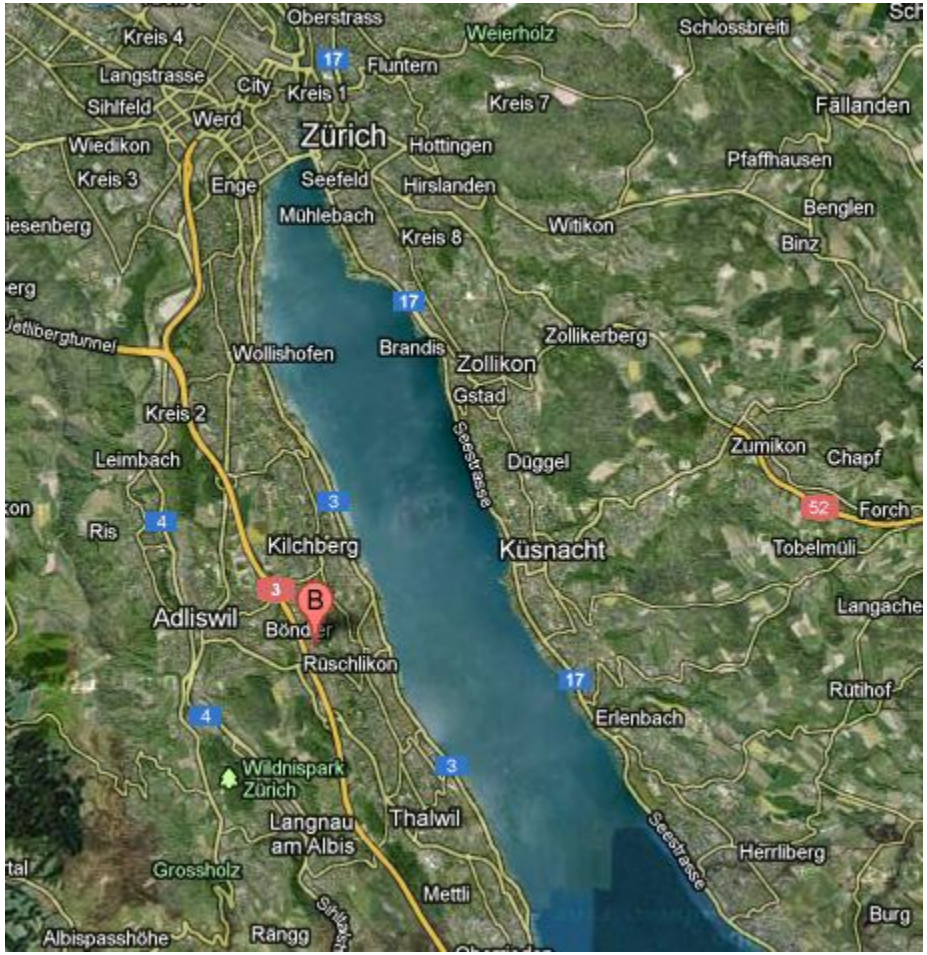
FUNMOLS IBM


Oberstrass
Kreis 4
Weierholz
Schlossbreiti
Langstrasse
City
Kreis 1
Fluntern
Sihlfeld
Werd
Kreis 7
Fällanden
Zürich
Hottingen
Wiedikon
Pfaffhausen
Kreis 3
Enge
Seefeld
Hirslanden
Mühlebach
Witikon
Benglen
Kreis 8
Binz
Zollikerberg
Wollishofen
Brandis
Zollikon
Gstad
Kreis 2
Leimbach
Düggel
Zumikon
Chapf
Forch
Ris
Kilchberg
Küsnacht
Tobelmüli
Adliswil
Rüschlikon
Langache
Rütihof
Erlenbach
Wildnispark Zürich
Langnau am Albis
Thalwil
Herrliberg
Grossholz
Mettli
Albispasshöhe
Rängg
Burg

micro-/nanoelectromechanical systems (MEMS/NEMS); spintronics/ magnetism; nanowires; carbon-based devices; organic electronics; functional materials; directed self-assembly; cooling; three-dimensional integration; optical interconnects; photonics; and simulation and theory

950 m^2 cleanroom facility

noise-free labs:

Mechanical vibrations: Velocity less than 500 nm/s (*x,y,z*), below 16 Hz and less than 100 nm/s above the 16 Hz band.

