

Charge Transport 101: A Few Major Mechanisms

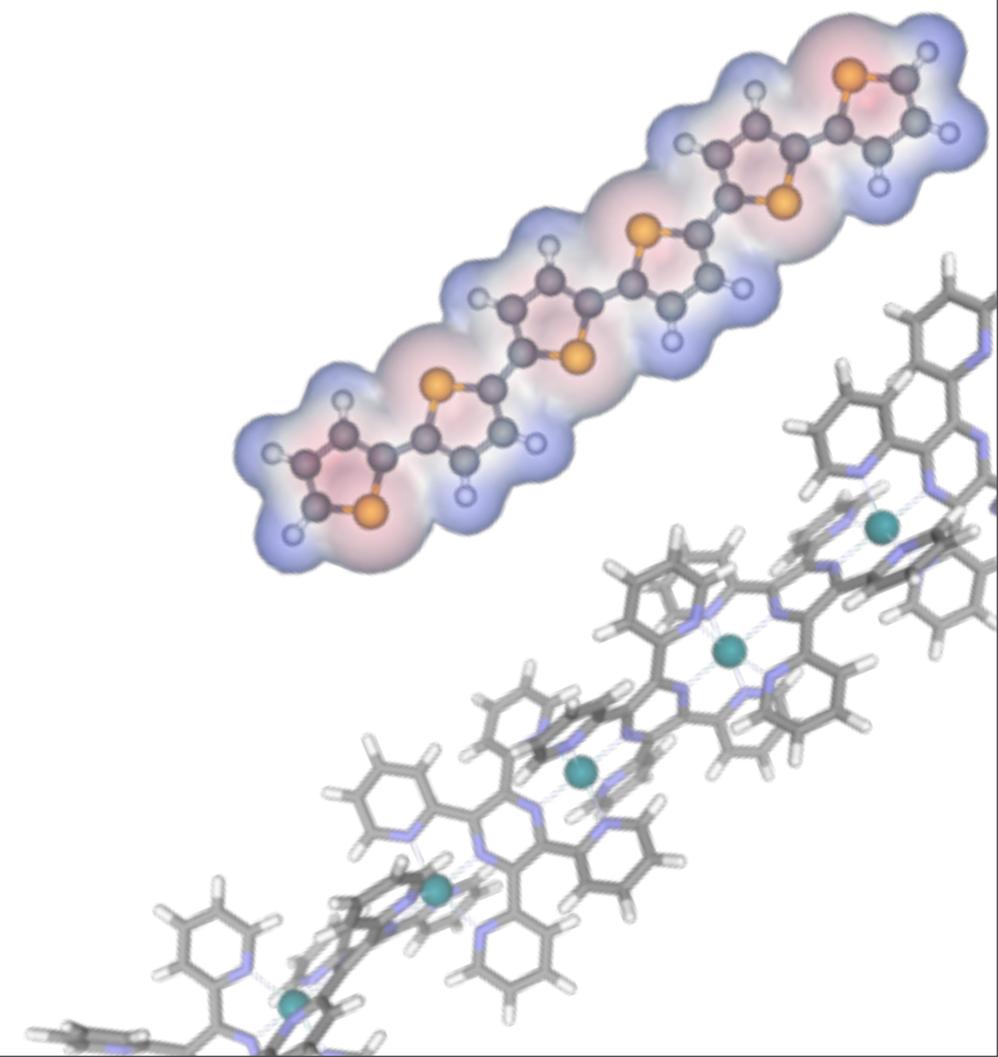


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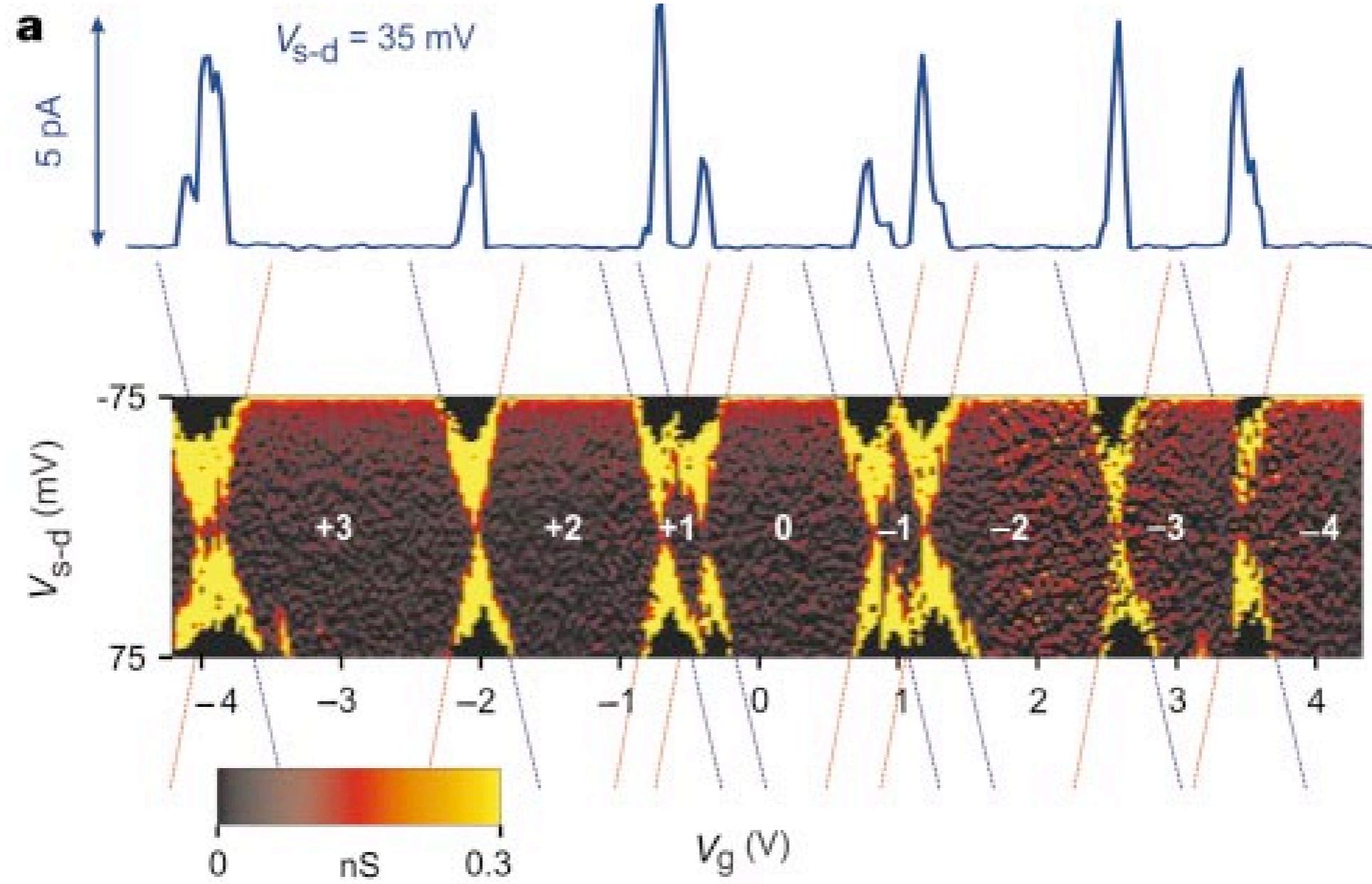
<http://hutchison.chem.pitt.edu>



