Huckel I-V 3.0: A Self-consistent Model for Molecular Transport with Improved Electrostatics

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I. Introduction

Huckel I-V 1.0

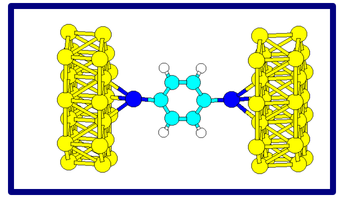
$V = ?V_{appl}$ (? theory)

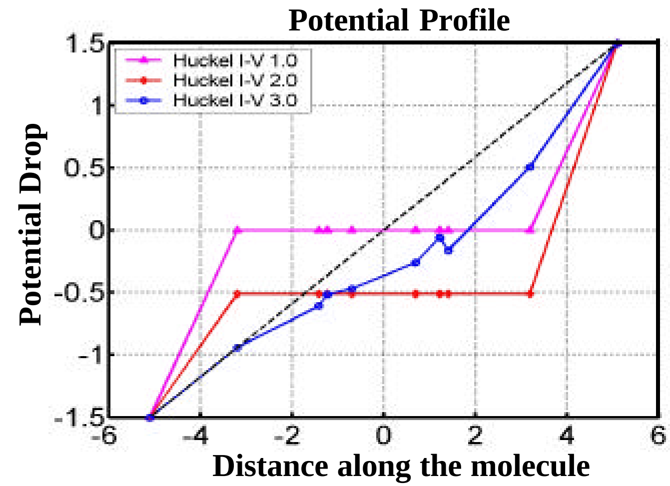
Huckel I-V 2.0

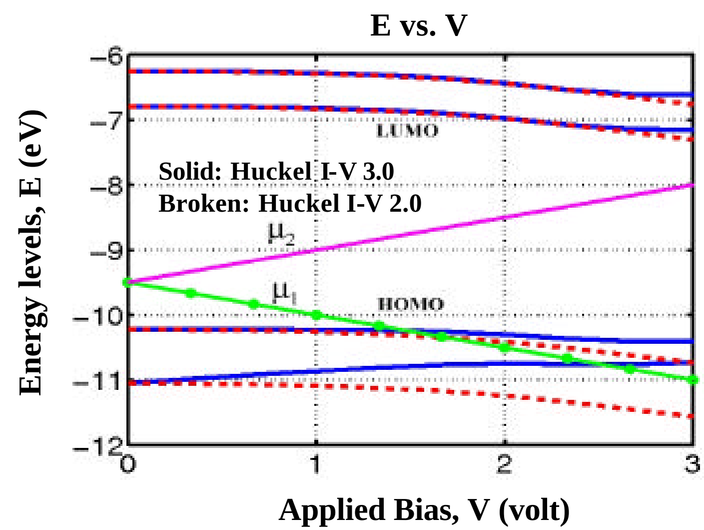
$V_{scf}(?N) = U_0 (N – N_{eq}) + 0.5V_{appl}$

