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: $G = \sum_i \frac{2e^2}{h} \tau_i$

Semiconductor heterostructures: $\lambda_F \gg$ atomic dimensions

Conductance quantization: $G = 2ne^2/h$ ($\tau_i \equiv 1$)

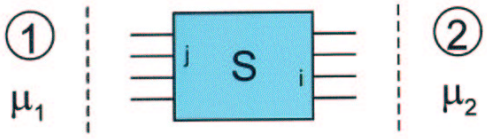
Metals: discrete atomic structure important because $\lambda_F \approx a$

$G \neq 2ne^2/h$, but $G \approx 2e^2/h$

for lowest conductance plateau

How can one determine τ_i ? Superconductivity

Conductance of a one-dimensional system



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:

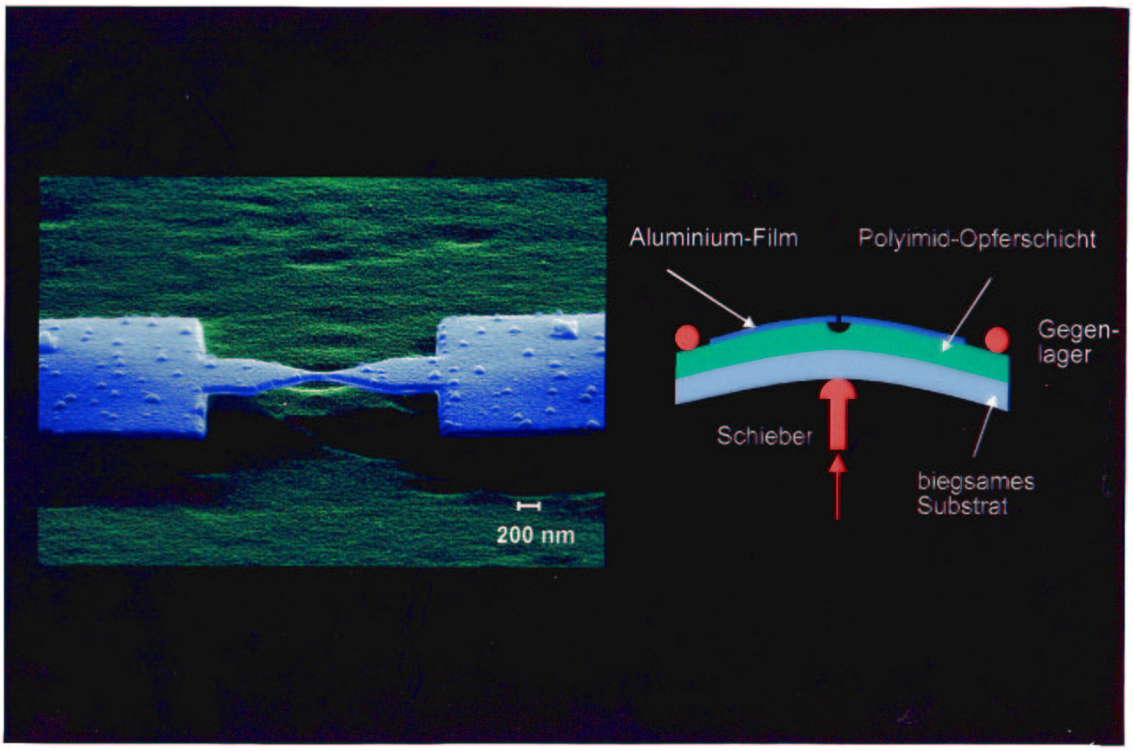
$$I_j = ev_j \frac{dn_j}{dE} (\mu_1-\mu_2)$$

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 $I = \Sigma I$ at voltage $U = (\mu_1-\mu_2)/e$

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

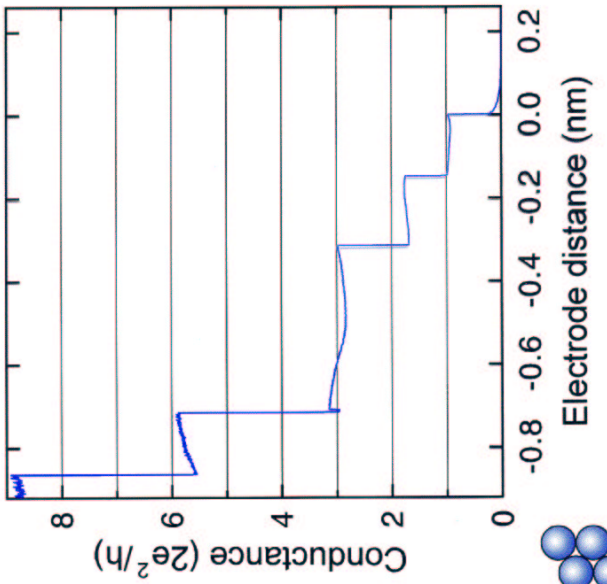


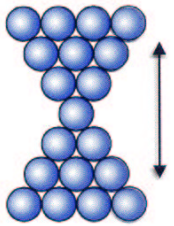
Nanostructures as electronic wave guides

Metallic structures:
Cu, Au, Al

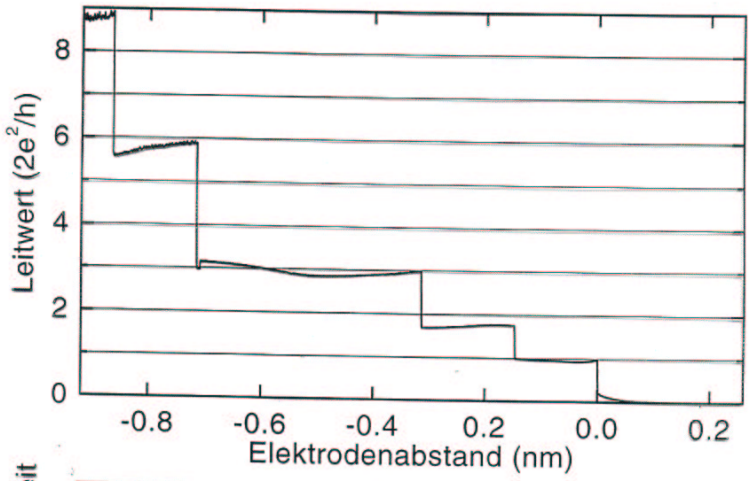
$\lambda_F \approx$ interatomic distance

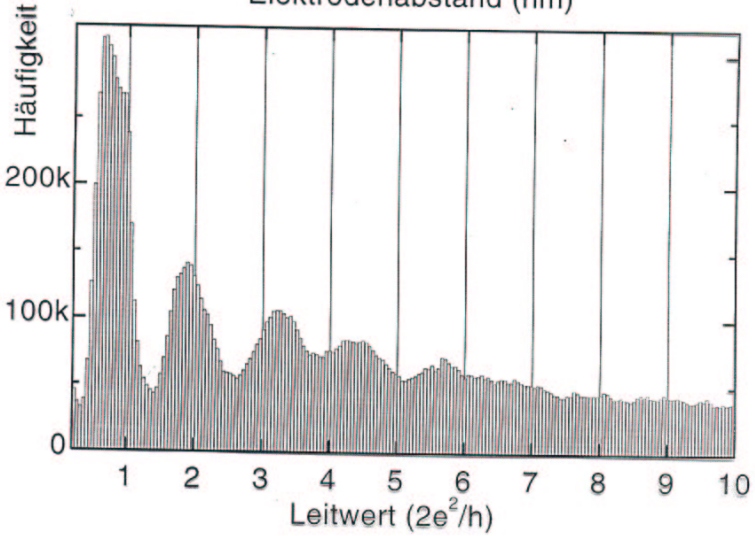
Realisation:
scanning tunneling microscope
break junctions