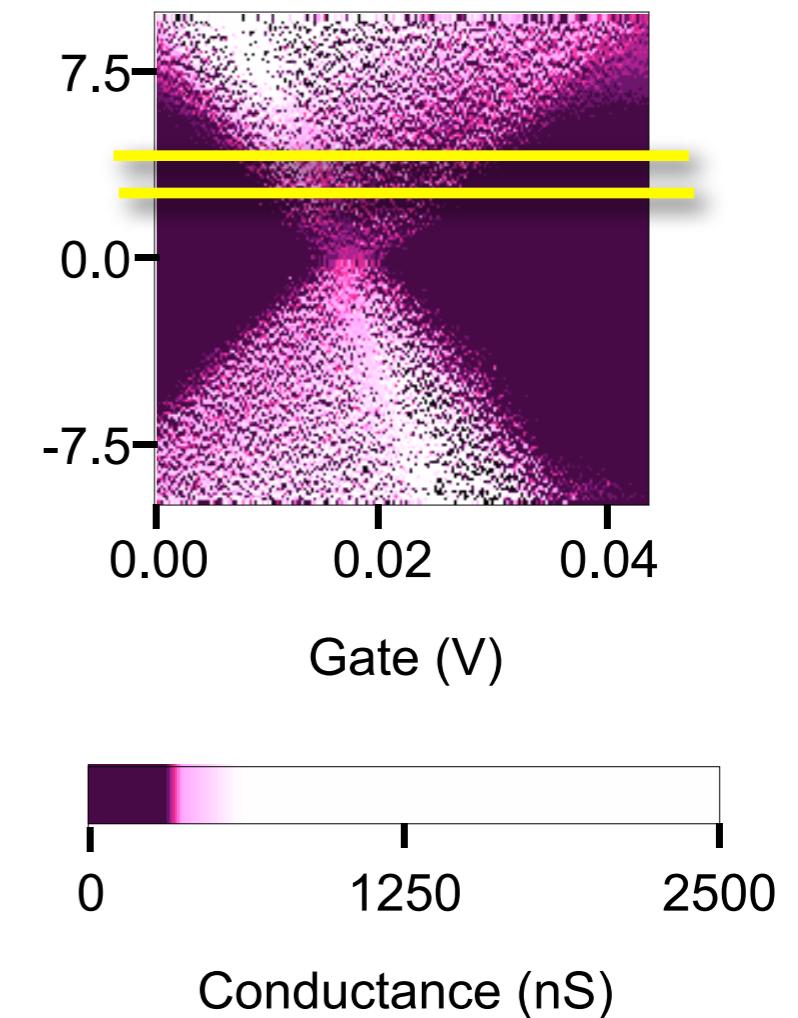
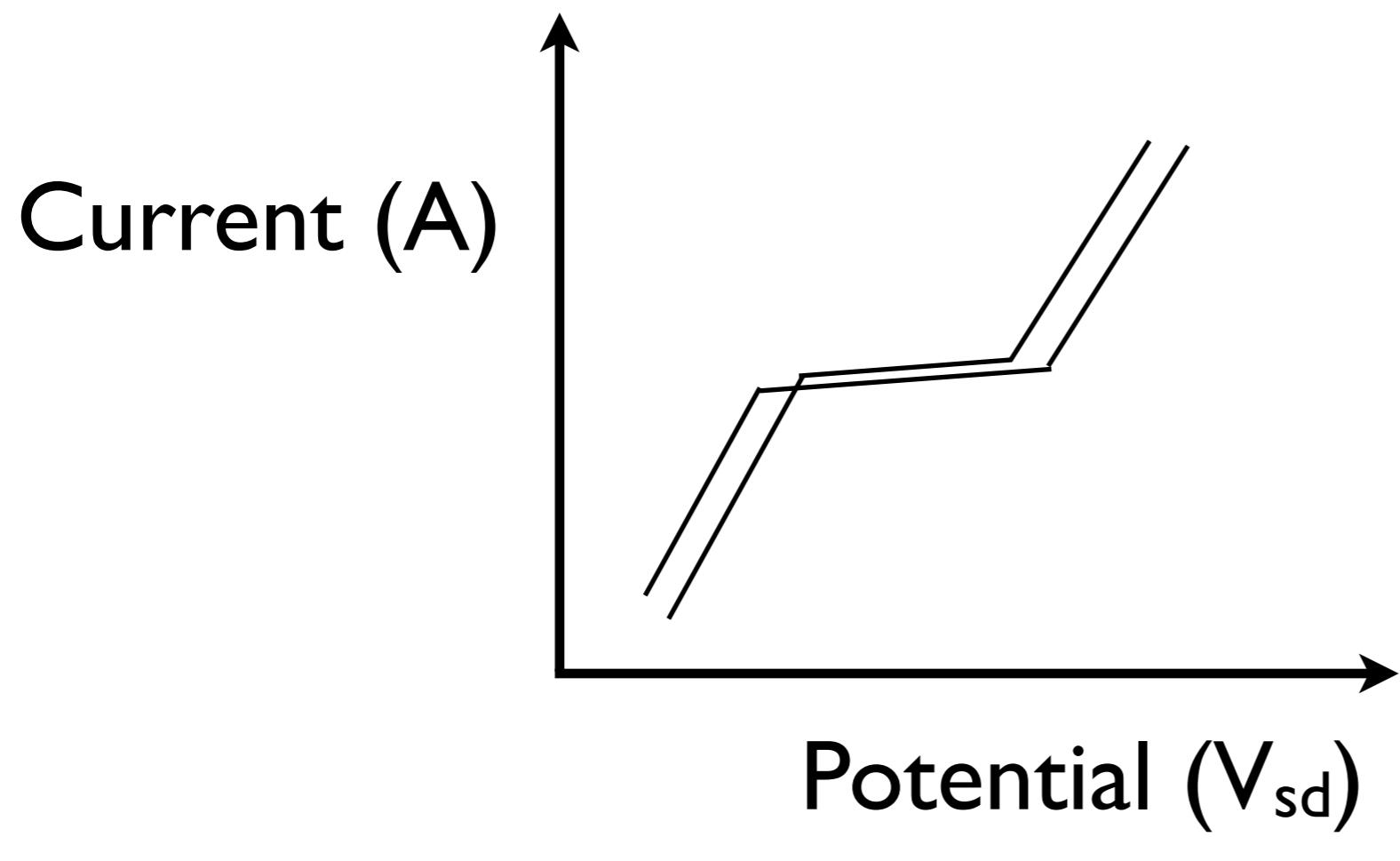
Outline

- Superexchange
- Basic Hopping
- Metallic Transport (e.g., Drude Model)
- Coulomb Blockade (continued)
- Kondo Effect
- Negative Differential Resistance
- Electron-Vibrational Effects

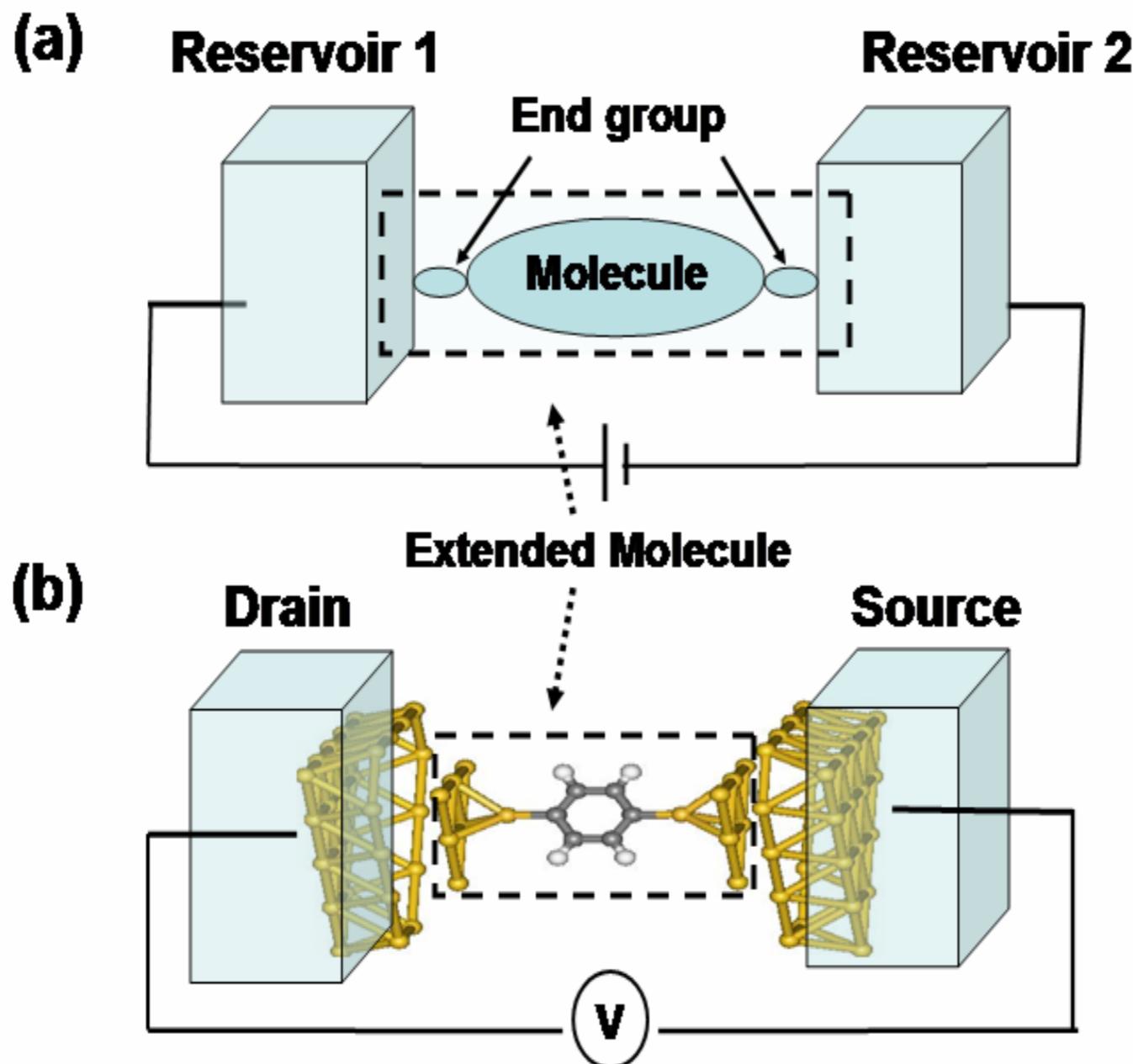
Coulomb Blockade Again...