Huckel I-V 3.0

$V_{scf}(??) = V_{Laplace} + V_{Poisson}(??) + V_{image}(??)$







I. Introduction

Complete description of the self-consistent potential

Spatial features retained

Both charging and screening effects included

Image corrections included

Three terminal calculations with proper electrostatics

Degrees of freedom: number of gates, oxide thickness, oxide dielectric constant

Computationally inexpensive

Useful to do calculations on large molecular systems

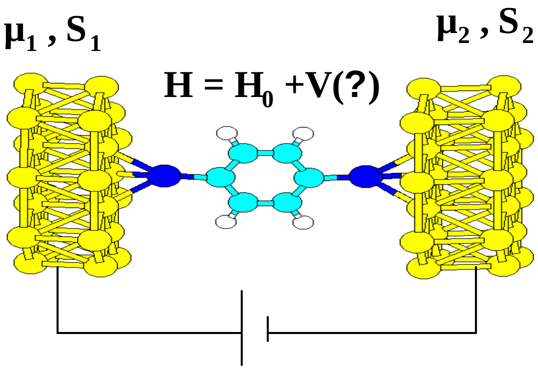
I. Introduction

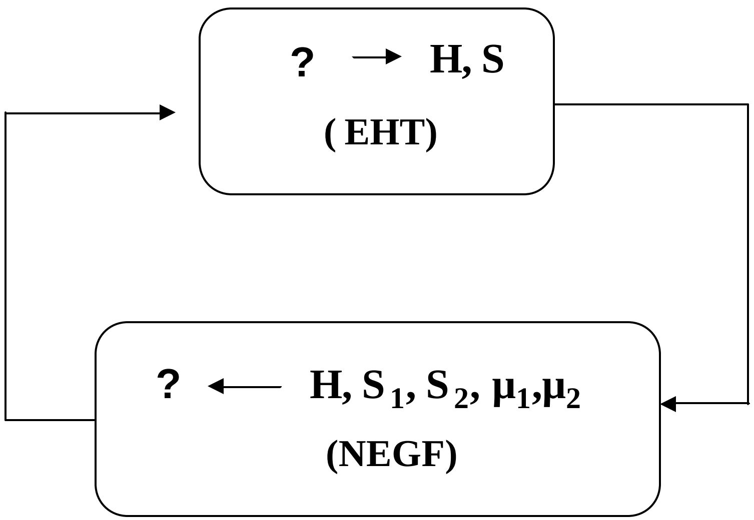
Previous Huckel I-V models are on the Nanohub for public use

Huckel I-V 3.0 will be on the hub soon

www.nanohub.org

II. Description of the Model





Hamiltonian (H) and Overlap (S) matrices from EHT

Self-consistent potential V(?) using any suitable scheme

Self-energies ($S_{1,2}$) from the surface Green's function of the contacts

Density matrix (?) using NEGF

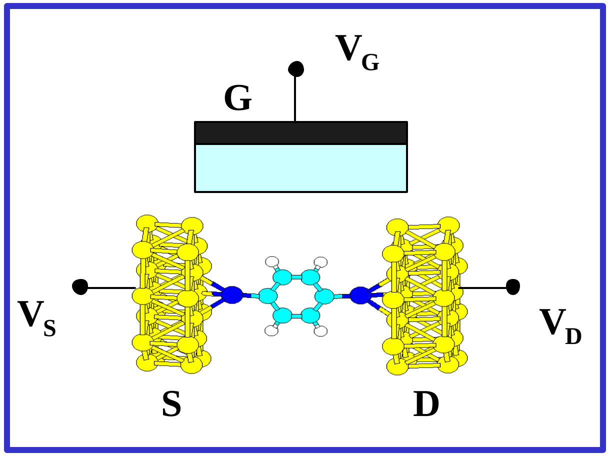
II. Description of the Model

Self-consistent Potential

$$V_{scf}(r) \rightarrow V_{scf}(\Delta r) = V_{Poisson}(\Delta r) + V_{image}(\Delta r) + V_{Laplace}$$

From CNDO using the Hartree term

Solving 3D Laplace in real space using FEM



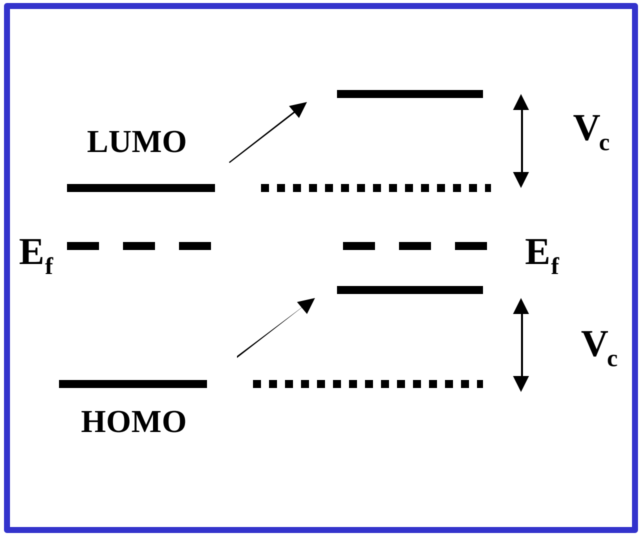
II. Description of the Model

Fitting parameter

Only one fitting parameter (V_c)

