Basics of quantum transport in single-molecule junctions

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The advances in nanofabrication techniques have made possible to study the electronic transport through single atoms and molecules, which has given rise to new field of **Molecular Electronics**.

**Fundamental issues:**
- New physical phenomena
- Potential applications
Molecular electronics: Experimental techniques

1. Scanning tunneling microscope

2. Break-junctions

3. Electrochemical methods

4. Electromigration

Source-Drain electrodes

Au

SiO₂

Si
gate electrode
**Molecular electronics: Functional structures**

1. **Diode:** Au-SAM-Ti-Au (Nanopore) 4-thioacetatebiphenyl, M. Reed, APL (1997)

![Diode image]

2. **Switch:** Nanopore (60 K) M. Reed et al., Science (1999)

![Switch image]


![Transistor image]
Molecular electronics: Goals for the theory

- Understanding of the transport mechanisms at the molecular scale.
- Quantitative description of the transport properties.
Outline of these lectures

**Lecture 1:** “*Coherent transport through single-molecule junctions*”.
- 1.1 Landauer approach: relation conductance-transmission.
- 1.2 Some lessons from the resonant tunneling model.
- 1.3 Green’s functions.
- 1.4 Length dependence of the conductance.
- 1.5 Role of the molecular conjugation.
- 1.6 Quantum interferences: Fano resonances.
- 1.7 Ab initio methods: density functional theory.
- 1.8 Validity of the coherent picture.

**Lecture 2:** “*Single-molecule transistors: Coulomb blockade and Kondo physics*”.
- 2.1 Introduction and experimental motivation.
- 2.2 Coulomb blockade regime: rate equations.
- 2.3 The Kondo effect.
- 2.4 Experimental observation of Coulomb blockade and Kondo effect.

**Lecture 3:** “*Inelastic current: role of the vibration modes*”.
- 3.1 Experimental motivation.
- 3.2 Simple theoretical model: Different transport regimes.
- 3.3 First-principle calculations.
References


Main reference of these lectures:

Lecture 1: “Coherent transport through single-molecule junctions”

Reference

Chapters 13 and 14
Molecular Electronics: An Introduction to Theory and Experiment,
1.1 Landauer approach to electron transport

[Landauer, IBM J. Res. Dev. 1, 223 (1957)]

**real system**

\[ G = \frac{2e^2}{h} T(E_F) \]

- **Landauer formula**
- **incoming** \( N_L \)
- **outgoing** \( N_R \)

**electron reservoirs**

**scattering region**

\( E_F + eV \)

\( E_F \)

\( S \)

- **G** = conductance;
- **\( T(E_F) \)** = transmission at the Fermi energy.
1.1 Understanding the Landauer formula

Electronic transport as scattering problem

Current density:

\[ J = \frac{e\hbar}{2mi} \{ \psi^* \nabla \psi - \psi \nabla \psi^* \} = ev_k T(k) \]

In a solid state device:

\[ I = \frac{2e}{h} \int_{-\infty}^{\infty} dE \ T(E) \left[ f_L - f_R \right] \]

Linear response: \( I = GV; \ G = \text{Conductance} \). At low temperatures:

\[ G = G_0 T(E_F) \]

\[ G_0 = \text{Conductance quantum} \]

\[ G_0 = \frac{2e^2}{h} \approx (12.9 \ \text{k}\Omega)^{-1} \]

\( T = \text{Transmission coefficient} \)
1.1 Landauer formula and simple tunneling models

**Simmons’ model**: a frequently used model in molecular electronics.

Example: barrier height = 4 eV and barrier width = 1 nm.

High bias: Fowler-Nordheim regime
1.2 Some lessons from the resonant tunneling model

Often the transport through a molecular junction is dominated by a single molecular orbital. Those situations can be described with the resonant tunneling model.
1.2 Some lessons from the resonant tunneling model

Landauer formula:
\[ I(V) = \frac{2e}{h} \int_{-\infty}^{\infty} dE \ T(E,V) \left[ f(E - eV/2) - f(E + eV/2) \right] \]

Breit-Wigner formula:
\[ T(E,V) = \frac{4\Gamma_L \Gamma_R}{\left[ E - \epsilon_0(V) \right]^2 + \left[ \Gamma_L + \Gamma_R \right]^2} \]