Coulomb Blockade I/V Curves



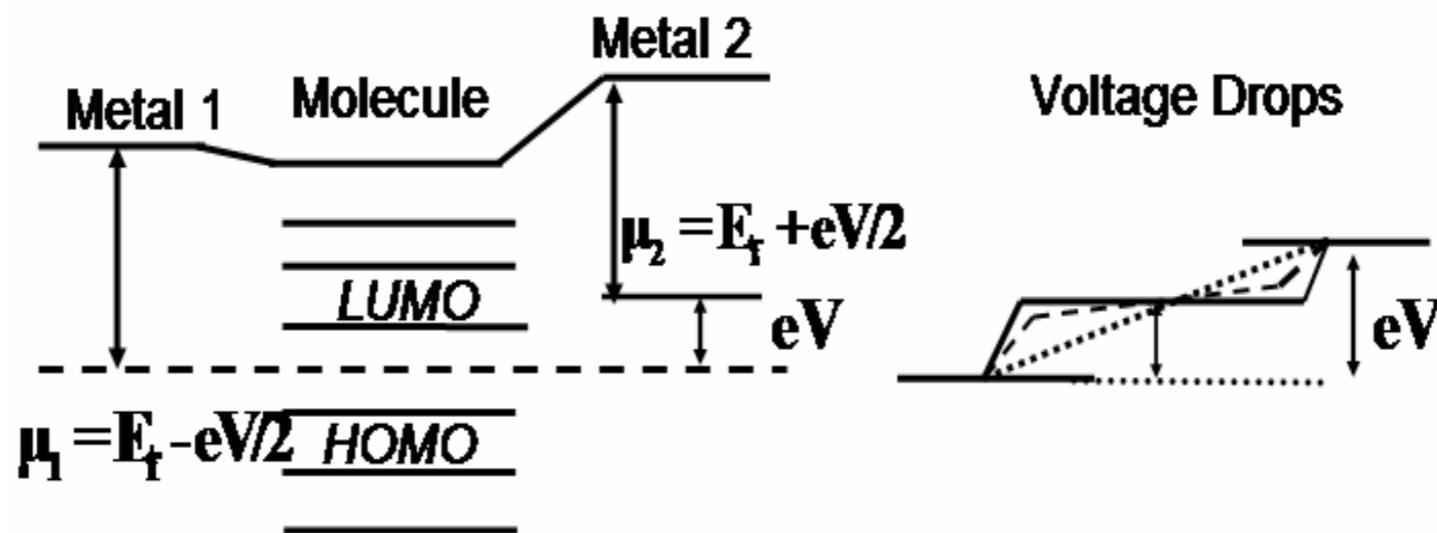
Calculations on Coulomb Blockade



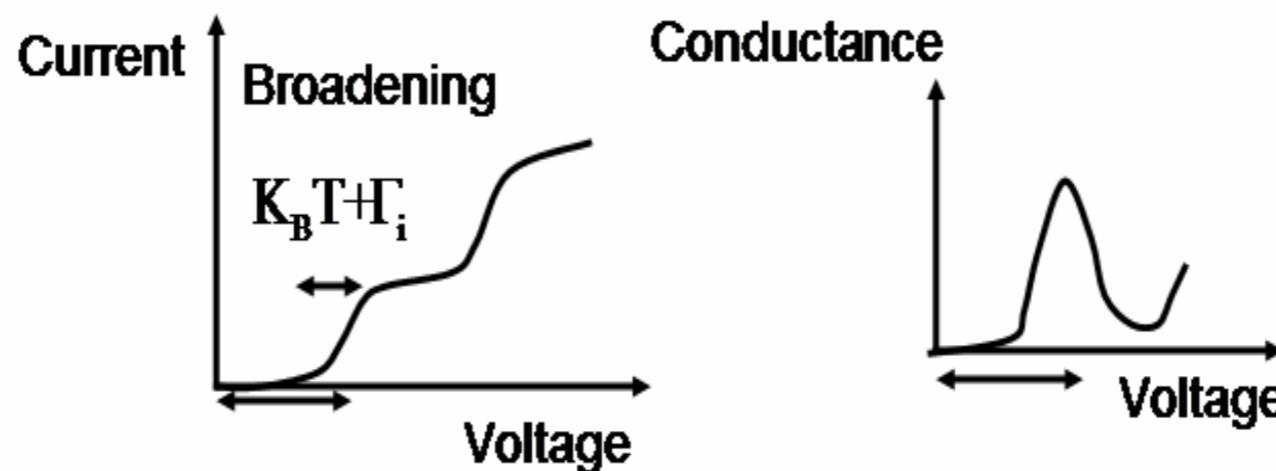
Simulating Coulomb Blockade

(a)

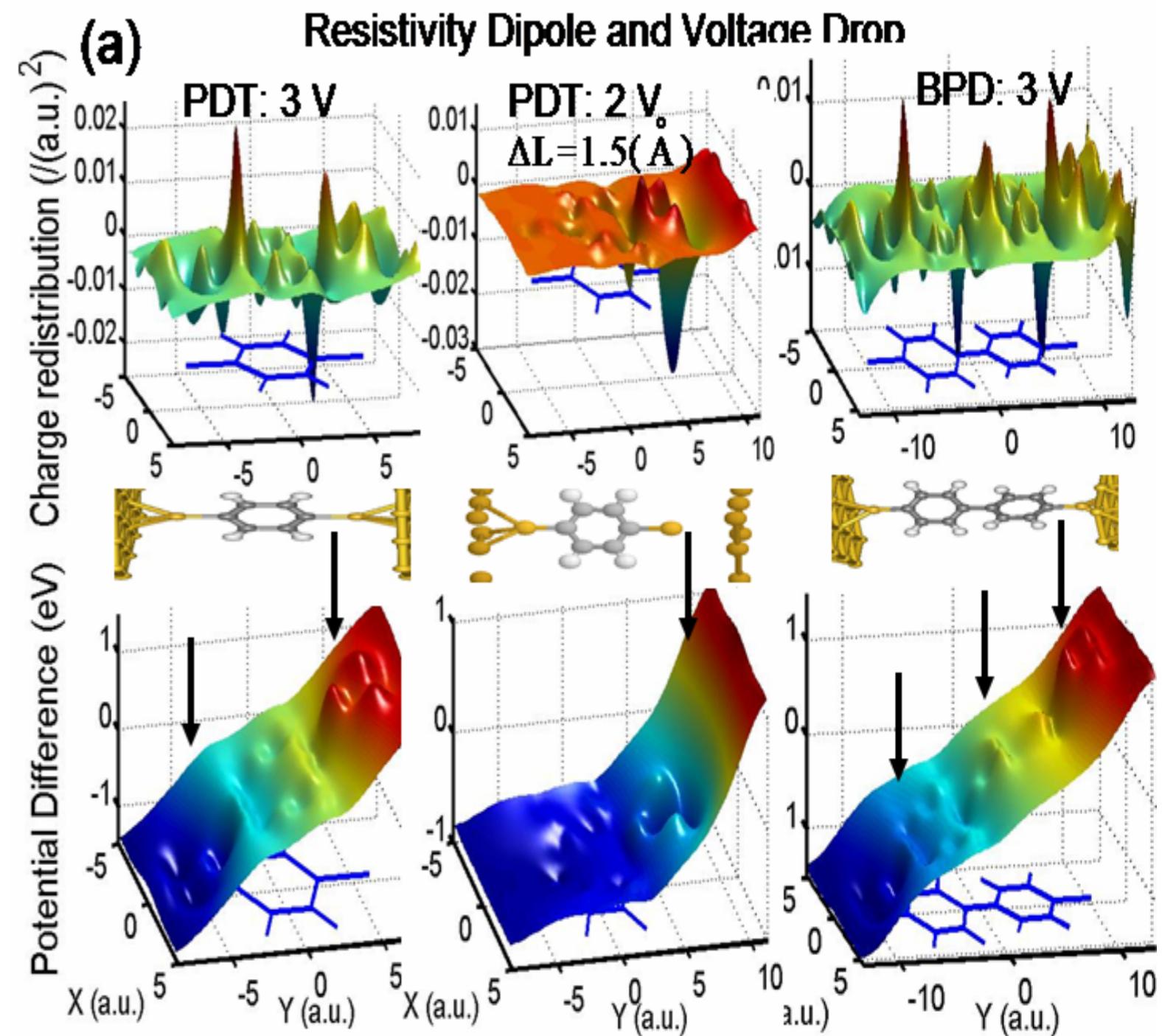
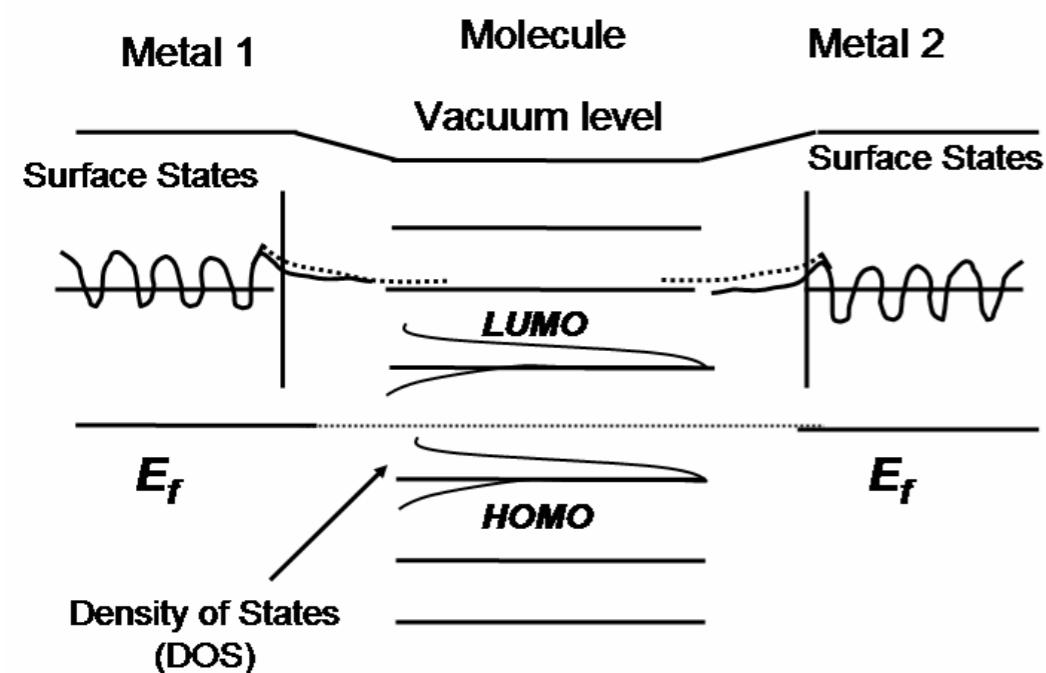
"Band" Diagram at Non-Equilibrium



(b)



