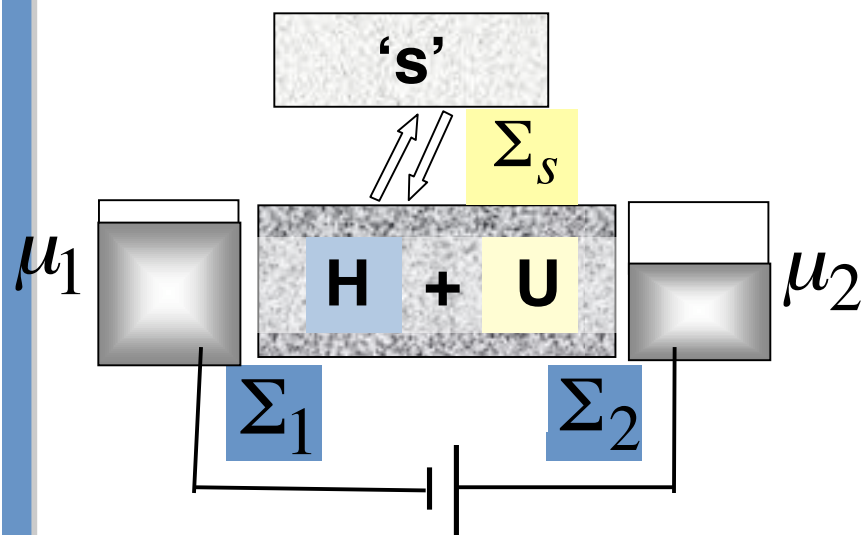


Molecular desorption ?



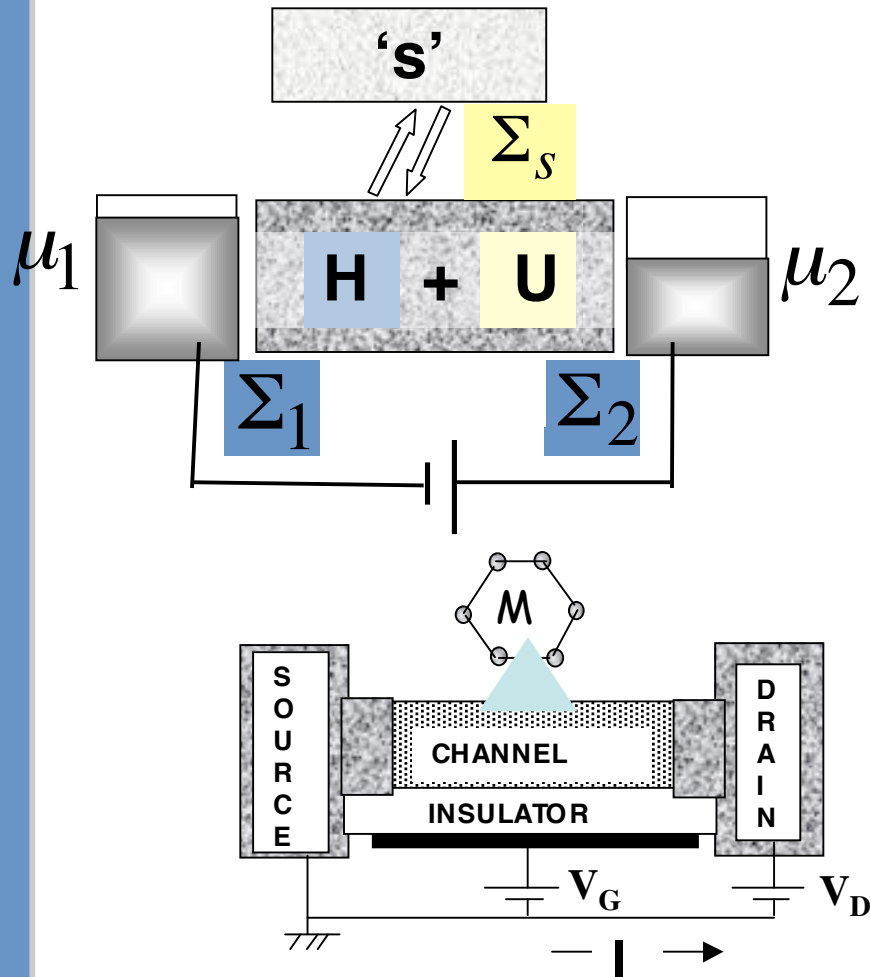
Modeling "hot contacts"

Unified Model



Supplement **device**
equations with
separate equation
for "contact"

Unified Model

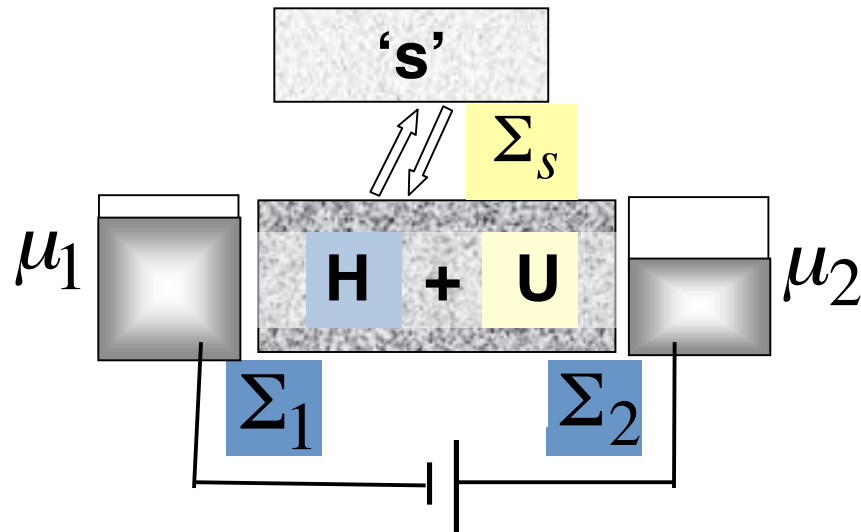


Supplement **device equations** with **separate equation** for "contact"

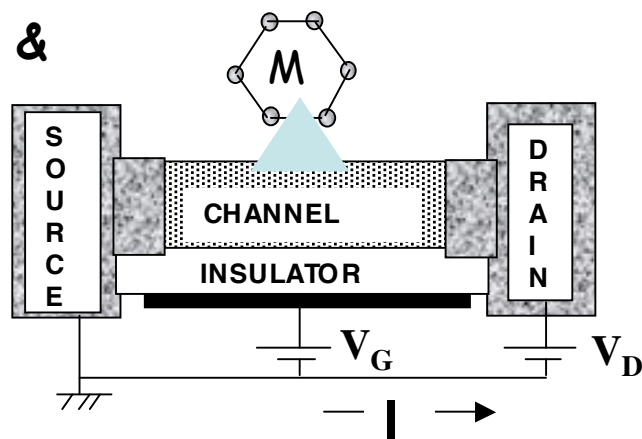
Contacts can involve different degrees of freedom:

- Mechanical
- Spin

Unified Model



Electronics & Sensing



- Conceptual Understanding
- Theoretical Approaches
- Educational Resources
- Simulation Tools
- Professional Leadership

www.nanohub.org

"Hot contacts"