- \( \epsilon_0 = \) level position
- \( \Gamma_L + \Gamma_R = \) level width
1.2 Shape of the I-V curves

\[ \varepsilon_0 = 1 \text{eV}; \quad k_B T = 0.025 \text{ eV (room temperature)} \]

\[ \Gamma_L = \Gamma_R = 0.1 \text{eV} \]
\[ \Gamma_L = \Gamma_R = 0.05 \text{eV} \]
\[ \Gamma_L = \Gamma_R = 0.02 \text{eV} \]

(a) \[ \varepsilon_0 \]
(b) \[ \varepsilon_0 \]
(c) \[ \varepsilon_0 \]
1.2 Molecular contacts as tunnel junctions

Low bias region: \( |eV| \ll |\epsilon_0| \)

Low-bias expansion: \( I(V) \approx AV + BV^3 \Rightarrow G(V) \approx A + 3BV^2 \)
1.2 Single molecules as tunnel junctions

Cui et al. (Lindsay’s group), Science 294, 571 (2001)

A trans-Platinum(II) Complex as a Single-Molecule Insulator**

Marcel Mayor,* Carsten von Hänisch, Heiko B. Weber,* Joachim Reichert, and Detlef Beckmann
1.2 Temperature dependence of the current

Wang, Lee and Reed, PRB 68, 035416 (2003)

Voltage dependence: Again a tunnel junction!

Current independent of the temperature

FIG. 5. Measured CI2 /V data (circle symbol) is compared with calculation (solid curve) using the optimum fitting parameters of $\Phi_0 = 1.42$ eV and $\alpha = 0.65$. The calculated $I$ (V) from a simple rectangular model ($\alpha = 1$) with $\Phi_e = 0.85$ eV is also shown as the dashed curve.

$CH_3(CH_2)_{n-1}SH$
1.2 Temperature dependence of the current

$\varepsilon_0 = 1\,\text{eV}; \quad \Gamma_L = \Gamma_R = 2\,\text{meV}$

- **Off-resonant transport** $\Rightarrow T$ independent
- **On-resonant transport** $\Rightarrow T$ dependent (as long as $T > \Gamma$)
1.2 Temperature dependence of the current

Within the resonant tunneling model, the temperature dependence of the linear conductance is given by:

\[
G(T) = \left(\frac{2e^2}{h}\right) \frac{1}{4k_BT} \int_{-\infty}^{\infty} dE \left[\frac{4\Gamma_L\Gamma_R}{(E-\epsilon_0)^2 + (\Gamma_L + \Gamma_R)^2}\right] \frac{1}{\cosh^2(\beta E/2)}; \quad \beta = 1/k_BT
\]

- **Off-resonant tunneling:** \(|\epsilon_0| >> \Gamma, k_BT\)
  \[
  G(T) = \left(\frac{2e^2}{h}\right) \frac{4\Gamma_L\Gamma_R}{\epsilon_0^2}
  \]
  (temperature-independent)

- **Weak coupling regime:** \((\Gamma << k_BT)\)
  \[
  G(T) = \left(\frac{2e^2}{h}\right) \frac{\pi\Gamma_L\Gamma_R}{\Gamma_L + \Gamma_R} \frac{1}{k_BT \cosh^2(\beta \epsilon_0/2)}
  \]

In this limit, the conductance decreases as the temperature increases.
1.2 Symmetry of the I-V curves

“Molecular rectifiers”
Arieh Aviram and Mark A. Ratner

“The construction of a very simple electronic device, a rectifier, based on the used of a single organic molecule is discussed. The molecular rectifier consists of a donor pi system and an acceptor pi system, separated by a sigma-bonded (methylene) tunneling bridge. The response of such a molecule to an applied field is calculated, and rectifier properties indeed appear.”

(...) 23 years later

R. Metzger et al., JACS 1997
1.2 Symmetry of the I-V curves

Single-level model: asymmetric coupling

\[ \varepsilon_0(V) = \varepsilon_0 + \frac{\left( \Gamma_L - \Gamma_R \right) eV}{2} \]

\[ \begin{aligned} \varepsilon_0 &= 1 \text{ eV} \\ \Gamma_R &= 20 \text{ meV} \end{aligned} \]
1.2 The resonant tunneling model at work

1.3 Calculation of the transmission: Green’s functions

\[ G_{i\alpha,j\beta}(t,0) = -i \langle c_{i\alpha}(t) c_{j\beta}^+(0) \rangle \]

**Green’s function**

**Equation of motion?**

\[ \frac{d c_{i\alpha}(t)}{d t} = \frac{i}{\hbar} \left[ c_{i\alpha}(t), \hat{H} \right] \]

\[ \hat{G}^{r,a}(E) = \left[ E \pm i\eta - \hat{H} \right]^{-1} \]