Voltage Drop

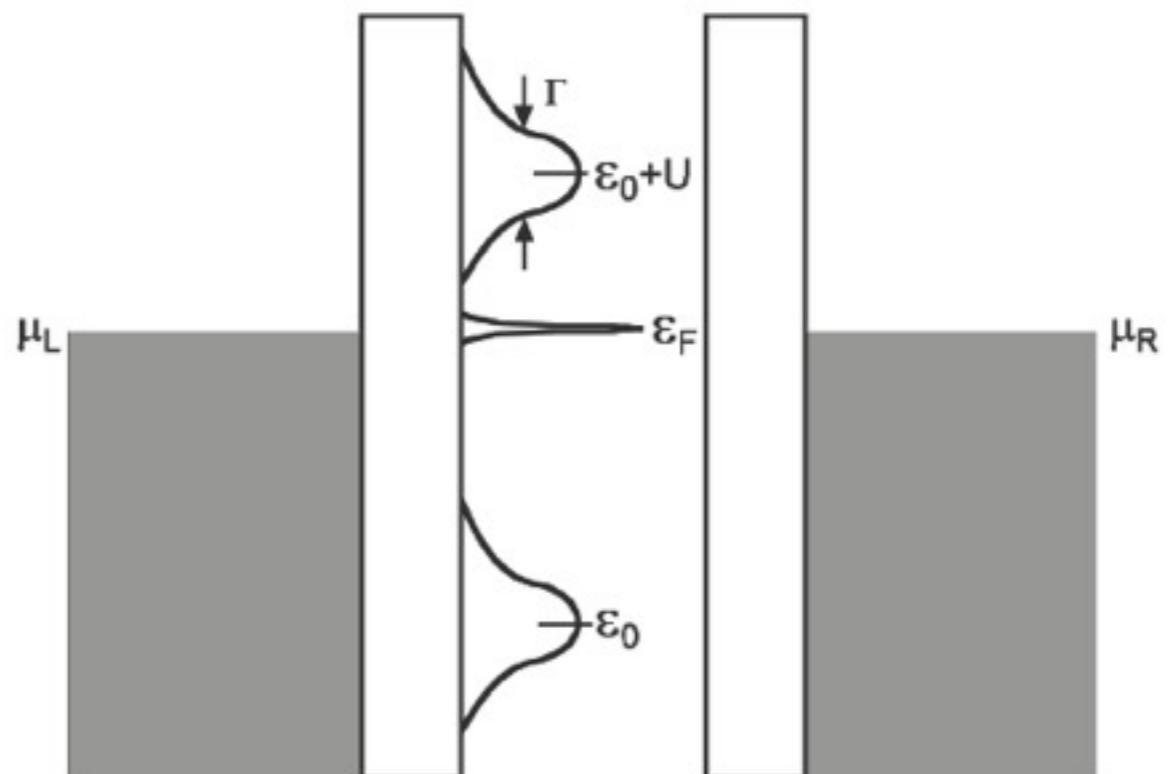
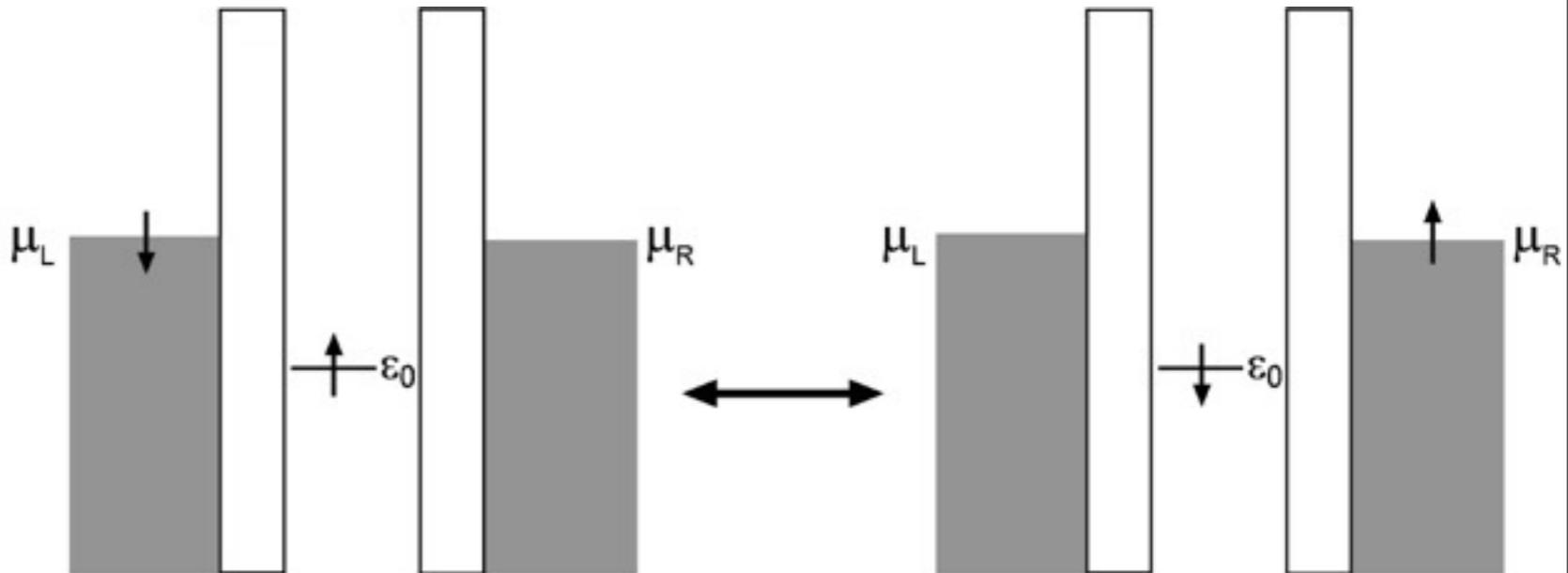


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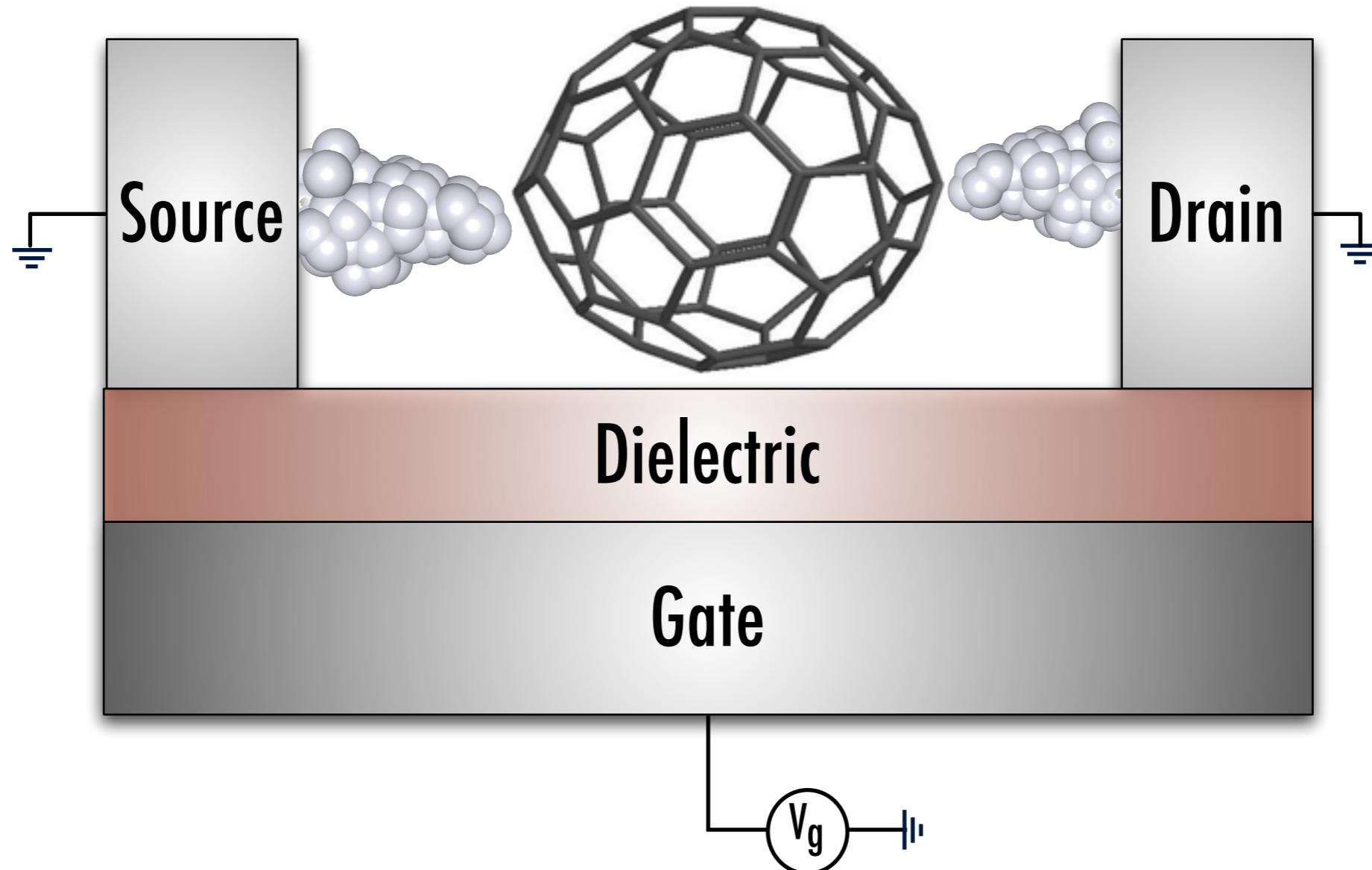
Kondo Effect

- A localized spin is screened by conduction electrons.
- This leads to a resonance at the Fermi Energy.
- A signature in transport is a peak in dI/dV at zero bias.
- Energy scale:
Kondo Temperature, T_K .