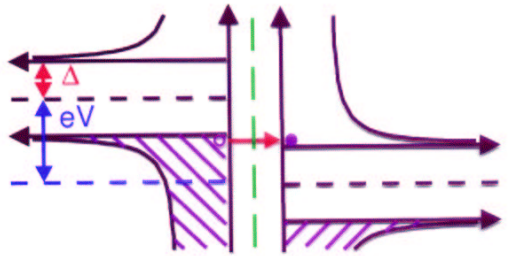
Conductance plateaus in atomic-size contacts of Al





Yanson, Ruitenbeek et al.

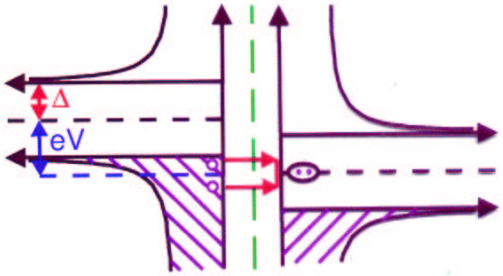
One electron transport:



$eV \geq 2\Delta/1$

$P \propto \tau^1$

2 electrons:

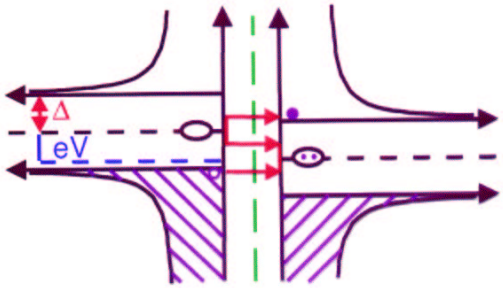


$eV \geq 2\Delta/2$

$P \propto \tau^2$

Andreev-reflection

3 electrons:



$eV \geq 2\Delta/3$

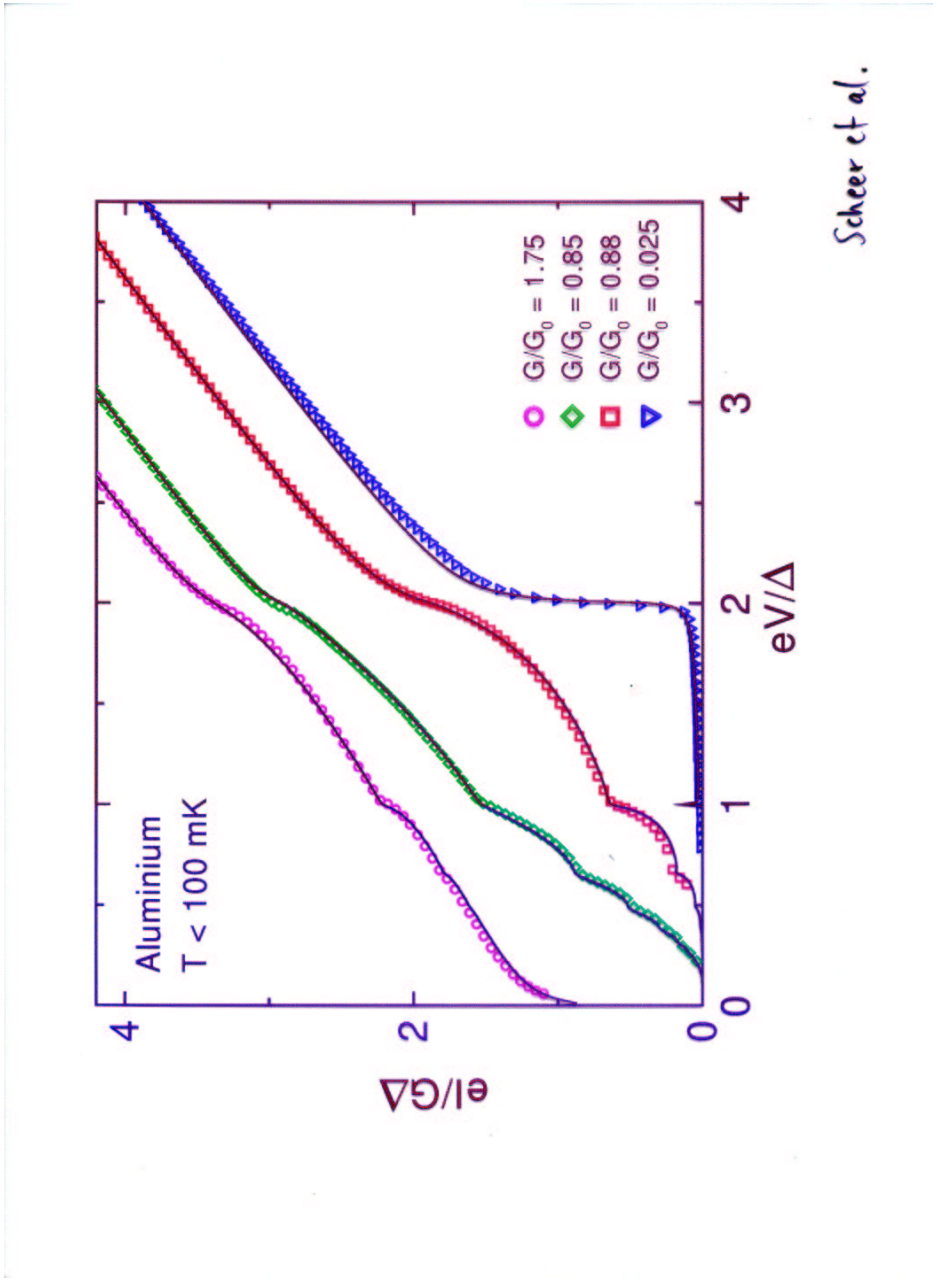
$P \propto \tau^3$

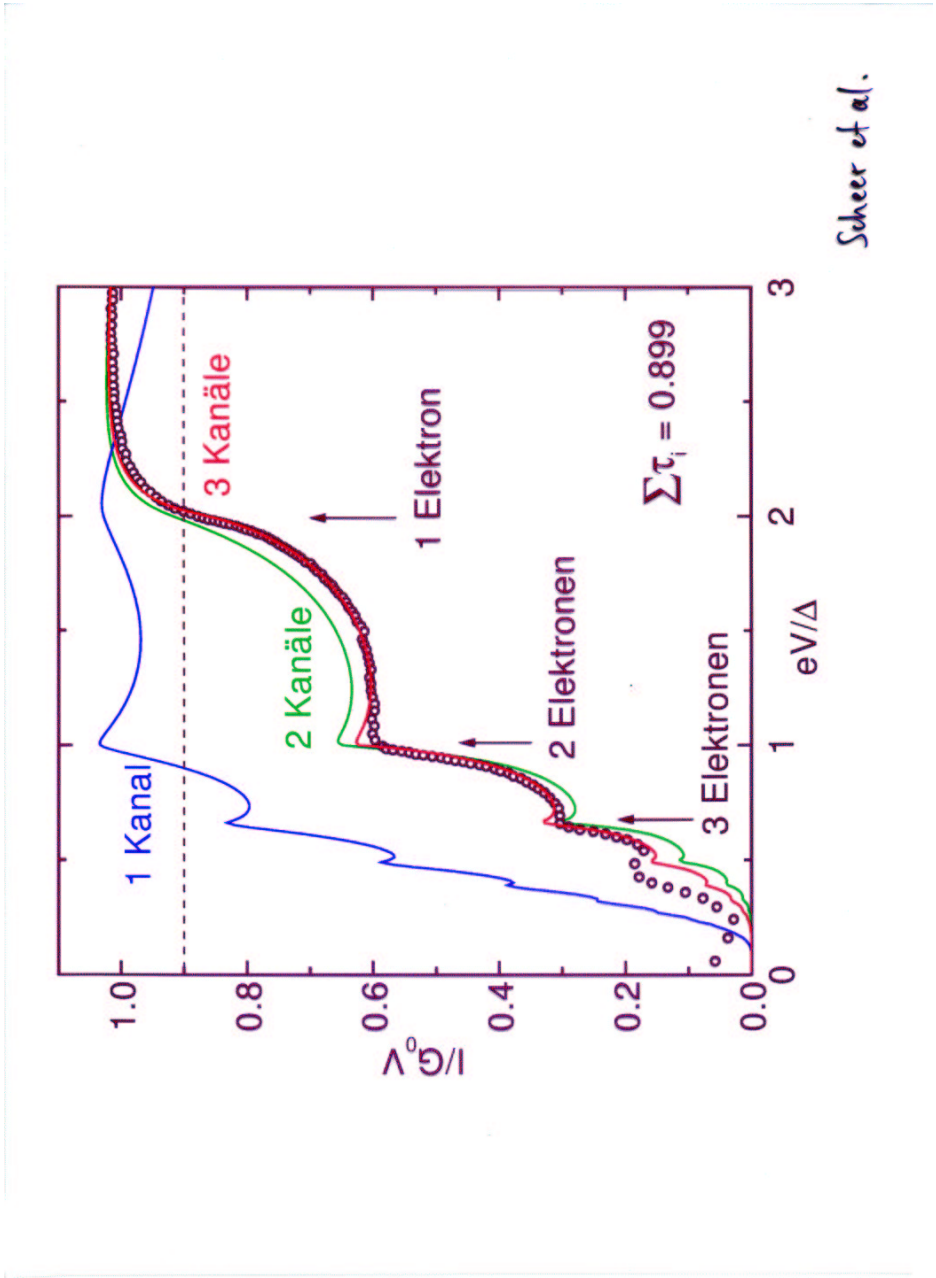
multiple Andreev-reflection (MAR):

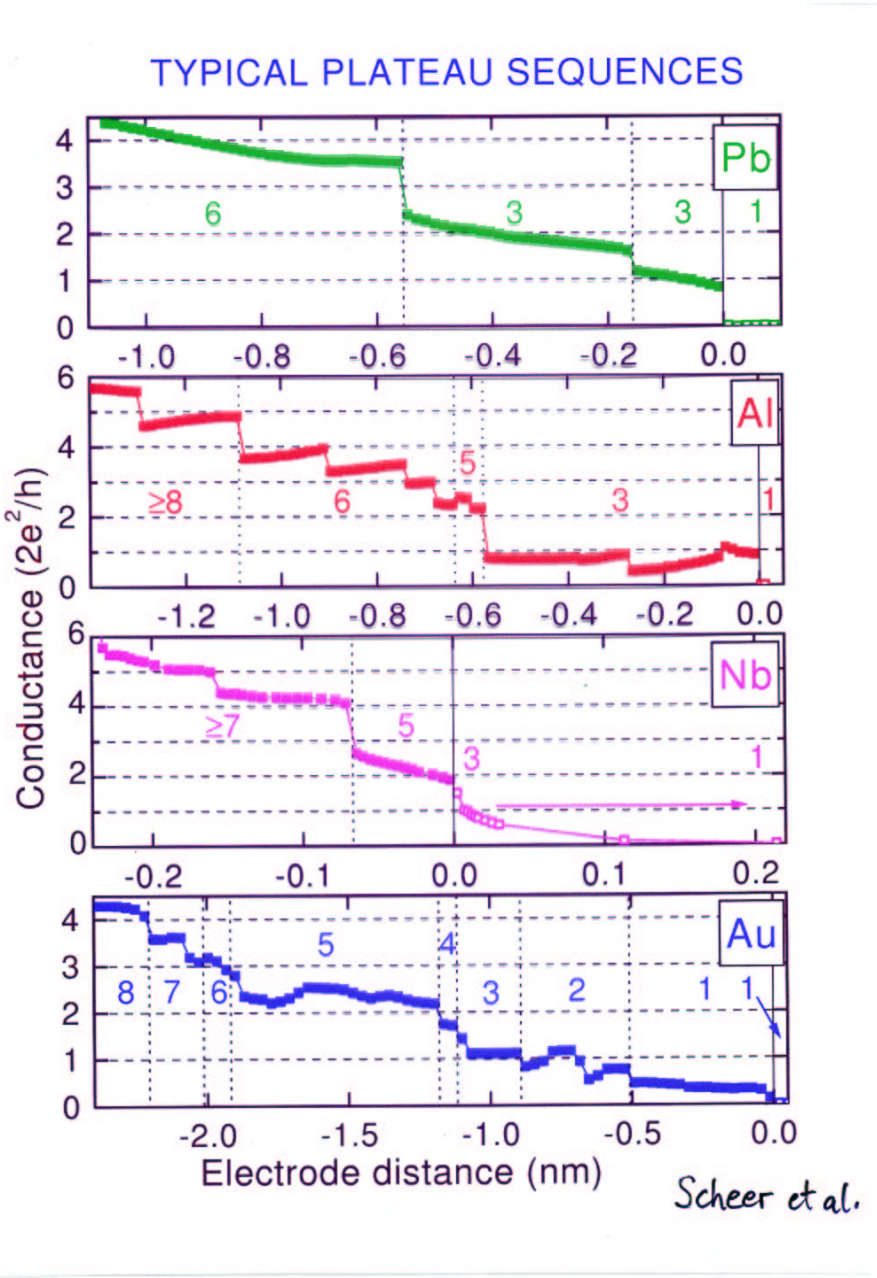
n electrons:

$eV \geq 2\Delta/n$

$P \propto \tau^n$




Scheer et al.
1 Kanal
3 Kanäle
2 Kanäle
1 Elektron
2 Elektronen
3 Elektronen
$\Sigma\tau_i = 0.899$
G/G_0
eV/Δ


TYPICAL PLATEAU SEQUENCES
Pb
Al
Nb
Au
Conductance ($2e^2/h$)
Electrode distance (nm)
Scheer et al.