(\( \eta = 0^+ \))

\[ \hat{H} = \hat{H}_L + \hat{H}_R + \hat{H}_C + \left( \hat{V}_{LC} + \hat{V}_{RC} + h.c. \right) \]

Three subsystems: left (L), right (R) and center (C)
1.3 Calculation of the transmission: Green's functions

\[
\hat{H} = \begin{pmatrix}
\hat{H}_L & \hat{V}_{LC} & 0 \\
\hat{V}_{CL} & \hat{H}_C & \hat{V}_{CR} \\
0 & \hat{V}_{RC} & \hat{H}_R
\end{pmatrix}
\]

\[\hat{G}_{CC}^{r,a}(E) = \left[ E \pm i\eta - \hat{H}_C - \hat{\Sigma}_{L}^{r,a} - \hat{\Sigma}_{R}^{r,a} \right]^{-1} \]

where \( \hat{\Sigma}_{\mu}^{r,a}(E) = \hat{V}_{\mu}[E \pm i\eta - \hat{H}_\mu]^{-1} \hat{V}_{\mu} \) \( (\mu = L, R) \) are the self-energies

\( \hat{\Gamma}_\mu = \text{Im}(\hat{\Sigma}_\mu) \quad \text{---> scattering rates} \)

\[
T(E) = 4 \text{Tr}\left[\hat{\Gamma}_L(E)\hat{G}_{CC}^{r}(E)\hat{\Gamma}_R(E)\hat{G}_{CC}^{a}(E)\right]
\]

\[
\hat{t} = 2\hat{\Gamma}_L^{1/2} \hat{G}_{CC}^{r} \hat{\Gamma}_R^{1/2}
\]

**Box:**

\[
T(E) = \text{Tr}\left[\hat{tt}^+\right]
\]
1.3 Example: resonant tunneling model

- Derivation of the Breit-Wigner formula for the transmission through a single electronic level from the general expression of the transmission.

\[ H_C = \varepsilon_0 \]

- Self-energies:
  \[ \Sigma_{L,R}^a = i \Gamma_{L,R} = (\Sigma_{L,R}^r)^* \]

- Scattering rates:
  \[ \Gamma_{L,R} = \text{Im}(\Sigma_{L,R}^a) \]

- Green's functions:
  \[ \hat{G}_{cc}^{r,a}(E) = \left[ (E \pm i\eta)\hat{1} - \hat{H}_C - \hat{\Sigma}_{L,R}^r - \hat{\Sigma}_{L,R}^a \right]^{-1} \]

Transmission (Breit-Wigner formula)

\[ T(E) = 4 \text{Tr} \left[ \hat{\Gamma}_L(E) \hat{G}_{cc}^{r}(E) \hat{\Gamma}_R(E) \hat{G}_{cc}^{a}(E) \right] = \frac{4 \Gamma_L \Gamma_R}{(E - \varepsilon_0)^2 + (\Gamma_L + \Gamma_R)^2} \]
1.3 Two-level model: Conductance of a hydrogen molecule


- The hydrogen molecule forms a stable bridge between Pt electrodes.

- The conductance is $G \sim G_0$ and it is largely dominated by a single conduction channel.
### 1.3 Two-level model

- Derivation of the expression of the transmission through a hydrogen molecule.

\[ \begin{align*}
\text{Hamiltonian:} & \quad \hat{H}_C = \begin{pmatrix} \varepsilon_0 & t_H \\ t_H & \varepsilon_0 \end{pmatrix} \\
\text{Self-energies:} & \quad \hat{\Sigma}_L^a = \begin{pmatrix} i\Gamma_L & 0 \\ 0 & 0 \end{pmatrix}; \quad \hat{\Sigma}_R^a = \begin{pmatrix} 0 & 0 \\ 0 & i\Gamma_R \end{pmatrix} \\
\text{Scattering rates:} & \quad \hat{\Gamma}_{L,R} = \text{Im}(\hat{\Sigma}_{L,R}^a) \\
\text{Green's functions:} & \quad \hat{G}_{CC}^{r,a}(E) = \left[ (E \pm i\eta)\hat{1} - \hat{H}_C - \hat{\Sigma}_L^a - \hat{\Sigma}_R^a \right]^{-1}
\end{align*} \]