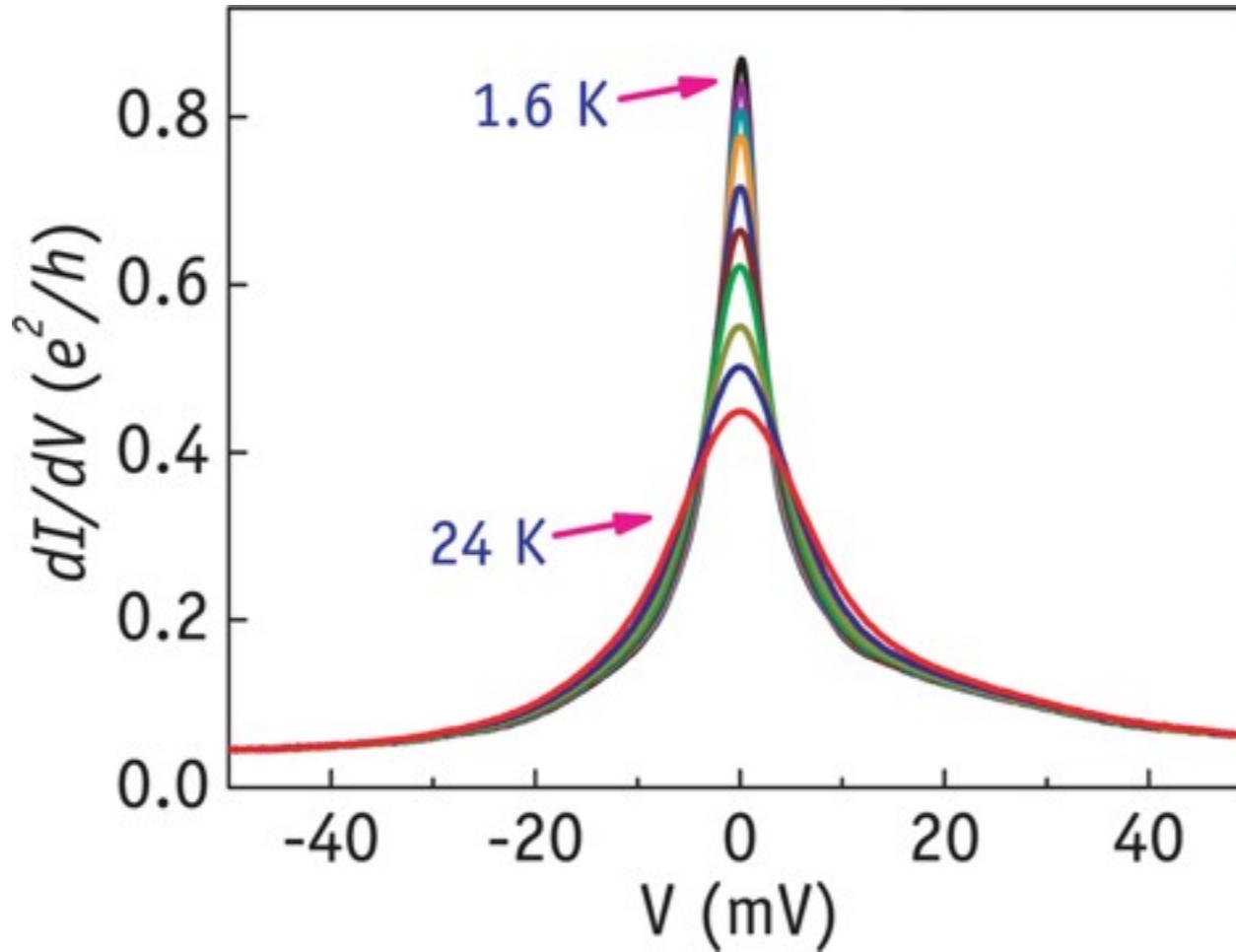


Device Schematic

Need good coupling to both electrodes...



Kondo Effect in C₆₀ Devices



- In 15% of devices, we observed a prominent zero-bias peak in dI/dV , which is suppressed as a function of temperature.
- In ~ 300 control samples, zero-bias features were observed in < 2% of devices.
- Fits yield $T_K = 28.2 \pm 0.3$ K, in agreement with FWHM ~ 30 K.

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Negative Differential Resistance

- Normal resistance: positive slope of I/V curve
- “Dynamic” resistance: resistance changes in a certain region

Why?

- Logic (switching)
- Amplifiers, etc.

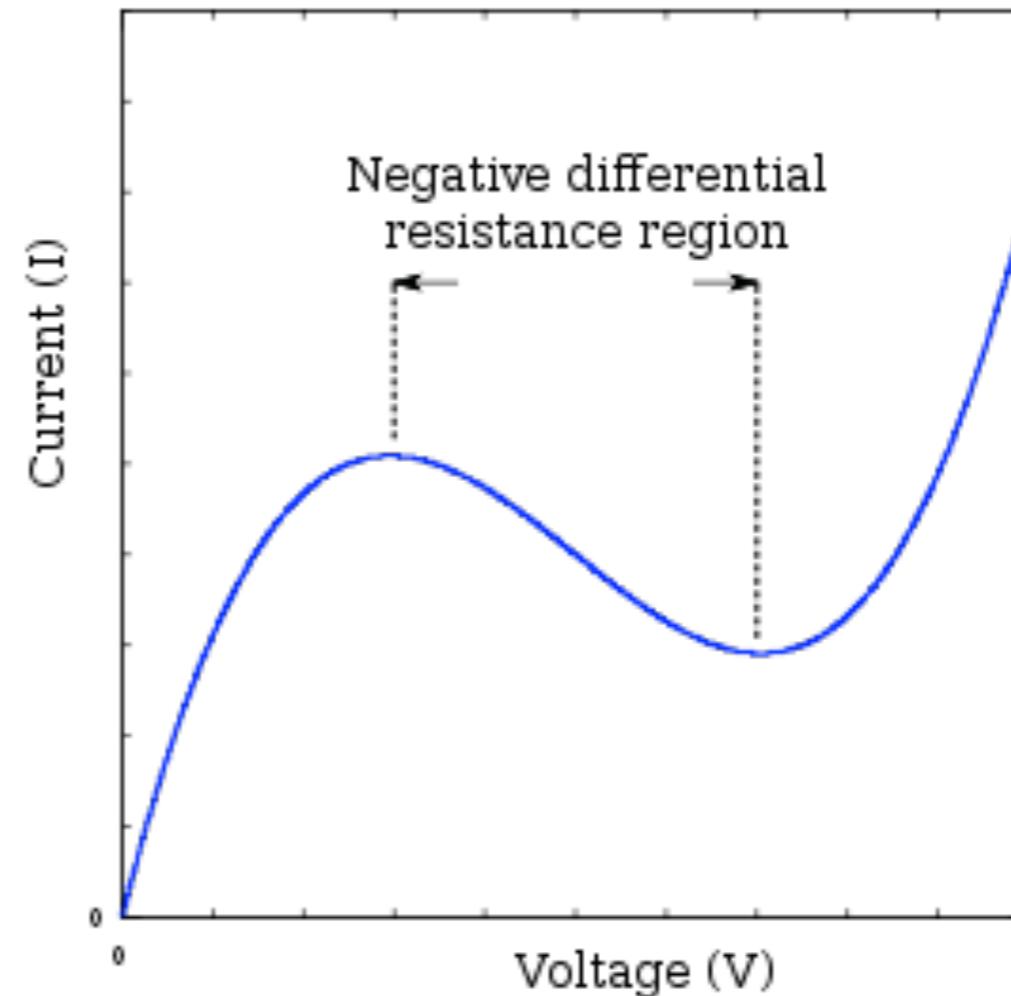
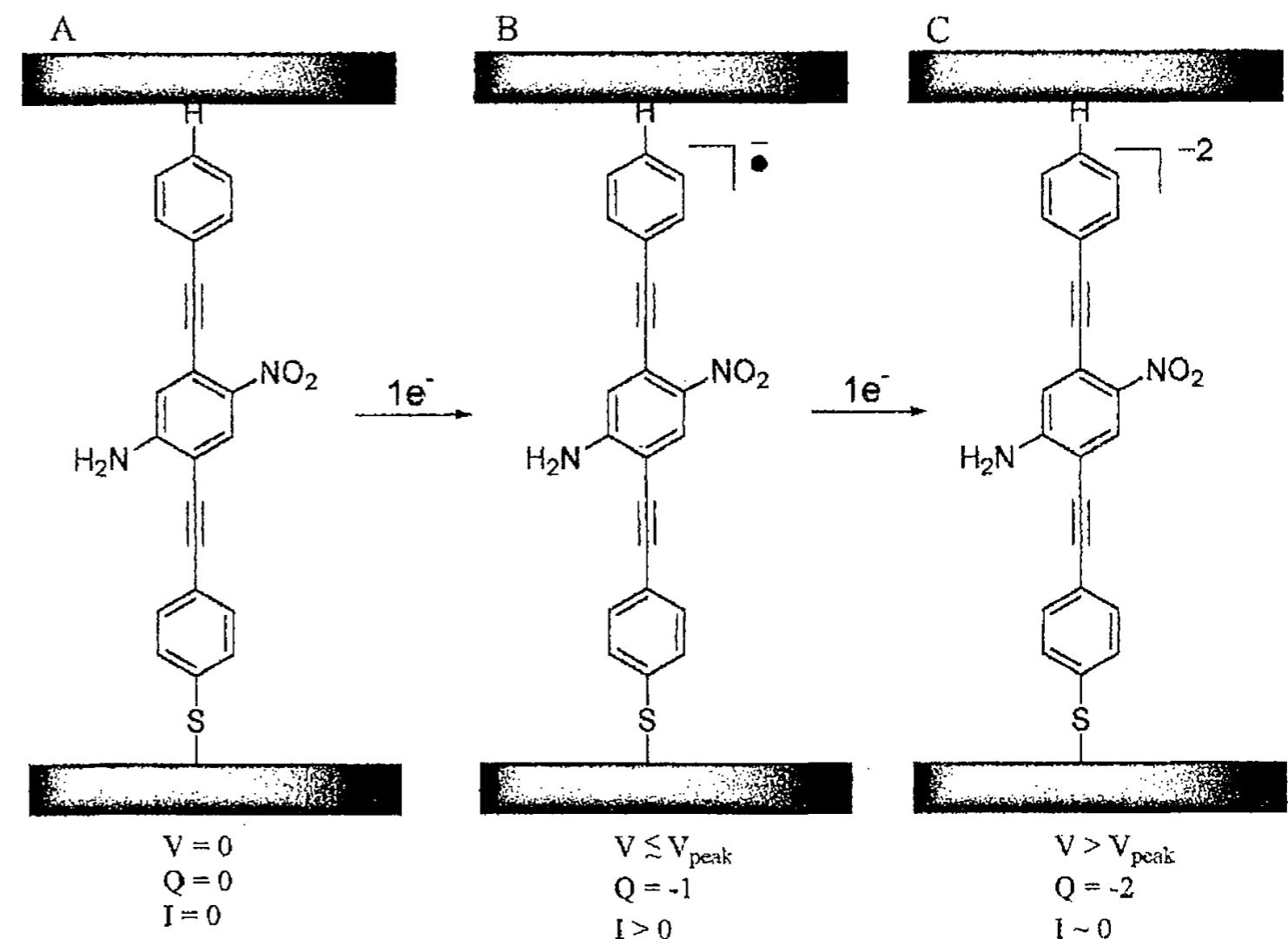
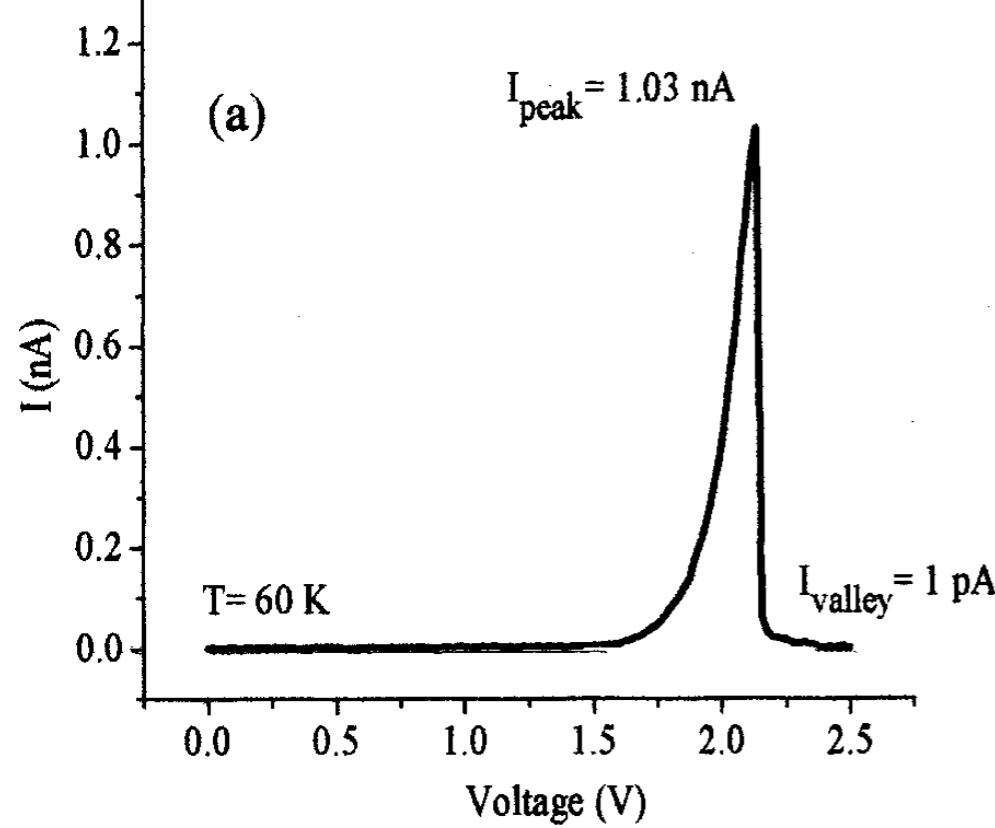