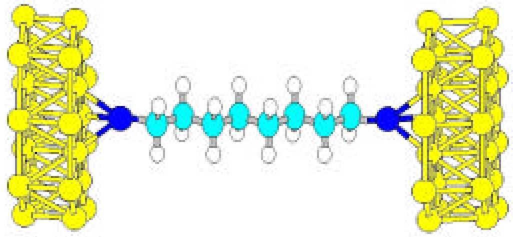
V_c **is a constant potential added to the molecular Hamiltonian**

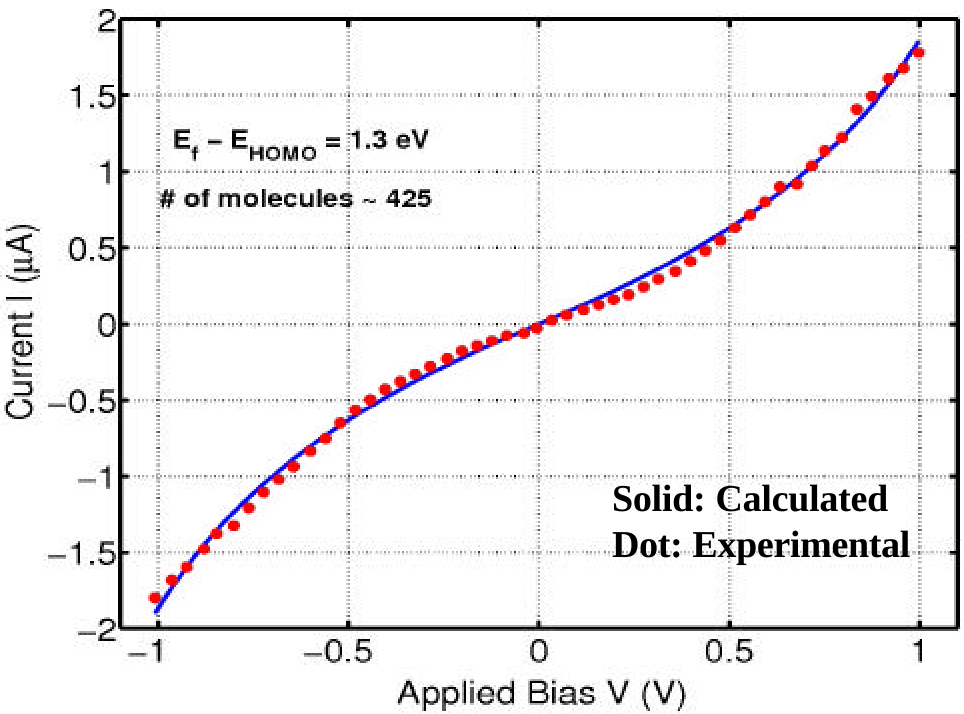
Fermi level of the device is kept fixed at the contact Fermi energy (-9.5 eV)