**Transmission**

\[
T(E) = 4\text{Tr}\left[ \hat{\Gamma}_L(E)\hat{G}_{CC}^r(E)\hat{\Gamma}_R(E)\hat{G}_{CC}^a(E) \right] = \frac{4\Gamma^2 t_H^2}{[(E - \varepsilon_+)^2 + \Gamma^2][(E - \varepsilon_-)^2 + \Gamma^2]}
\]

where \( \varepsilon_\pm = \varepsilon_0 \pm t_H \) (bonding and anti-bonding states).
1.3 Two-level model

Bonding and antibonding states:

\[ \varepsilon_{\pm} = \varepsilon_0 \pm t_H \]

Transmission:

\[ T(E) = \frac{4\Gamma^2 t_H^2}{[(E - \varepsilon_+)^2 + \Gamma^2][ (E - \varepsilon_-)^2 + \Gamma^2]} \]
1.4 Length dependence of conductance

Wang, Lee and Reed, 

The conductance often decays exponentially with the length of the molecule

\[ G = G_0 e^{-\beta d} \]

Typical values of \( \beta \) range from 2-4 nm\(^{-1}\) for conjugated molecules to 8-12 nm\(^{-1}\) for aromatic compounds.
1.4 Length dependence of conductance

\[ I(V) = \frac{2e}{h} \int_{-\infty}^{\infty} dET(E,V) [f_L - f_R] \]

\[ G = \frac{2e^2}{h} T(E_F) \]

\[ T(E) = 4 \Gamma_L \Gamma_R |G_{1N}(E)|^2 \]

Off-resonant tunneling: \( \max(t_{i,i+1}) \ll \min(|E - \epsilon_i|) \Rightarrow G_{1N} \approx \frac{1}{E - \epsilon_N} \prod_{i=1}^{N-1} \frac{t_{i,i+1}}{E - \epsilon_i} \)

Homogeneous bridge: \( t_{i,i+1} = t \) and \( \epsilon_i = \epsilon \)

\[ \Rightarrow T(E) \approx \frac{4 \Gamma_L \Gamma_R}{|t|^2} \left| \frac{t}{E - \epsilon} \right|^{2N} \propto e^{-\beta(E)L} \]

\[ \beta(E) = \frac{2}{\alpha} \ln \left| \frac{E - \epsilon}{t} \right| \]

\( \alpha = \) lattice constant; \( Na = L \)
1.5 Role of the conjugation in $\pi$-electron systems

Hückel model for a benzene molecule:

Eigenenergies and eigenfunctions:

\[
\begin{align*}
E_1 &= \varepsilon_0 - 2|t|; & E_2 &= E_3 = \varepsilon_0 - |t|; \\
E_4 &= E_5 = \varepsilon_0 + |t|; & E_6 &= \varepsilon_0 + 2|t| \\
\end{align*}
\]

\[
\begin{align*}
|\phi_1\rangle &= \frac{1}{\sqrt{6}} (|1\rangle + |2\rangle + |3\rangle + |4\rangle + |5\rangle + |6\rangle); & |\phi_2\rangle &= \frac{1}{\sqrt{12}} (2|1\rangle + |2\rangle - |3\rangle - 2|4\rangle - |5\rangle + |6\rangle); \\
|\phi_3\rangle &= \frac{1}{2} (|2\rangle + |3\rangle - |5\rangle - |6\rangle); & |\phi_4\rangle &= \frac{1}{\sqrt{12}} (2|1\rangle - |2\rangle - |3\rangle + 2|4\rangle - |5\rangle - |6\rangle); \\
|\phi_5\rangle &= \frac{1}{2} (|2\rangle - |3\rangle + |5\rangle - |6\rangle); & |\phi_6\rangle &= \frac{1}{\sqrt{6}} (|1\rangle - |2\rangle + |3\rangle - |4\rangle + |5\rangle - |6\rangle)
\end{align*}
\]
1.5 Role of the conjugation in π-electron systems

Computation of the transmission through a benzene junction using a Hückel model to describe the π-electrons in this molecule.