Electromagnetic fields (EMF):

Flux density less than B = 5 nT RMS in an integral spectrum between 0 and 625 Hz

Noise power: < 10-12 V2 RMS up to 1 kHz without 50 Hz, < 10-10 V2 RMS up to 1 kHz for 50 Hz and harmonics , < 10-10 V2 RMS above 1 kHz

Temperature stability: 0.1 °C/1 h and 0.5 °C/24 h

These challenging specifications will be achieved by the following measures:

Mechanical vibrations Separated tool platform vibro-acoustically decoupled from building and operator platform. Massive concrete pedestal (> 65 tons), suppressing frequencies above 25 Hz

Tool platform with passive mechanical damping, suppressing frequencies above 3 Hz

Active mechanical damping down to 0.5 Hz

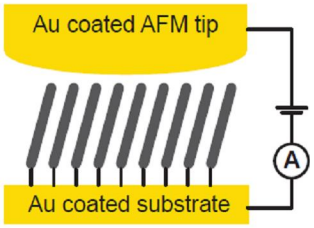
Operator platform decoupled from tool platform.

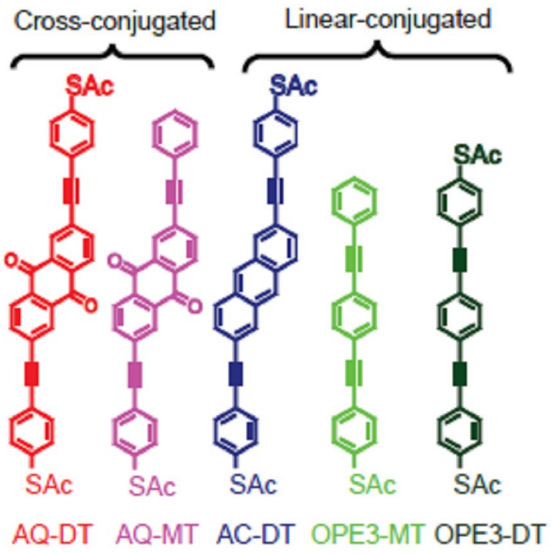
Electro-magnetic fields (EMF) Passive mu-metal shielding of each lab to screen external EMF and to reduce EMF within the lab to B < 20 nT. Active EMF cancellation system consisting of 3 pairs of Helmholtz coils to cancel the remaining EMF and to guarantee B < 5 nT.

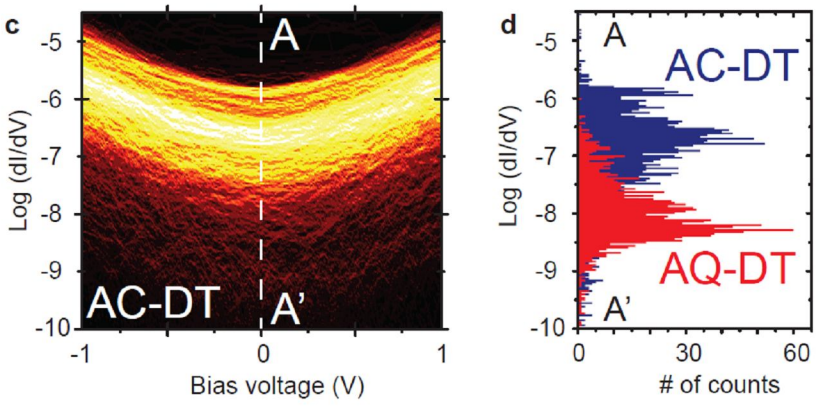
Chamber concept All additional sources of noise, such as pumps, transformers, and power supplies, will be placed remotely in chambers adjacent to each lab.

