Single Molecule Transistors

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Motivation

Single molecule transistors

Carbon Nanotube Single Molecule Transistors
Two-terminal configurations

- Nanopore structures
- Crossed wires
- Mechanical Break Junctions
- Scanning Tunneling Microscope
- Conducting Probe

Atomic Force Microscope

- High Bias Voltage
  - significant mechanical deformation
  - careful study of these systems is difficult
Three-terminal configurations

- Metallic Source and Drain Electrodes
- Bridged by Single Molecule
- Gate Couples Electromagnetically
- Tunnel Junctions to the Source and Drain Electrodes
- Gate Shifts the Source and Drain Fermi Levels
Fabrication

- Inter-electrode gap \( \sim 1 \text{nm} \)
- Electron-beam lithography
- Electromigration technique
  - Scattering - conduction electrons
  - Momentum transfer to lattice
- Oxidation of metal
- Positioning of a metallic gate electrode
  - small enough
    - gate manipulation
  - large enough
    - no current
Molecules

- C60 molecules
  - Bonds Au
  - Charge transfer
  - Beyond Van der Waals bonding

- Transition Metal Coordination Complexes (TMCCs)
  - two planar, conjugated ligands
  - octahedral crystal field
  - Co, Cu, Zn, individual ligands, and alkane chain

- Vanadium
  - Two atoms
  - Gold electrodes

- Phenyl Dithiol
  - Two different geometric configurations
  - Gold electrodes
- Chemical bonding
- Placement of the molecules - statistical
- No atomic-scale imaging
- Estimate of success rate can be made
Non Resonant Transport
- molecule acts as a potential barrier in the device
- current decreases exponentially with the molecule

Resonant Transport
- nonlinear conduction
- electronic properties similar to single-electron transistors
Electron Addition Energy (Eₐ)

- Single particle level spacing ($\delta E$)
- Promoting an electron
  - HOMO: from the Highest Occupied Molecular Orbital
  - LUMO: to the Lowest Unoccupied Molecular Orbital
- Charging energy (Eₖ)
  - Coulomb interactions
  - Defined as $Eₖ = e^2/C$
Coulomb Blockade

- Thermal Energy $kBT \ll Ea$
- Large source-drain voltage (compared to $E_a$)
  - allows resonant tunneling
- Applying Voltage to the gate electrode
  - Changes the electrostatic potential near molecule
- Cotunneling
- Slow internal relaxation rate
Molecule as a Tunnel Junction
- insulating layer between the two electrodes
- electrons quantum-mechanically tunnel

Tunneling Current
- dependent on the cross-sectional area
- length of the molecule.
- ionization potential of the molecule
- source-drain bias voltage
- length increases - conductance decrease exponentially
Coulomb Blockade Cont.

- Sequential Tunneling Model
- Two tunnel barriers
- Transparency of Tunnel Barriers
- Rate of Electron Relaxation - Fast
- Electron Tunneling Rate - Slow
- Neglects Higher-Order Tunneling
- All Molecule Devices
Simple Energy Level Analysis

Graph 1: Current vs Voltage
- Symmetric
- Asymmetric

Graph 2: Conductance vs Voltage
- Conductance gap
Energy Levels

Probability of...

Molecule losing an electron: $e^{(WF-IP)/kT}$

Molecule gaining an electron: $e^{(EA-WF)/kT}$
Energy Levels Cont.

HOMO: Highest Occupied Molecular Orbital
LUMO: Lowest Unoccupied Molecular Orbital

WF: Metal Work Function
CP: Contact Potential
Non-equilibrium Current Flow

\[ \frac{\Gamma_1}{\hbar} \quad \text{and} \quad \frac{\Gamma_2}{\hbar} \]
Number of Electrons

\[ N_1 = 2f(\varepsilon, \mu_1) \]
\[ N_2 = 2f(\varepsilon, \mu_2) \]

\[ I_L = \frac{e\Gamma_1}{\hbar} (N_1 - N) \]
\[ I_R = \frac{e\Gamma_2}{\hbar} (N - N_2) \]

Steady State \( I_L = I_R \)

\[ \therefore N = 2 \frac{\Gamma_1 f(\varepsilon, \mu_1) + \Gamma_2 f(\varepsilon, \mu_2)}{\Gamma_1 + \Gamma_2} \]

where

\[ I = \frac{2e}{\hbar} \frac{\Gamma_1 \Gamma_2}{\Gamma_1 + \Gamma_2} [f(\varepsilon, \mu_1) - f(\varepsilon, \mu_2)] \]
\[ \mu_1 = E_f - \frac{eV}{2} \]
\[ \mu_2 = E_f - \frac{eV}{2} \]
\[ E_f = -5eV \]
\[ \epsilon_0 = -5.5eV \]
\[ \Gamma_1 = \Gamma_2 = 0.2eV \]
Molecule Charging Effects

Charging Effects 0 eV

Charging Effects 1 eV

https://nanohub.org/mw/invoke/molctoy?appcaption=MolCToy&version=1
Co Tunneling Theory

- Simultaneous Tunneling
  - 2+ Electrons

- Elastic cotunneling
  - Energy unchanged
  - Low Voltages

- Inelastic cotunneling
  - Electron from a Lower Energy State
  - Excited State - Vibration
  - Certain Bias Voltages
Kondo Theory

- Accounts for Electron Spin
- 0, 1 with a magnetic moment, or 2 electrons
- Still needs $E_a$
- Change gate voltage -SMT- magnetic moment
Non-Equilibrium Green Function

\[ G(E) = \left[ E - \varepsilon + i \frac{\Gamma_1 + \Gamma_2}{2} \right]^{-1} \]

\[ D(E) = \frac{A(E)}{2\pi} \]

\[ A(E) = -2\text{Im}\{G(E)\} \]

\[ N = \frac{2}{2\pi} \int_{-\infty}^{\infty} dE \left[ |G(E)|^2 \Gamma_1 f(E, \mu_1) + |G(E)|^2 \Gamma_2 f(E, \mu_2) \right] \]

\[ I = \frac{2e}{\hbar} \int_{-\infty}^{\infty} dE \Gamma_1 \Gamma_2 |G(E)|^2 \left[ f(E, \mu_1) - f(E, \mu_2) \right] \]
Ex: Quantum Point Contact
Ex: Phenyl Dithiol
Conclusion

- Single Molecule Transistors
- Fabrication Problems
- Electron Transport
- International Technology Roadmap for Semiconductors
  - Miniaturization – 1E-12
  - Speed – 1 THz
  - Highest binary throughput
QUESTIONS?

Illustration: Robert Dickson, Tae-Hee Le