Effect of V_c

III. Results: I-V for Octane Dithiols



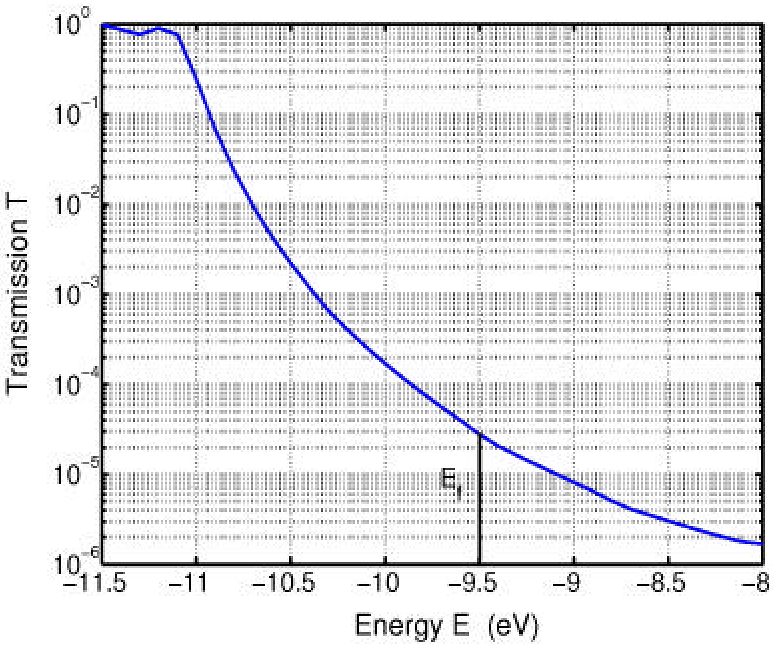


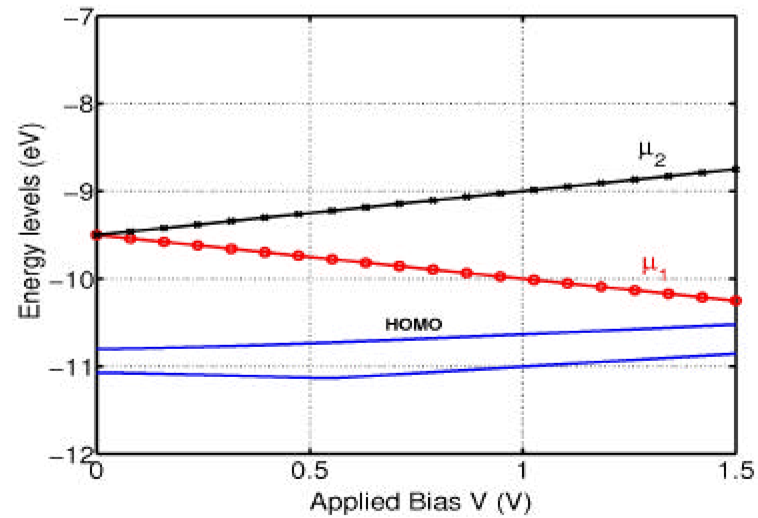
Two fitting parameters:
V_c (i.e. E_f-E_{HOMO}) and effective number of molecules

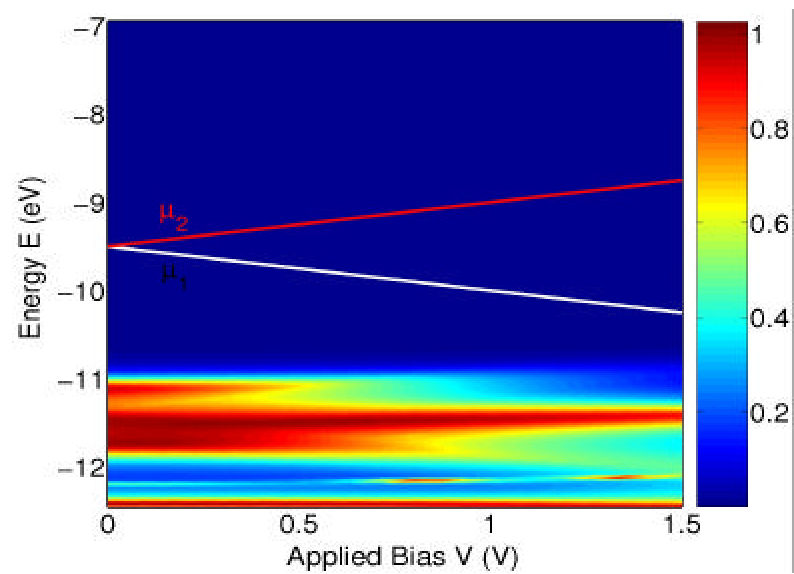
Strong coupling on both sides
S-Au bond length = 2.53 A^o

Nanopore data:
Reed, Nanoletters, v. 4, p. 643 (2004)