S.J. v. d. Molen: QM interference in molecular charge transport

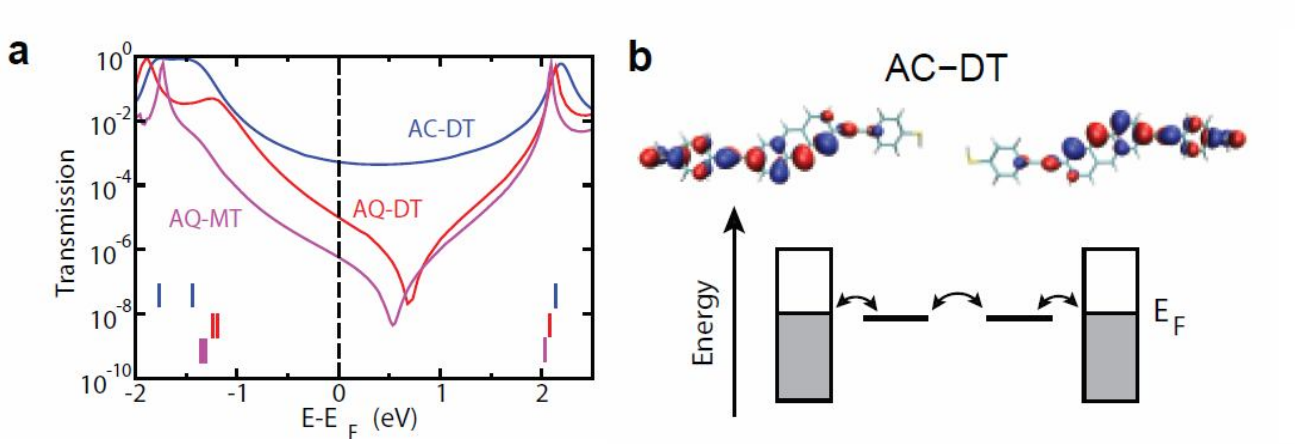
-Set of molecules: linearly and cross-conjugated
- Conducting probe AFM
- Measure I-V-s on with several molecules in the junction
- Plot 2D I-V histograms
- Cross conjugated has lower conductance, although HOMO-LUMO gap is the same