Image: Wikipedia

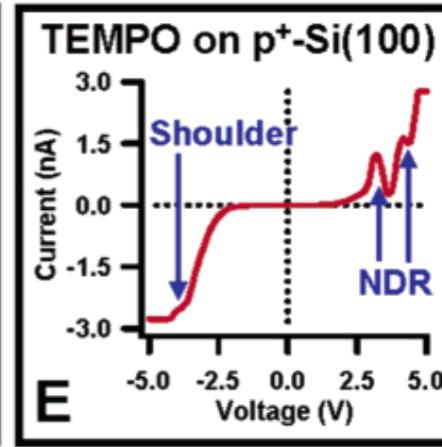
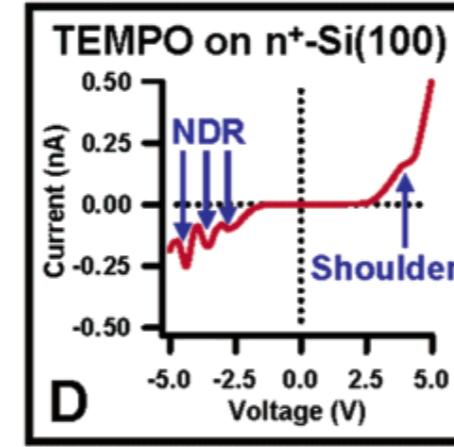
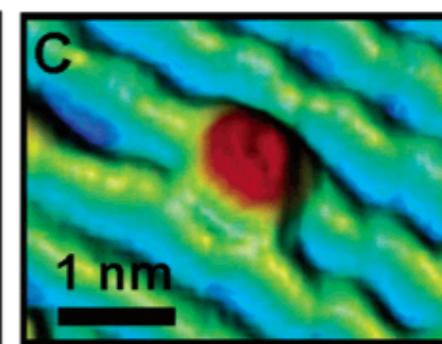
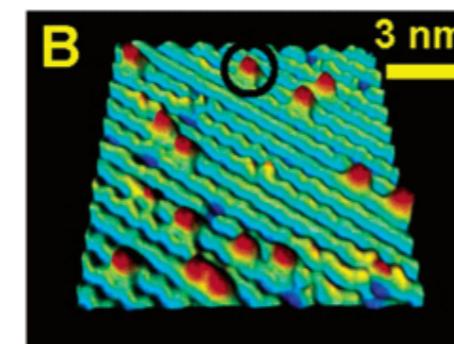
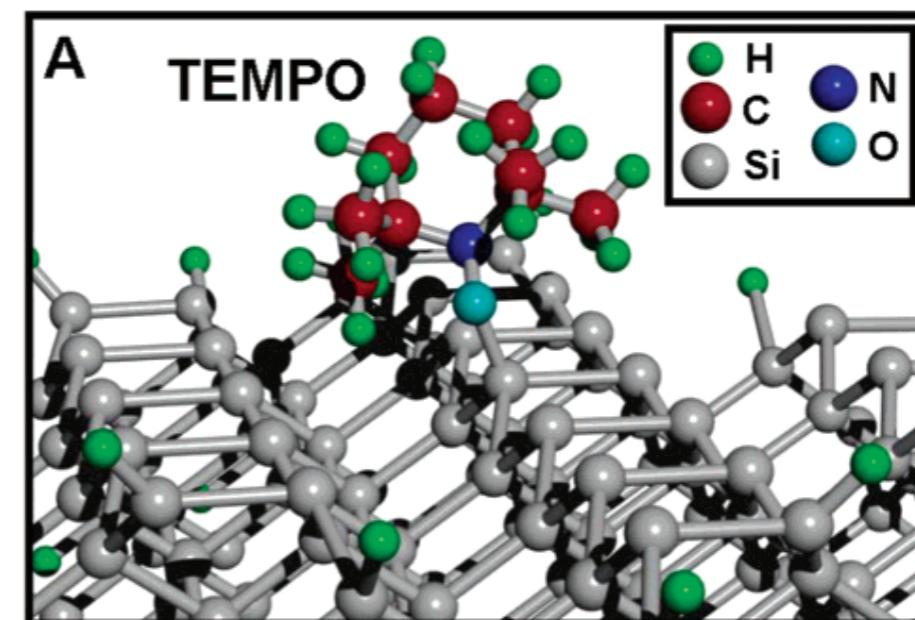
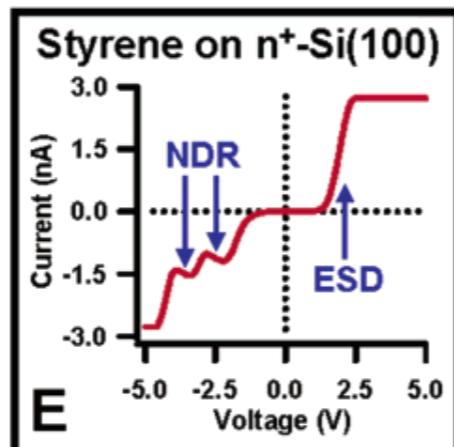
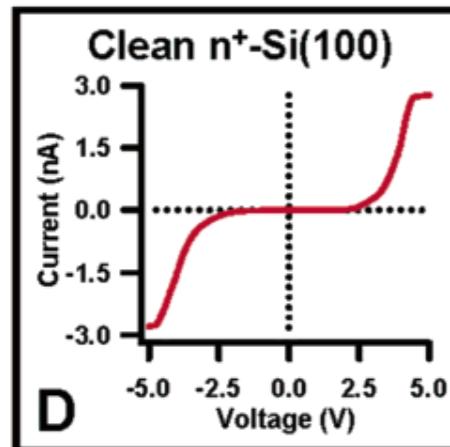
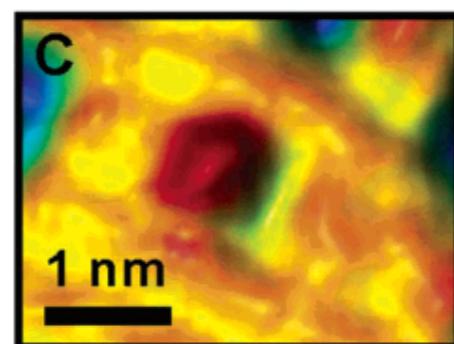
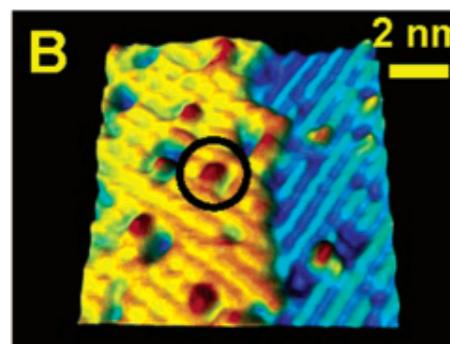
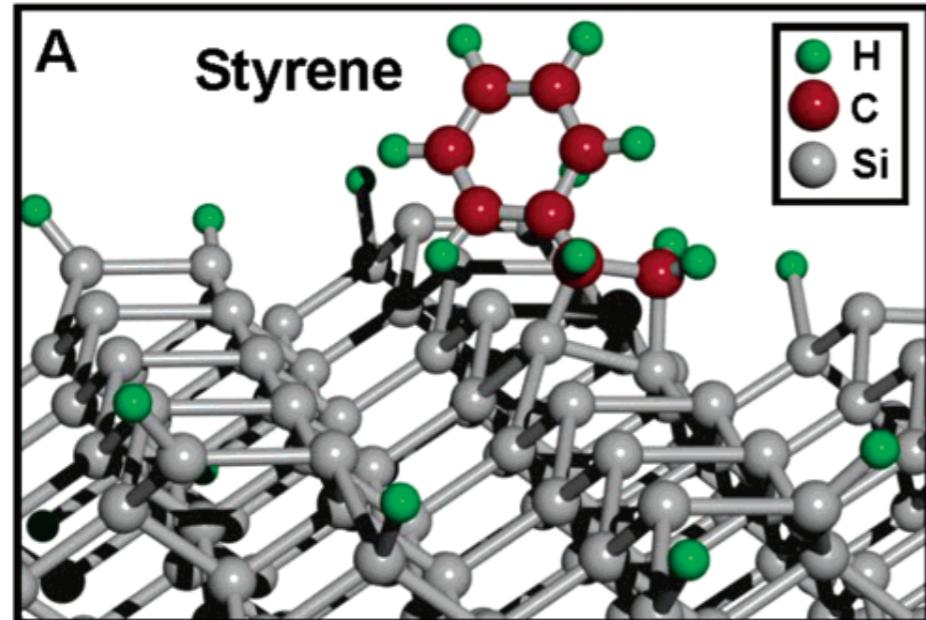
NDR Example