Model for the metal-benzene-metal junction:

- Hamiltonian:
  \[
  \hat{H}_C = \begin{pmatrix}
  \varepsilon_0 & -t & 0 & 0 & 0 & -t \\
  -t & \varepsilon_0 & -t & 0 & 0 & 0 \\
  0 & -t & \varepsilon_0 & -t & 0 & 0 \\
  0 & 0 & -t & \varepsilon_0 & -t & 0 \\
  0 & 0 & 0 & -t & \varepsilon_0 & -t \\
  -t & 0 & 0 & 0 & -t & \varepsilon_0 \\
  \end{pmatrix}
  \]

- Self-energies:
  \[
  (\Sigma^a_L)_{ij} = \begin{cases} 
  i\Gamma_L & \text{if } i = j = 1 \\
  0 & \text{otherwise} 
  \end{cases}
  \]
  \[
  (\Sigma^a_R)_{ij} = \begin{cases} 
  i\Gamma_R & \text{if } i = j = 4 \\
  0 & \text{otherwise} 
  \end{cases}
  \]
1.5 Role of the conjugation in \( \pi \)-electron systems

- Scattering rates: \( \hat{\Gamma}_{L,R} = \text{Im}(\Sigma^a_{L,R}) \)

- Green’s functions: \( \hat{G}_{CC}^{r,a}(E) = \left[(E \pm i\eta)\hat{1} - \hat{H}_C - \hat{\Sigma}_{L}^{r,a} - \hat{\Sigma}_{R}^{r,a}\right]^{-1} \)

- Transmission: \( T(E) = 4 \text{Tr}\left[\hat{\Gamma}_L(E)\hat{G}_{CC}^{r}(E)\hat{\Gamma}_R(E)\hat{G}_{CC}^{a}(E)\right] = 4\Gamma_L\Gamma_R\left|\hat{G}_{1,4}^{a}(E)\right|^2 \)

**Examples:**

![Graph showing transmission as a function of \((E-\varepsilon_0)/\Gamma\) for different \(\Gamma\) values. Symmetric junction: \(\Gamma_L = \Gamma_R = \Gamma\).]
1.5 Role of the conjugation in π-electron systems

LETTERS

Dependence of single-molecule junction conductance on molecular conformation

Latha Venkataraman1,4, Jennifer E. Klare2,4, Colin Nuckolls2,4, Mark S. Hybertsen1,4 & Michael L. Steigerwald2

Influence of the conjugation (two-ring molecules)
1.5 Role of conjugation in $\pi$-electron systems: origin of $\cos^2 \theta$

Off-resonant tunneling: $\max(t_{i,i+1}) << \min(|E - \epsilon_i|)$ \implies $G_{1N} \approx \frac{1}{E - \epsilon_N} \prod_{i=1}^{N-1} \frac{t_{i,i+1}}{E - \epsilon_i}$

In a conjugated molecule, the coupling between different segments is mediated by a $\pi - \pi$ hopping element:

$t_{\pi-\pi} = t_0 \cos \theta \implies T \propto \cos^2 \theta$
1.6 Quantum Interferences: Fano Resonances

Anti-resonance (vanishing transmission):

\[ E = \varepsilon_0 \]

Transmission maxima:

\[ E = \varepsilon = \frac{1}{2} \left( \varepsilon + \varepsilon_0 \right) \pm \sqrt{\left( \varepsilon - \varepsilon_0 \right)^2 + 4t^2} \]

\[ \varepsilon_0 = 2 \text{ eV}; \varepsilon = 0.0 \text{ eV}; \Gamma_L = \Gamma_R = 0.1 \text{ eV} \]
1.7 Ab initio methods: Density functional theory

- **Hohenberg–Kohn Theorems:**
  - The energy of the ground state can be determined from the electron density $\rho$.

- **Kohn–Sham Approach:**
  - Functional: $E[\rho] = T_S[\rho] + J[\rho] + E_{\text{ext}}[\rho] + E_{\text{XC}}[\rho]$
    - Electron density $\rho$.
    - $T_S[\rho]$ exact kinetic energy of a non-interacting system with the same density as the interacting one.
    - $J[\rho]$ classical Coulomb part.
    - $E_{\text{ext}}[\rho]$ external part (nuclei, ...).
    - $E_{\text{XC}}[\rho]$ exchange correlation part.
      - BP86: exchange part Becke 1988 and correlation part Perdew 1986
### 1.7 Density functional theory

- Variational approach leads to **Kohn–Sham Equations**:

  - \( F_{KS}^{ij} = \varepsilon_{ij} \) (integro-differential equations)

  \[
  F_{KS} = -\frac{1}{2} \nabla^2 + \int \frac{\rho(\vec{r}_2)}{r_{12}} d\vec{r}_2 + V_{XC}(\vec{r}_1) - \sum_A \frac{Z_A}{r_{1A}}
  \]

- Linear combination of local orbitals:
  - \( j_i = \sum_n c_{ni} \phi_n \)

- Linear set of equations: \( F_{KS} C = \varepsilon SC \)

  - Kohn – Sham matrix: \((F_{KS})_{ij} = \int \phi_i(\vec{r}) f_{KS}(\vec{r}) \phi_j(\vec{r}) d\vec{r}\)
  - Coefficient matrix: \((C)_{ij} = c_{ij}\)
  - Overlap matrix: \((S)_{ij} = \int \phi_i(\vec{r}) \phi_j(\vec{r}) d\vec{r}\)
  - Diagonal matrix of the orbital energies \( \varepsilon \).
1.7 DFT in molecular electronics

**Challenge:**

- Ab initio description of the electronic structure of an infinite (non-periodic) system.