III. Results: I-V for Octane Dithiols



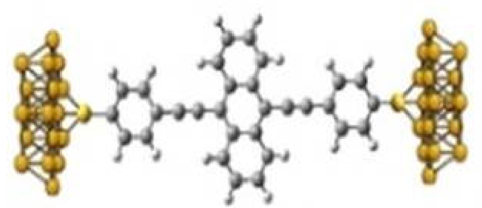


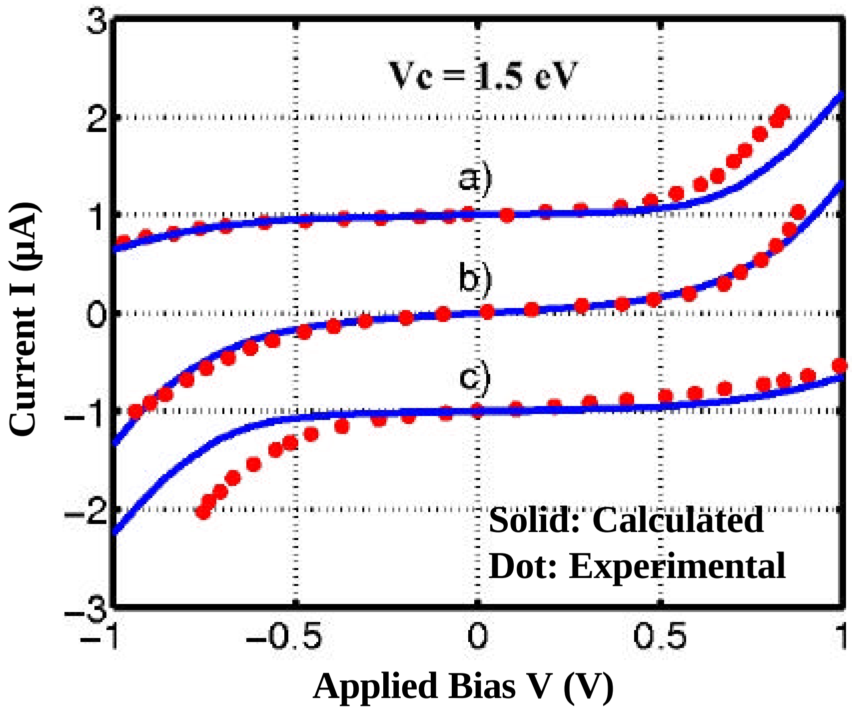


Conduction is in tunneling regime

low transmission, low current

III. Results: Asymmetric I-V





a) Left contact is weakly coupled

b) Symmetric coupling

c) Right contact is weakly coupled

Good quantitative match for both current value and shape

Asymmetry in the I-V is due to asymmetry in charging

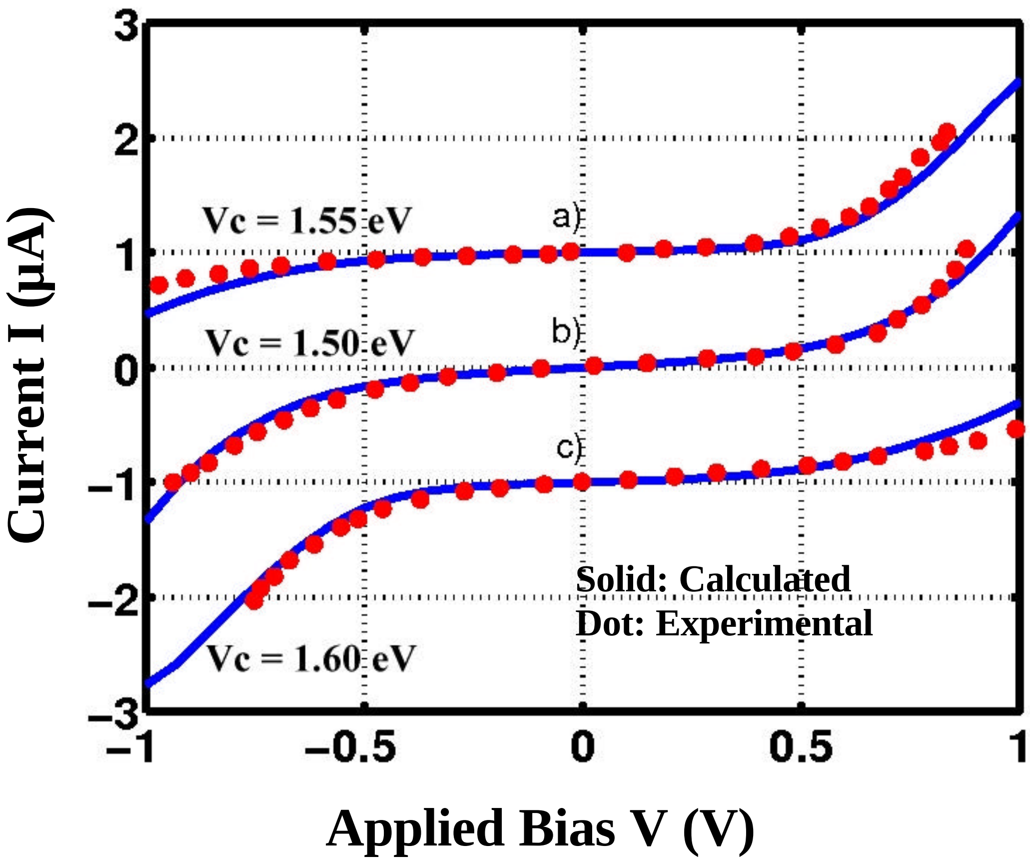
Weak coupling is simulated by stretching S-Au bond length from 2.53 A^o to 3.18 A^o