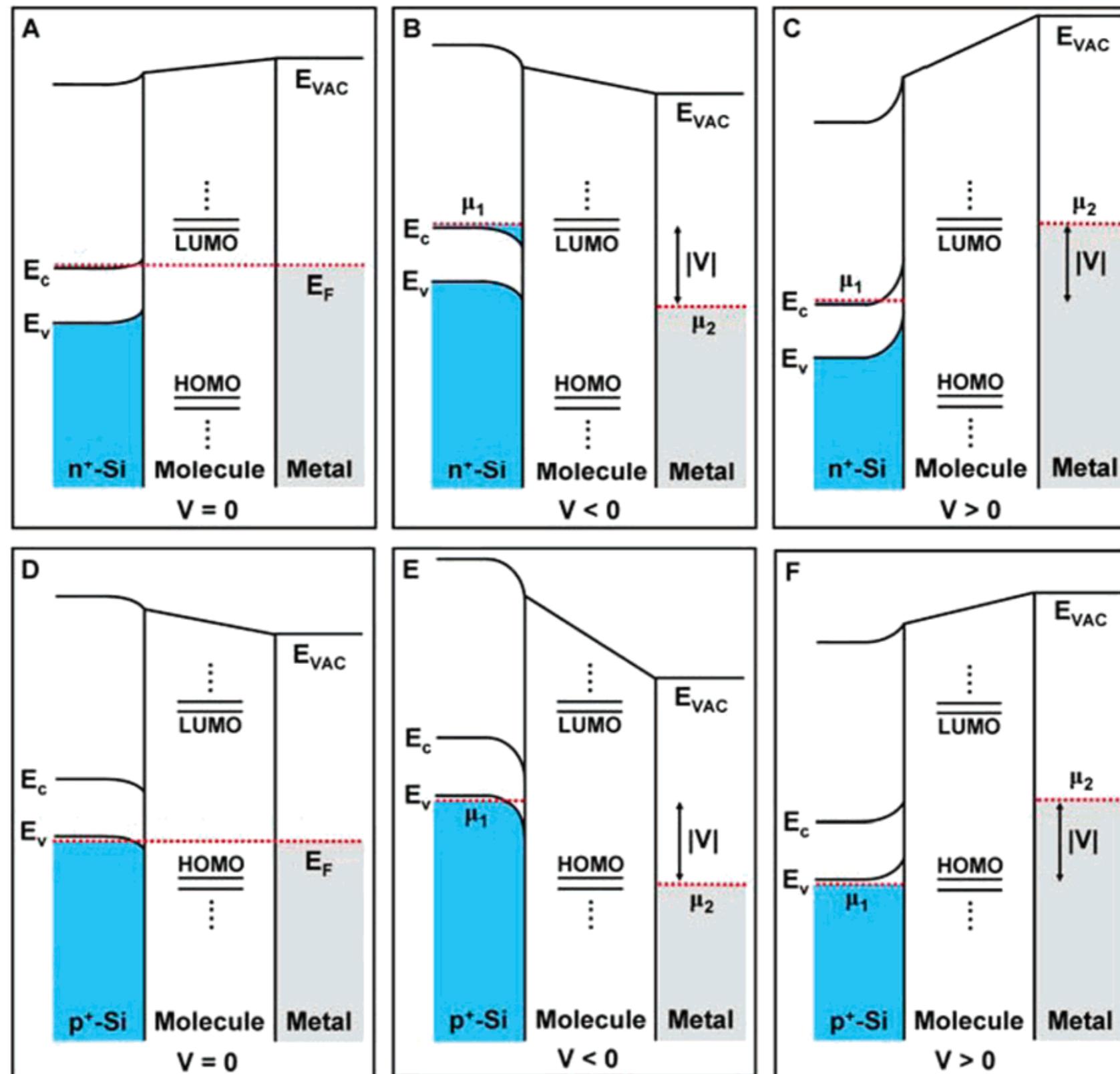
Science (1999) v286 p. 1550-1552

$$2V / 2\text{nm} \approx 1 \times 10^9 \text{ V/m}$$

More Negative Differential Resistance



Hersam / Dutta NDR Mechanism



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Electron-Vibrational Effects

- Many possible interactions...
- Reorganization energies imply electron-phonon coupling
- Inelastic Electron Tunneling Spectra (IETS)

Inelastic Electron Tunneling Spectra

- Even within coherent regime, possible for inelastic scattering
- Energy goes into normal mode
- Provides clear “molecular” signature

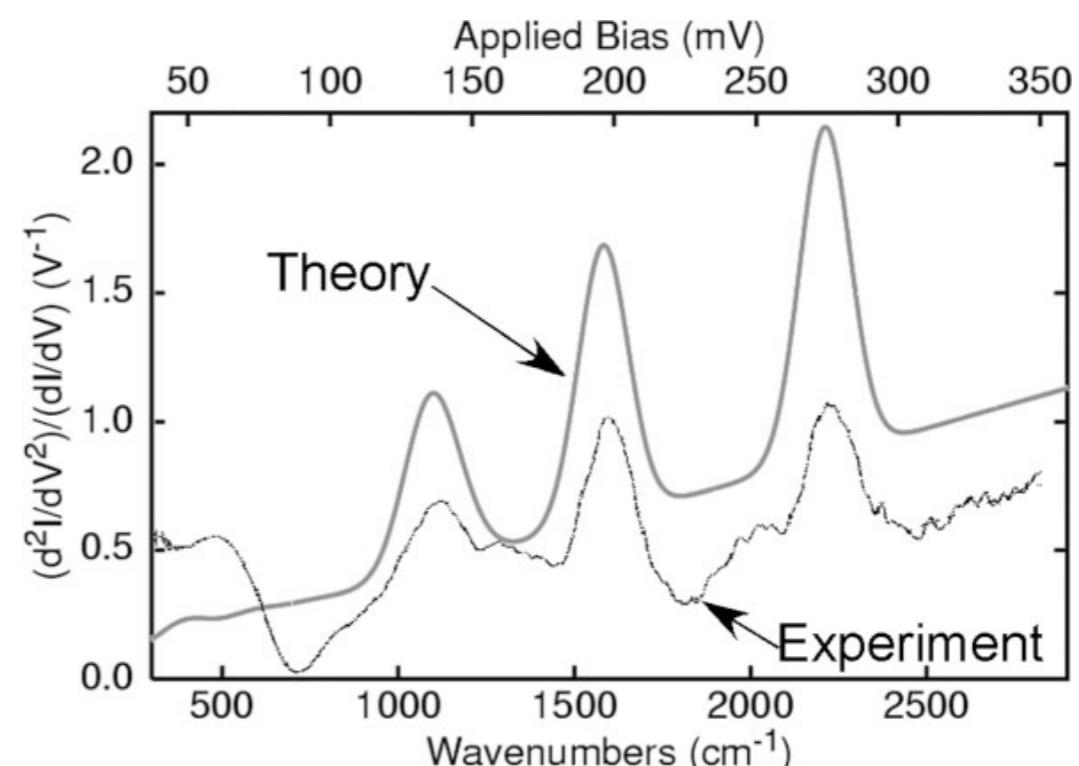
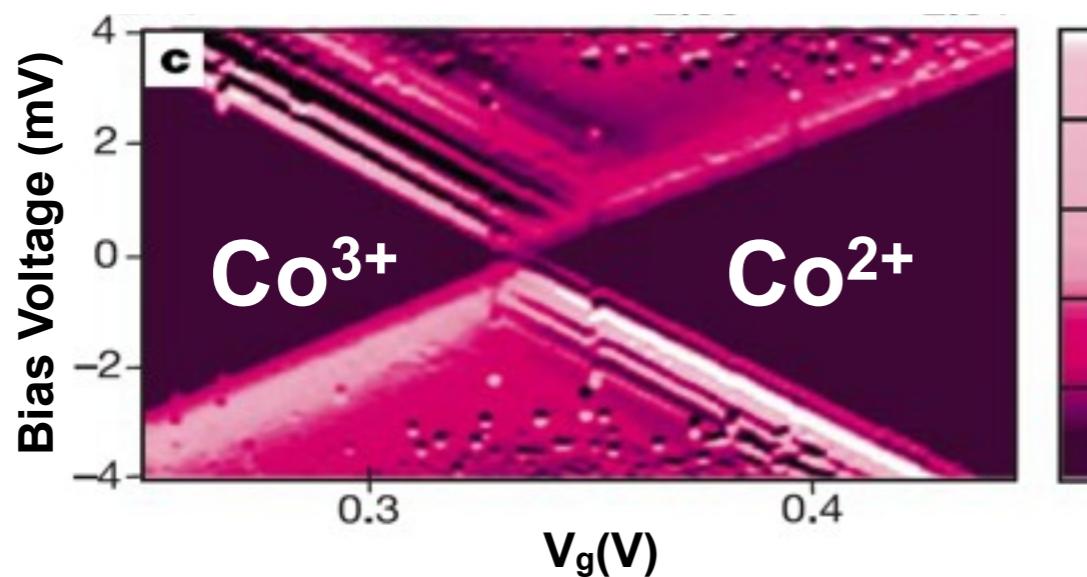
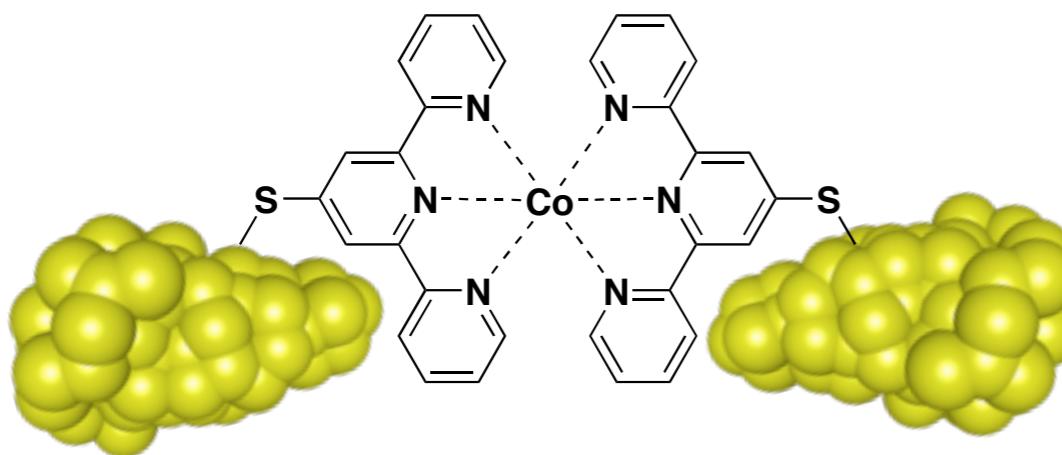