Transport channels through single atoms

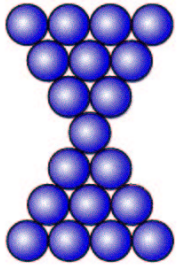
Determination of the number of channels N on each conductance plateau possible

first plateau: N depends on valence orbitals

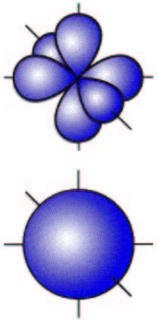
monovalent metals (Au, Na) $N_{max} = 1$
s orbitals

polyvalent metals (Al, Pb) $N_{max} = 4$
s and p orbitals

transition metals (Nb, W) $N_{max} = 6$
s and d orbitals



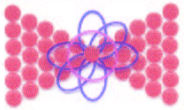
atomic orbitals



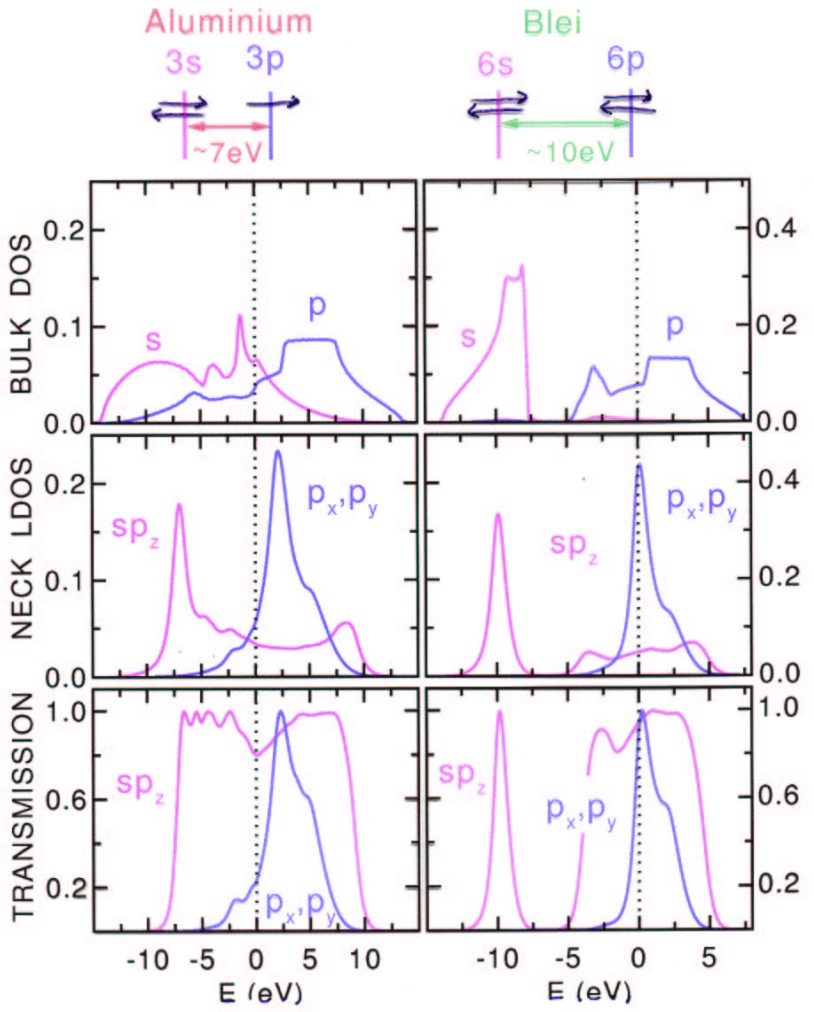
s orbital p orbitals

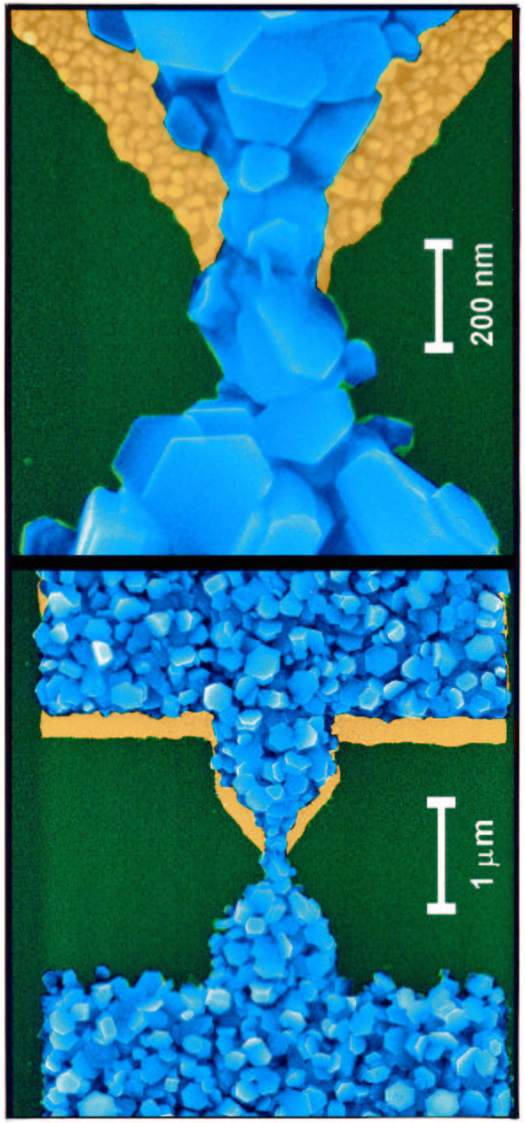
Transmission of each channel depends on local atom arrangement