Current is going through HOMO level and $E_f - E_{HOMO}$ is set to be 0.33 eV

Break Junction data:
Weber, PRL v. 88, 176804 (2002)

Our results:
PRB v. 70, 2004 (in production)

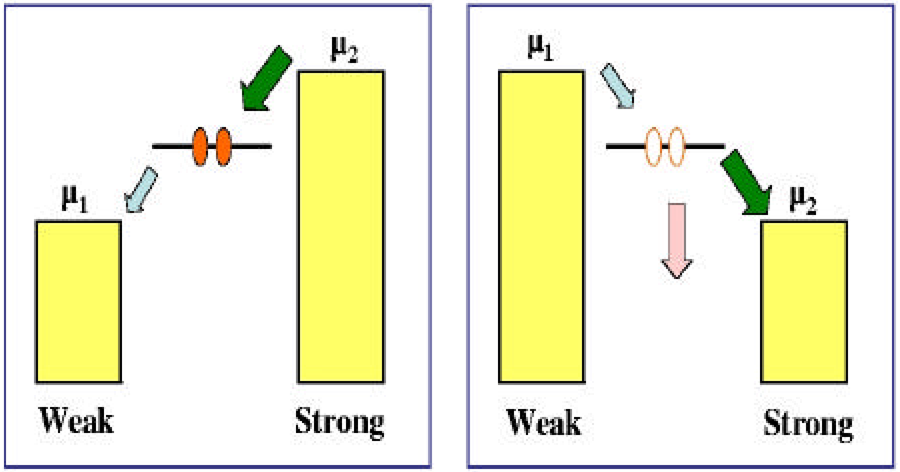
III. Results: Asymmetric I-V



A better match is obtained with different V_c values for each curve

III. Results: Asymmetric I-V

Origin of Asymmetry



