Electronic transport through single atoms and molecules

Hilbert v. Löhneysen

Physikalisches Institut, Universität Karlsruhe
and Forschungszentrum Karlsruhe, Institut für Festkörperphysik

Electron transport in atomic-size contacts
Current through single molecules
Au chains on vicinal Si(111) surfaces: first results

Transport channels for conduction electrons

Nanowire: waveguide for electrons when $d \approx \lambda_F$
Conductance: $G = \sum \frac{2e^2}{h} \tau_i$

Semiconductor heterostructures: $\lambda_F \gg$ atomic dimensions
Conductance quantization: $G = 2ne^2/h$ ($\tau_i = 1$)

Metals: discrete atomic structure important because $\lambda_F \approx a$
$G \neq 2ne^2/h$, but $G \approx 2e^2/h$
for lowest conductance plateau

How can one determine $\tau_i$? Superconductivity
Conductance of a one-dimensional system

1. $\mu_1$  
2. $\mu_2$

$\text{density of states for } d = 1$

$$\frac{dn_j}{dE} = \frac{1}{hv_j}$$

Current from reservoir 1 (channel $j$) into an elastically scattering random potential $S$:

$$I_j = ev_j \frac{dn_j}{dE} (\mu_1 - \mu_2)$$

Current from $S$ into reservoir 2 (channel 2):

$$I_i = \frac{e}{h} \sum_{j=1}^{N} |t_{ij}|^2 (\mu_1 - \mu_2)$$

Conductance: current $I = \Sigma I_j$ at voltage $U = (\mu_1 - \mu_2)/e$

$$G = \frac{I}{U} = \frac{Ie}{\mu_1 - \mu_2} = \frac{e^2}{h} \sum_{i=1}^{N} |t_{ij}|^2$$

![Image of conductance setup and measurement](image.png)

- Aluminium-Film
- Polyimide-Oberschicht
- Gegenlager
- Schieber
- Biegsames Substrat

200 nm
Nanostructures as electronic wave guides

Metallic structures:
Cu, Au, Al

Realisation:
\( \lambda_F \approx \text{interatomic distance} \)
scanning tunneling microscope
break junctions

Conductance plateaus in atomic-size contacts of Al

Yanson, Ruitenbeek et al.

Leitwert (2e^2/h)

Häufigkeit

Leitdenstand (nm)

Yanson, Ruitenbeek et al.
One electron transport:

\[ eV \geq \frac{2\Delta}{1} \]

\[ P \propto \tau^1 \]

2 electrons:

\[ eV \geq \frac{2\Delta}{2} \]

\[ P \propto \tau^2 \]

Andreev-reflection

3 electrons:

\[ eV \geq \frac{2\Delta}{3} \]

\[ P \propto \tau^3 \]

multiple Andreev-reflection (MAR):

\[ eV \geq \frac{2\Delta}{n} \]

\[ P \propto \tau^n \]

n electrons:
Transport channels through single atoms

Determination of the number of channels $N$ on each conductance plateau possible

first plateau: $N$ depends on valence orbitals

monovalent metals (Au, Na) $N_{\text{max}} = 1$

polivalent metals (Al, Pb) $N_{\text{max}} = 4$

transition metals (Nb, W) $N_{\text{max}} = 6$

Transmission of each channel depends on local atom arrangement

atomic orbitals

s orbital  p orbitals

s orbital

s orbitals
Formation of a junction

Exponential regime
Plateau

Previous experiments

Reed et al 1997

Transport through symmetric and asymmetric π-chain-molecules
Calculation of the electrical current through a single molecule

Weigend, Köntopp, Evers

Self-consistent DFT calculation for the complete system consisting of molecule and contacts (55 Au atoms each)

\[ I(V) \sim \int \tau(E) f(E) - f(E + eV) \]

Dependence on whether the S atom binds to 1, 2 or 3 atoms

Inhomogeneous broadening by thermally fluctuating couplings

Plan: combination of DFT (HOMO position) and Hartree-Fock (wave functions)

Theoretical description of electronic transport through single molecules

Heurich, Cuevas, Wenzel, Schön, PRL 2002

Strong coupling between electrodes and molecule

Electron/hole remains only a short time on the molecule

Ballistic Transport: Landauer Theory

Density functional theory for the molecule and tight-binding approximation for the electrode

Conduction channels
Transport through a single molecule at low temperatures

Switching of a symmetric molecule between different contact bonding configurations
Transport through a molecule with interrupted π-chain

strongly insulating!
Electronic structure of Si(557):Au

M. Schöck, C. Sürgers

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Institut für Nanotechnologie - Molekulare Elektronik
DFG Center for Functional Nanostructures (CFN)