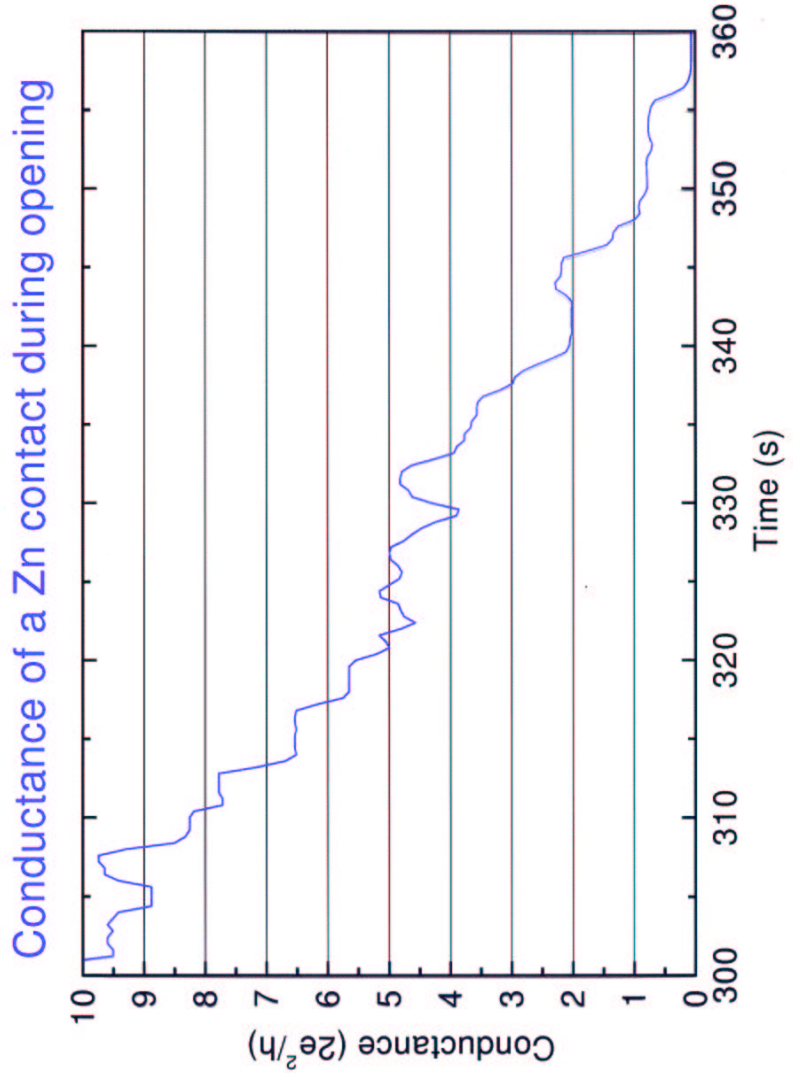
TRANSPORTKANÄLE IM LCAO-MODELL



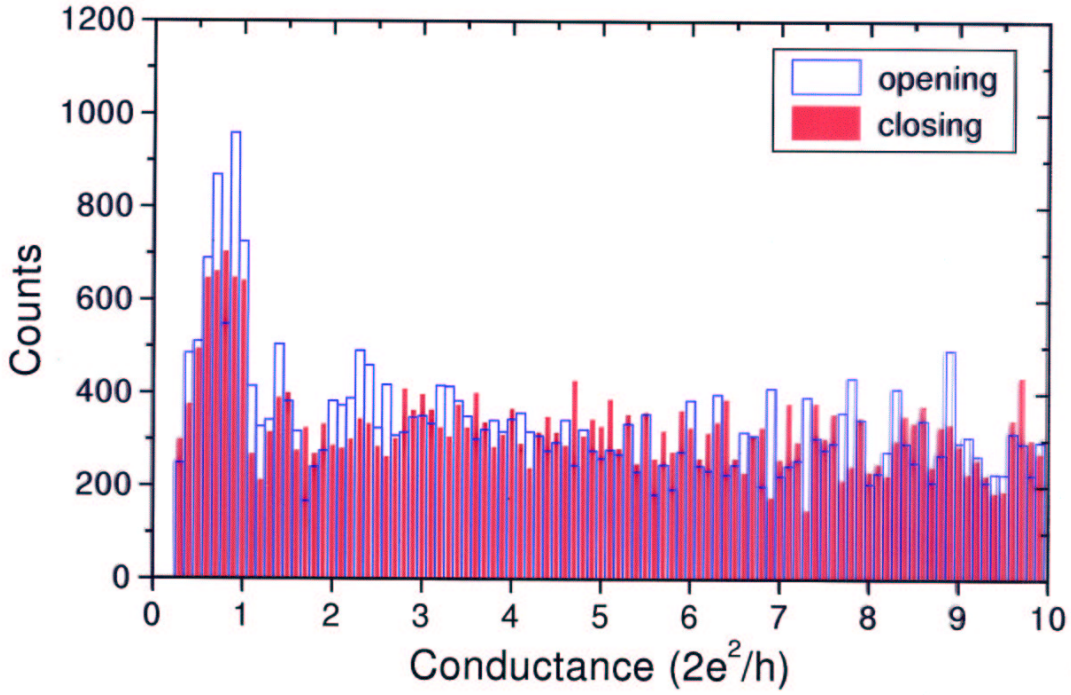
J. C. Cuevas et al.




200 nm
1 µm

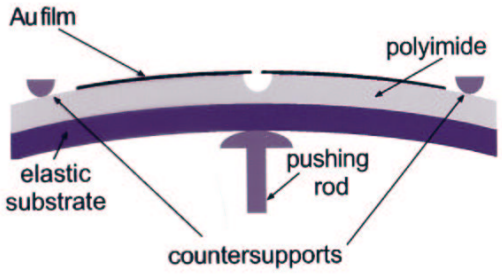

Conductance of a Zn contact during opening
Conductance (2e²/h)
Time (s)
0
1
2
3
4
5
6
7
8
9
10
300
310
320
330
340
350
360

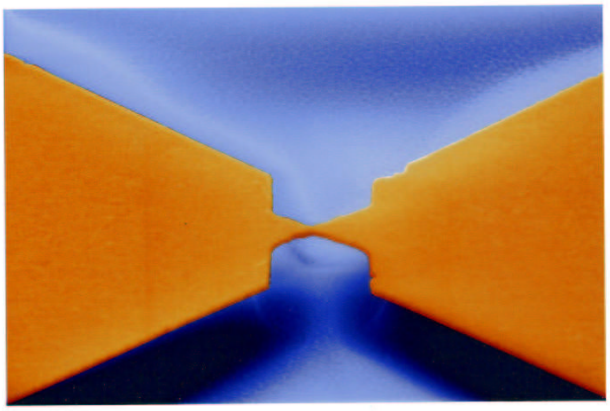
Histogram of conductance values of a Zn nanobridge



Forschungszentrum Karlsruhe
Technik und Umwelt
Institut für Nanotechnologie

Mechanically controlled break junction

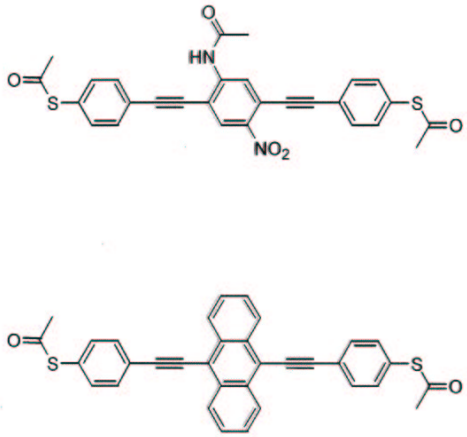


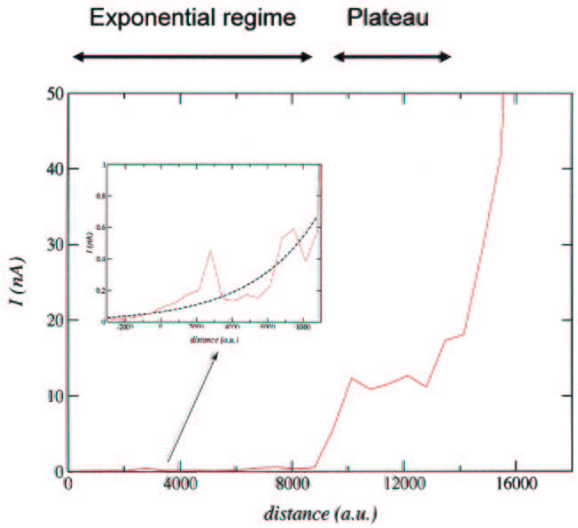


J. van Ruitenbeek et al
1995

Forschungszentrum Karlsruhe
in der Helmholtz-Gemeinschaft
Institut für Nanotechnologie