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

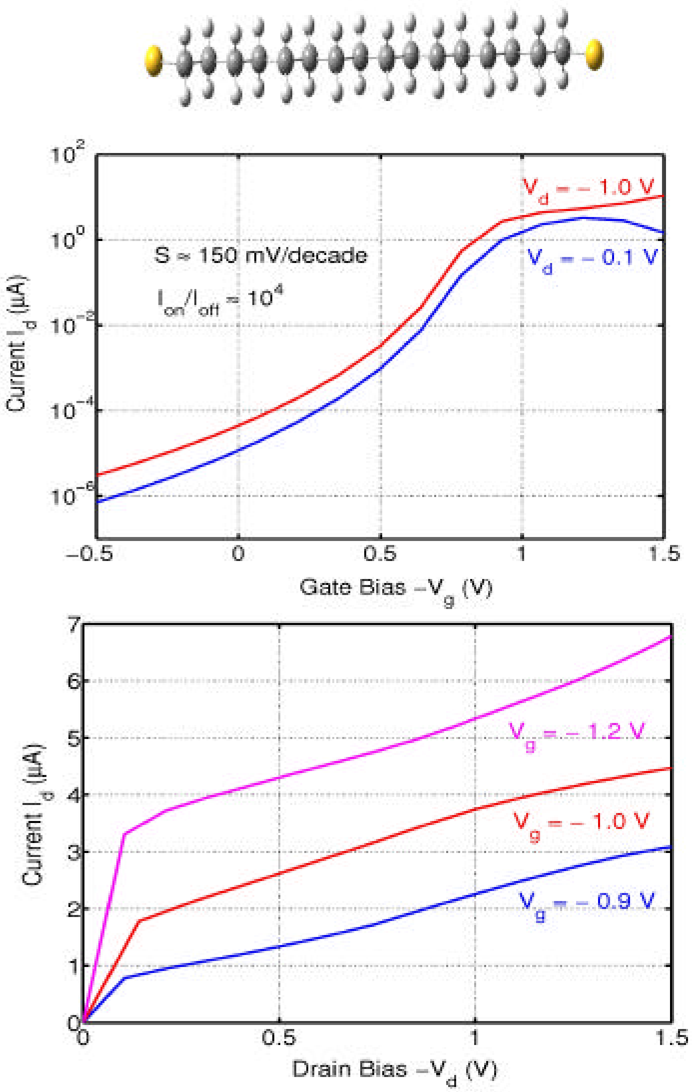
Asymmetric coupling gives rise to asymmetry in Charging

The molecule gets positively charged in the negative bias direction and that shifts the energy level down

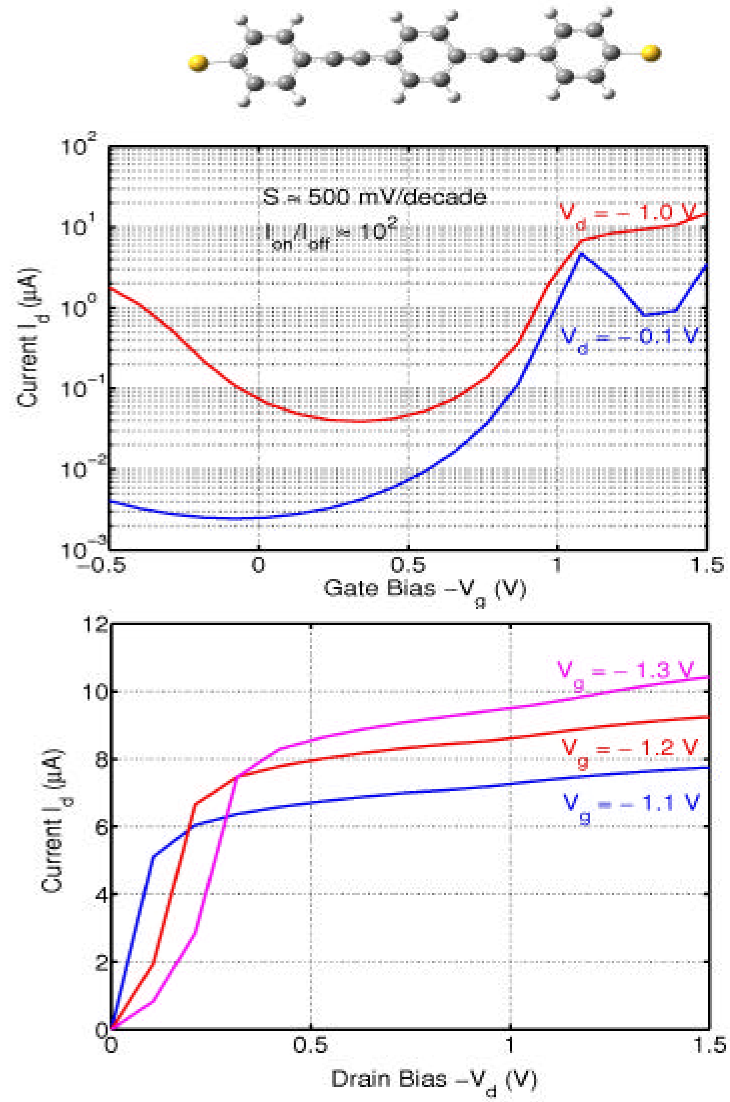
In the positive bias direction the energy level remains filled and there is no charging