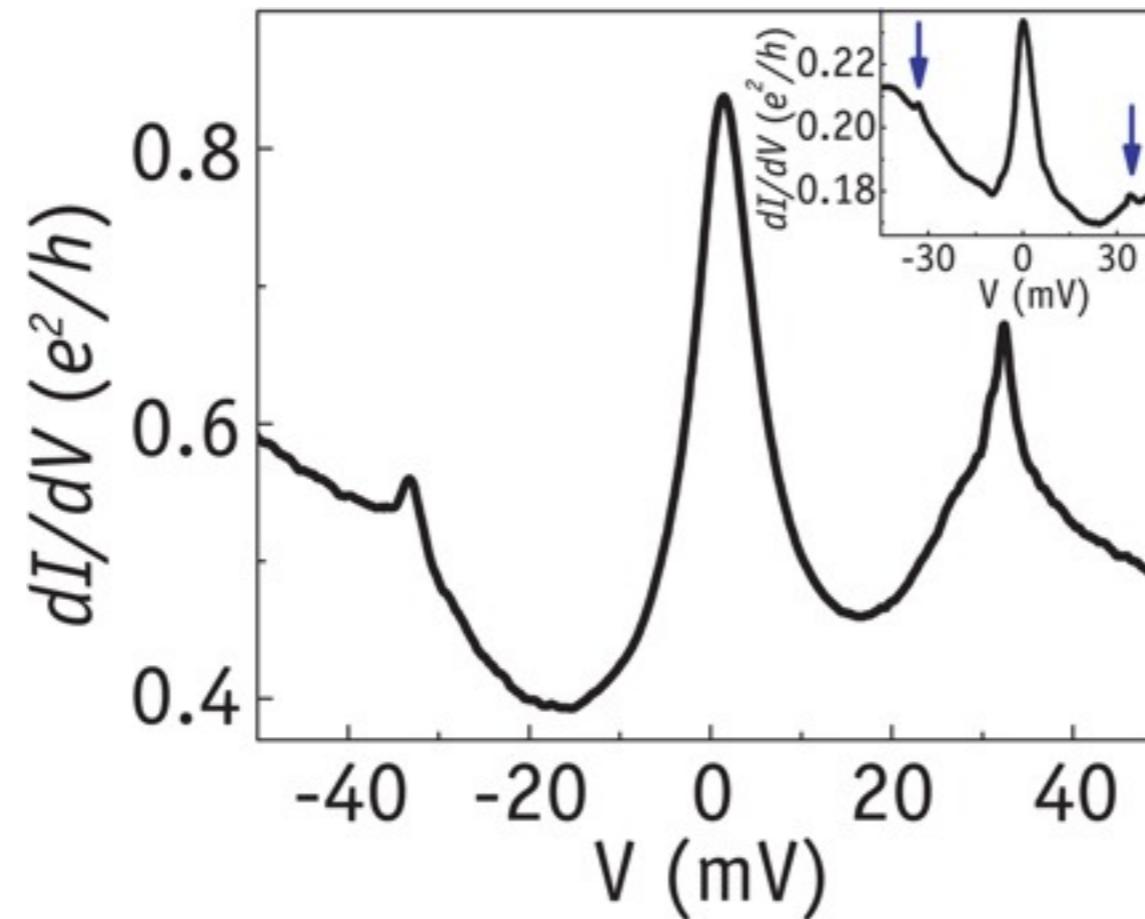
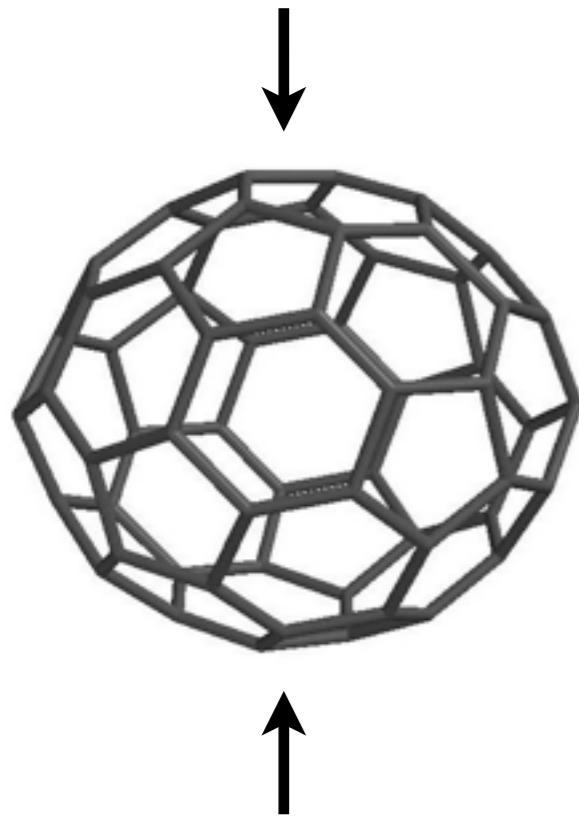
Figure 3. Experimental^[45] and calculated^[46] IETS spectra for the trimer of phenylene ethynylene between gold electrodes.

Electron-Vibrational Effects in Coulomb Blockade

- Single-Molecule Transistor
- $\text{Co}^{2+}/\text{Co}^{3+}$ Complexes



Inelastic Kondo Effect Observed: Electronic-Vibronic Coupling



- Position of features in 5 devices:
 - $\pm 29.6 \text{ mV}$
 - $\pm 32.8 \text{ mV}$
 - $\pm 33.5 \text{ mV}$
 - $\pm 36.9 \text{ mV}$
 - $\pm 37.2 \text{ mV}$

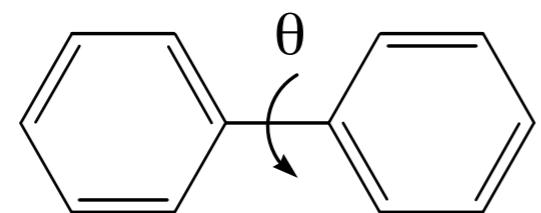
- We have observed additional finite-bias peaks near $\pm 33\text{mV}$, corresponding to the $H_g(I)$ vibrational mode of C_{60} .
- Electron-vibron coupling in the Kondo regime is predicted to lead to an inelastic Kondo effect.

Theory: J. Paaske and K. Flensberg, PRL (2005)

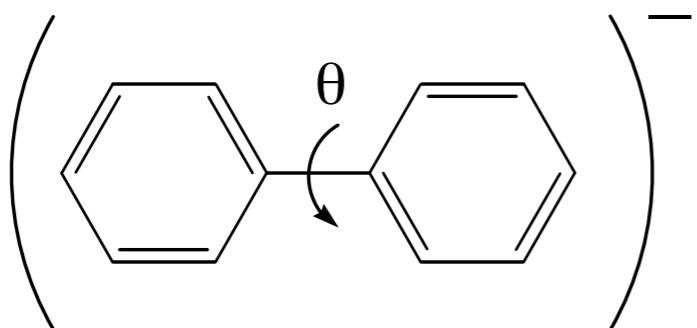
Finite-bias features: J. Park et al., Nature (2002), L.Yu et al., PRL (2004)

Gated Behavior: Twists & Turns

Anion Geometry \neq Cation Geometry \neq Neutral Geometry



$$\theta \approx 22^\circ$$



$$\theta \approx 0^\circ$$