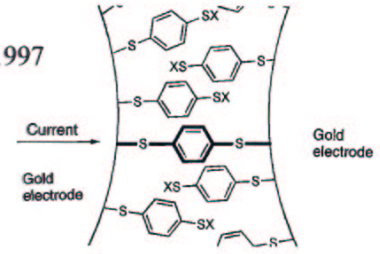
Formation of a junction

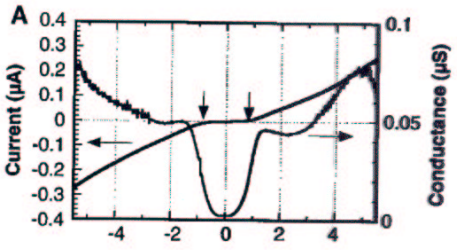




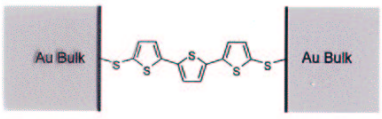
Previous experiments

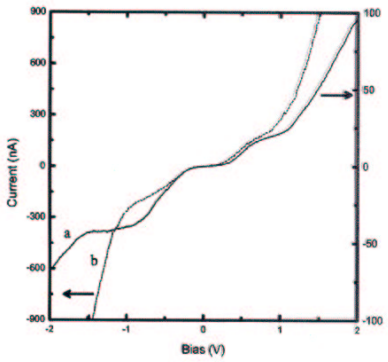
Reed et al 1997



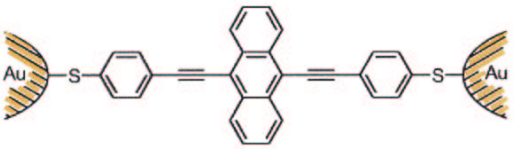


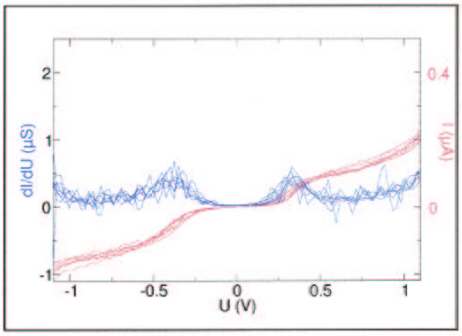
Kergueris et al (1999)

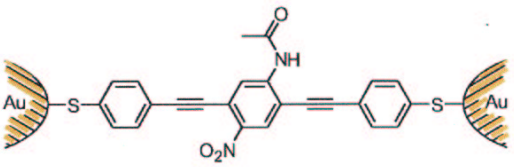


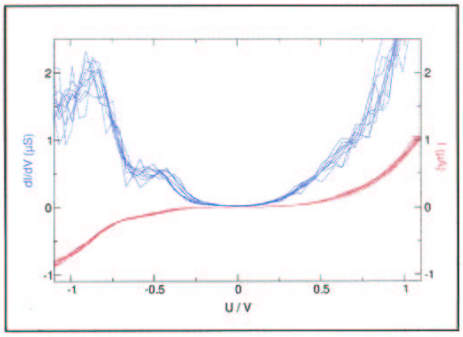


Transport through symmetric and asymmetric π-chain-molecules



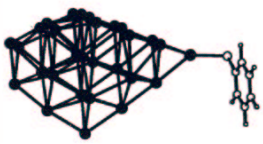


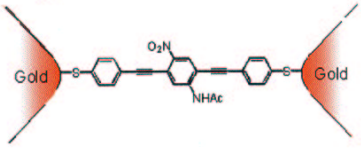


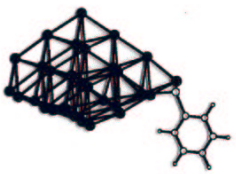


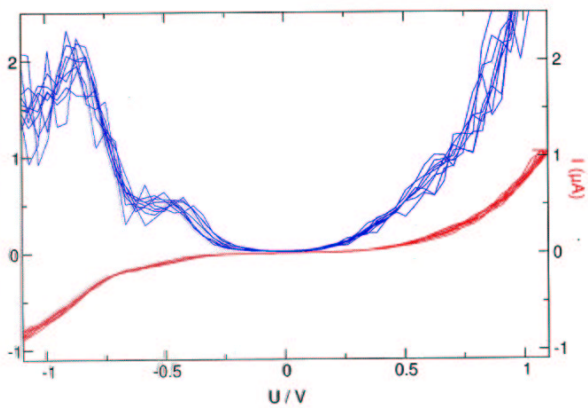
Forschungszentrum Karlsruhe
Technik und Umwelt
Institut für Nanotechnologie

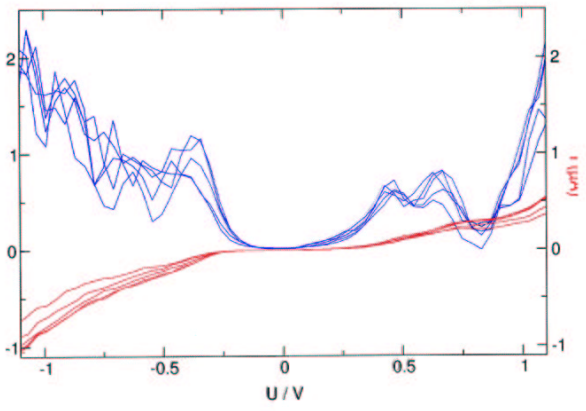
Asymmetric Molecule











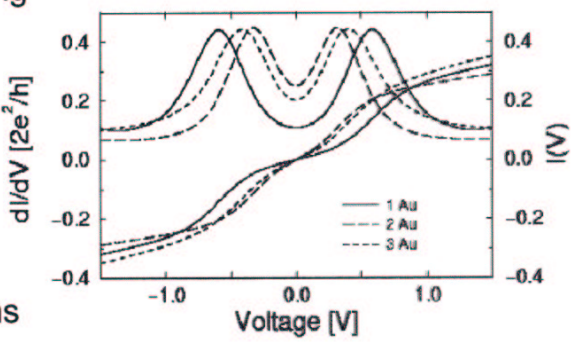
Calculation of the electrical current through a single molecule

Weigend, Köntopp, Evers

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

$$I(V) \sim \int T(E)\left[f(E) - f(E+eV)\right]$$

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



Inhomogenous 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

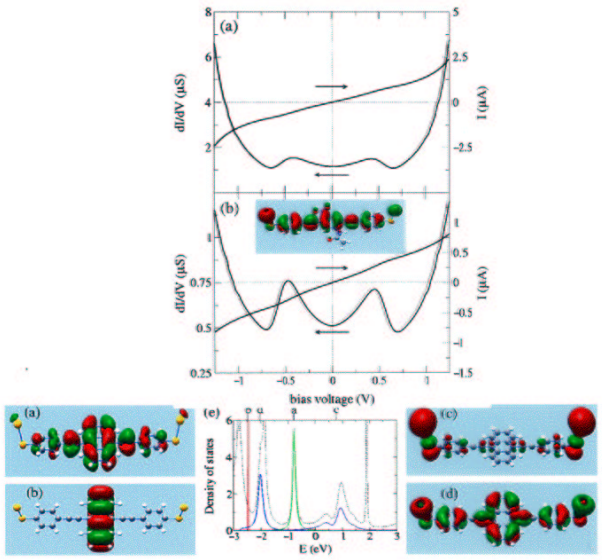
Strong coupling between
electrodes and molecule