III. Results: Gate effects

(A)



(B)

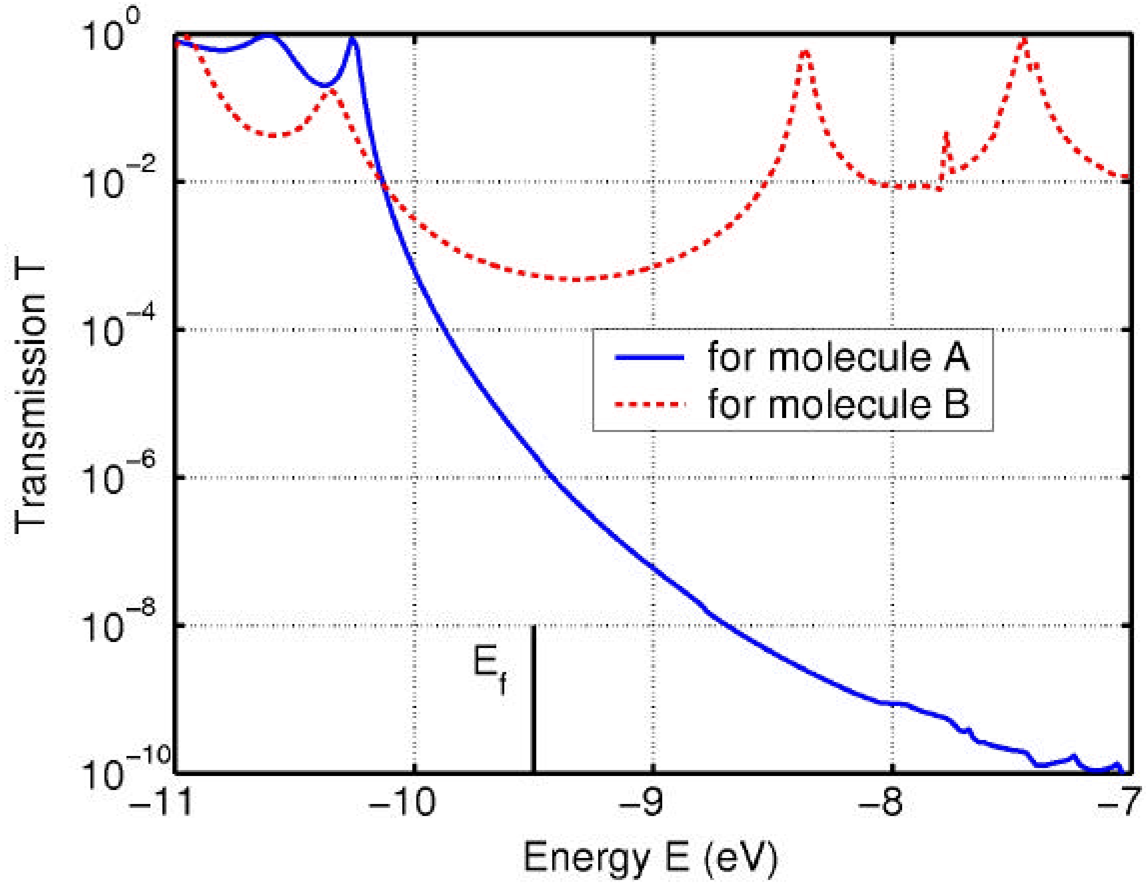


III. Results: Gate effects

Current is proportional to Transmission

Switching behavior is related to transmission

$I_{on}/I_{off} \sim T(E_{HOMO})/T(E_f)$



IV. Summary

Huckel I-V 3.0: A new transport model with better and improved electrostatics

Main strengths of the model:
full description of the potential profile
inclusion of gate electrodes
computationally inexpensive

Our calculations showed good agreement with few experimental results