- Corresponding description of the electronic transport.

**Density functional theory + Green’s function techniques**

*Quantum Chemistry Package TURBOMOLE: R. Ahlrichs, Universität Karlsruhe.*
1.7 Our approach: Cluster-based method


\[ G = \frac{2e^2}{h} T(E_F) = G_0 \text{Tr} \left[ \hat{t}^\dagger \hat{t} \right] (E_F) = G_0 \sum_i \tau_i(E_F) \]

\[ \hat{t}(E) = \hat{\Gamma}_L^{1/2}(E) \hat{G}_{CC}^a(E) \hat{\Gamma}_R^{1/2}(E) \]

- Green’s functions:
  \[ \hat{G}_{CC}^a = (E^a \hat{S}_{CC} - \hat{H}_{CC} - \hat{\Sigma}_L^a - \hat{\Sigma}_R^a)^{-1} \]

- self-energy:
  \[ \hat{\Sigma}_{XX}^a = (\hat{H}_{CX} - E \hat{S}_{CX}) \hat{\Sigma}_{XX}^a (\hat{H}_{XC} - E \hat{S}_{XC}) \]

- scattering rate:
  \[ \hat{\Gamma}_X = 2 \text{Im} \left\{ \hat{\Sigma}_X^a \right\} \]

Quantum Chemistry Package **TURBOMOLE**: R. Ahlrichs, Universität Karlsruhe
1.7 Our approach: Cluster-based method

- Bulk parameters extracted from large metal cluster to describe the lead Green’s functions.

Electrode surface Green’s functions constructed from bulk parameters with an iterative decimation technique.
1.7 An example: $C_{60}$ molecular junctions


Constant-current STM image of Cu(100)-$C_{60}$ at 8 K.
(Sample voltage $V = 1.7$ V, tunneling current $I = 1$ nA).

Conductance vs. tip displacement.
The tip is made of W.
1.7 Electronic structure of $C_{60}$

Electronic structure of an isolated $C_{60}$ molecule (DFT, BP86 functional, def-SVP basis set):

**HOMO**: $-5.90$ eV (5-fold degenerate)  
**LUMO**: $-4.26$ eV (3-fold degenerate)

($\text{HOMO-LUMO gap: } 1.64$ eV)
### 1.7 Conductance of ideal Au-C$_{60}$-Au junctions


**Top geometry:**
- Transport dominated by a single conduction channel.

**Hollow geometry:**
- Transport dominated by two conduction channels.

- $G_{\text{top}} = 0.55 \ G_0$
- $G_{\text{hollow}} = 1.85 \ G_0$

**Channel decomposition**

![Graph showing the transmission spectra for top and hollow geometries](image-url)
1.7 Determining the geometry of Au-C₆₀-Au junctions


Animation of the formation process of a Au-C₆₀-Au junction:
1.7 Transport properties of $\text{Au-C}_6\text{O-Au}$ junctions

- Binding energy of the molecular junction.
- Charge on the C60 molecule.
- Linear conductance.
- Thermopower (room temperature).

The most stable geometry the C$_{60}$ is not inside the gold junction.

Typically, the C$_{60}$ is negatively charged.

Conductance plateau: $0.07-0.2 \ G_0$.

Negative thermopower: LUMO-dominated transport.
\section*{1.8 Final remarks: Validity of the coherent picture}

\[ \Delta E = |\varepsilon_0 - E_F| = \text{injection energy} \]
\[ \Gamma = \Gamma_L + \Gamma_R = \text{level width} \]

\begin{itemize}
  \item **Traversal time:**
  \[ \tau = \frac{\hbar}{\sqrt{\Delta E^2 + \Gamma^2}} \]
  \item **Energy scales:**
  \[ e-e: U; e-ph: \lambda \]
\end{itemize}

\textbf{Coherent transport:}
\[ \tau \ll \min(\hbar/U, \hbar/\lambda) \]

\textbf{Incoherent transport:}
\[ \tau \gg \min(\hbar/U, \hbar/\lambda) \]