Electron/hole remains only
a short time on the molecule

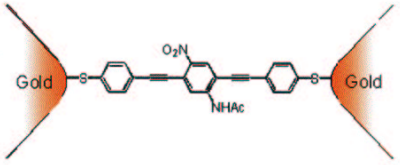
Ballistic Transport:
Landauer Theory

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

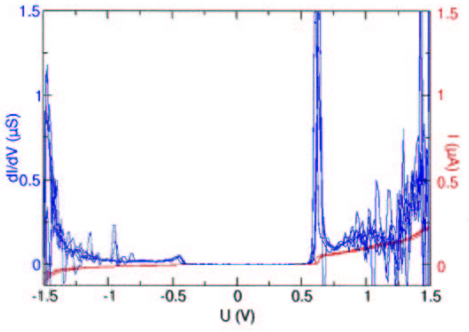
Conduction channels

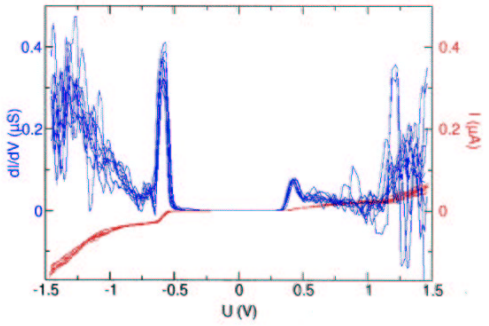


Transport through a single molecule at low tempereatures

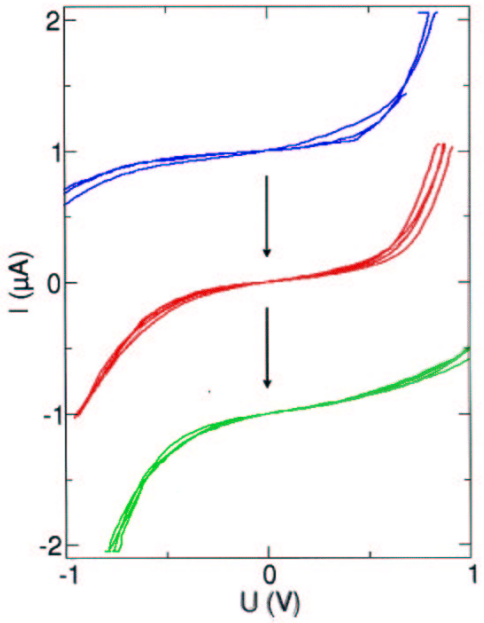


T=10 K

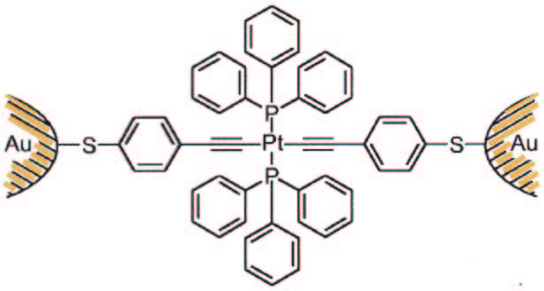


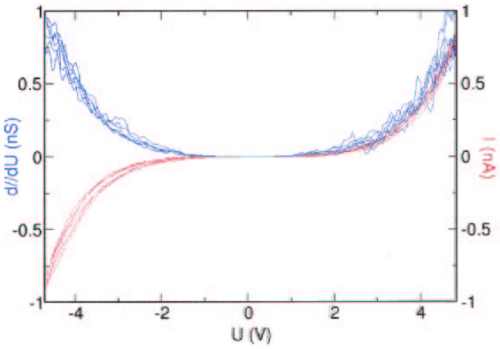


Switching of a symmetric molecule between different contact bonding configurations

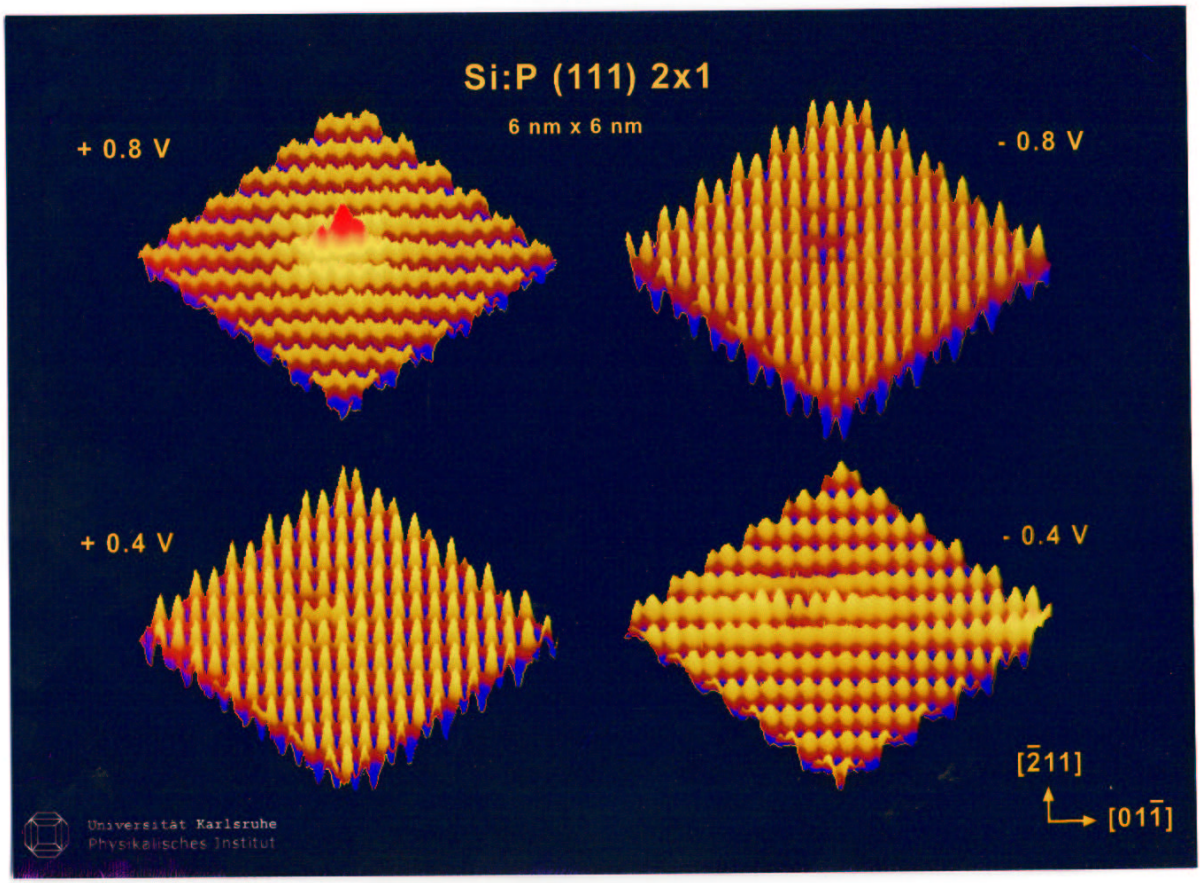


Transport through a molecule with interrupted π-chain

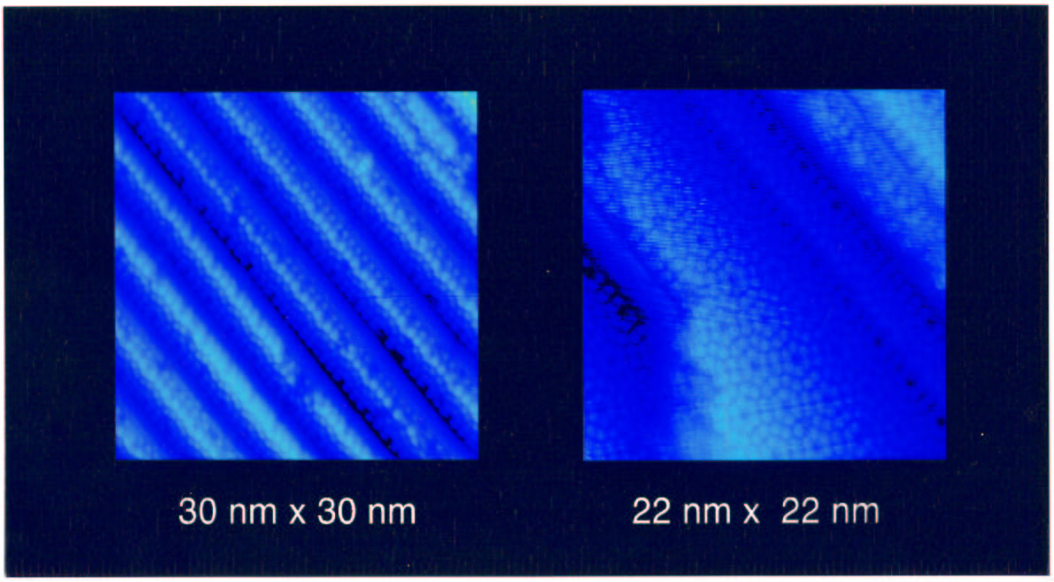




strongly insulating!

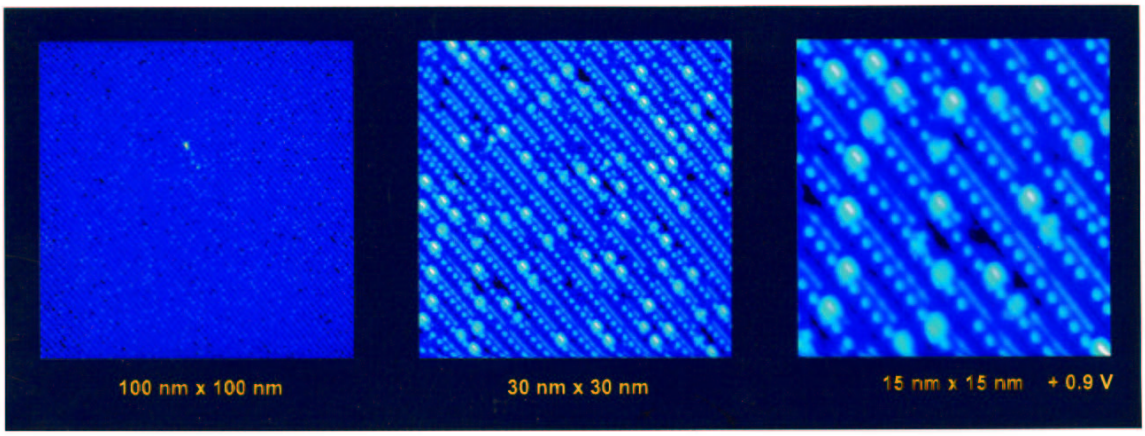


Si (111) - 7x7 10° off [$\bar{1}\bar{1}2$]



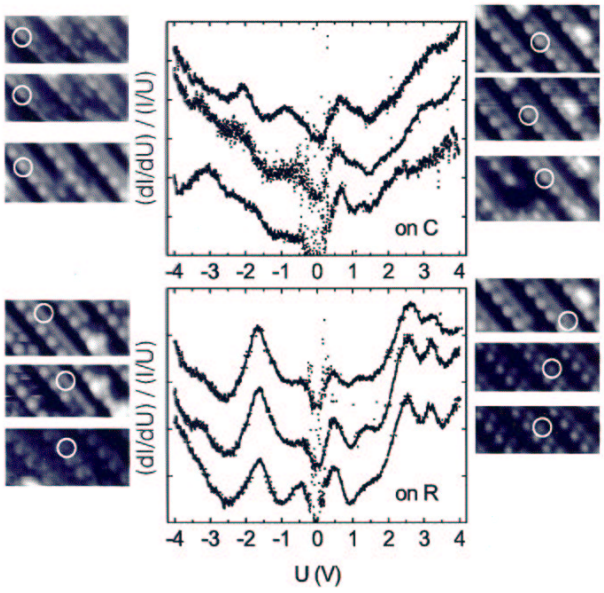
M. Schöck, C. Sürgers

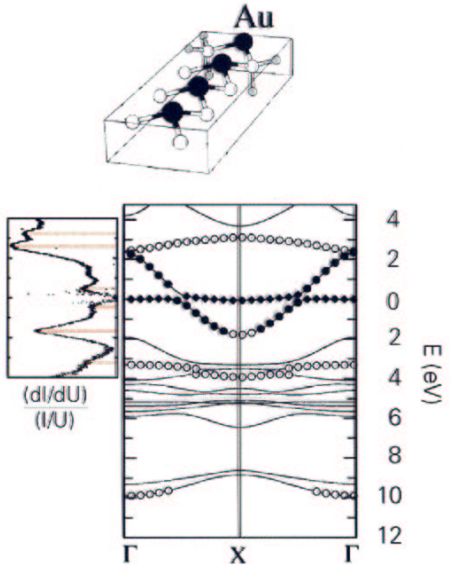
Si (111): Au 0.2 ML (10° off [$\bar{1}\bar{1}2$])



M. Schöck, C. Sürgers

Electronic structure of Si(557):Au





D. Sánchez-Portal et al.
Phys. Rev. B **65**, 081401 (2002)

M. Schöck, C. Sürgers

Acknowledgments

Elke Scheer
P. Joyez, D. Esteve, C. Urbina, M.-H. Devoret, CEA Saclay

H. Weber, R. Häussler, C. Paschke
J. Reichardt, D. Beckmann, R. Ochs, M. Mayor

H. Hein, P. Pfundstein - e^- beam

H. Kroha, A. Mirlin, P. Wölfle - theory

Universität Karlsruhe
Lokalisierung von Elektronen in makroskopischen und mikroskopischen Systemen

Forschungszentrum Karlsruhe
Institut für Nanotechnologie - Molekulare Elektronik

DFG Center for Functional Nanostructures (CFN)