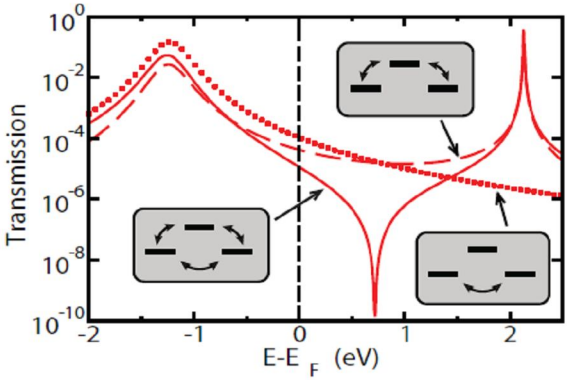


S.J. v. d. Molen: QM interference in molecular charge transport

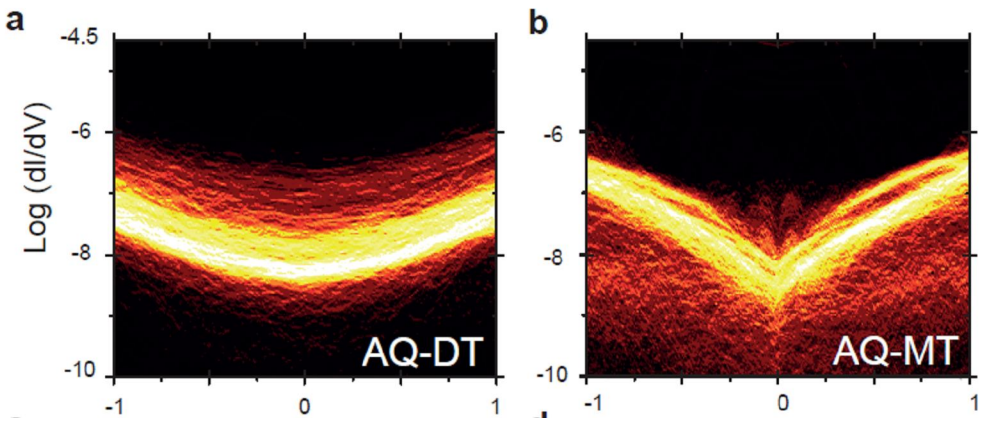


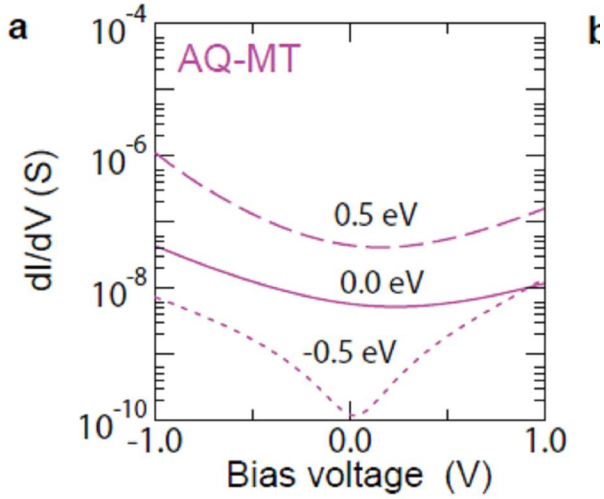
-Calculate T(e) and an antiresonance is seen for the cross conjugated
- Localized Molecular Orbitals: A linear combination of frontier orbitals
- For AQ the HOMO and HOMO-1 is almost degenerate (left and right) and a single LUMO
- The electrons can directly hop, or through the high energy level, these two interfere destructively

- For AC HOMO-1 is far, middle level is missing



S.J. v. d. Molen: QM interference in molecular charge transport

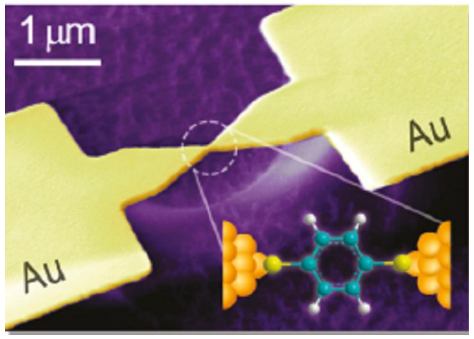


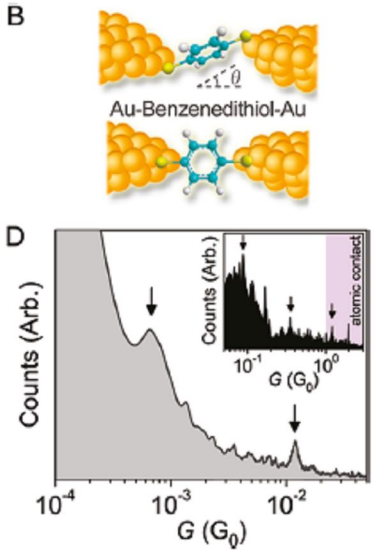


- However I-V curve is parabolic
- But for the mothiol, the dip is seen, dependence on E_f (since the current is the integral of T)
- Away from the antiresonance, the integral is symmetric

Results: Elke Scheer group – Konstanz

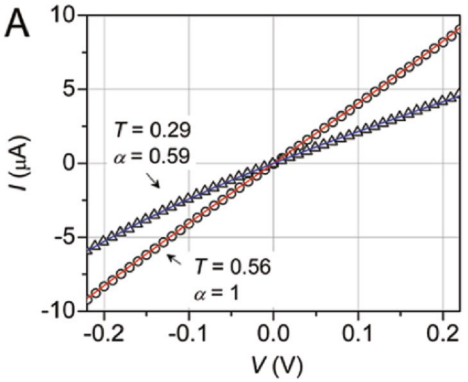
IETS-PCS transitions downscaled





different conductance, for different conformations (even highly conductive)

measure I-V curves:
from fit: symmetric or asymmetric coupling



$$I(V) = \frac{2e}{h}\int_{-\infty}^{\infty} T(E,V)\left[f(E-eV/2) - f(E+eV/2)\right] \mathrm{d}E$$

$$T(E,V) = \frac{4\Gamma_L\Gamma_R}{\left[E - E_0(V)\right]^2 + \left[\Gamma_L + \Gamma_R\right]^2}$$

$$E_0(V) = E_0 + \left(\frac{\Gamma_L - \Gamma_R}{\Gamma_L + \Gamma_R}\right)\frac{eV}{2}$$

Asymmetry scales crossover!

$$\alpha = \Gamma_R/\Gamma_L$$

$$T_{max} = 4\alpha/(1+\alpha)$$

$$T_{crossover} = T_{max}/2$$

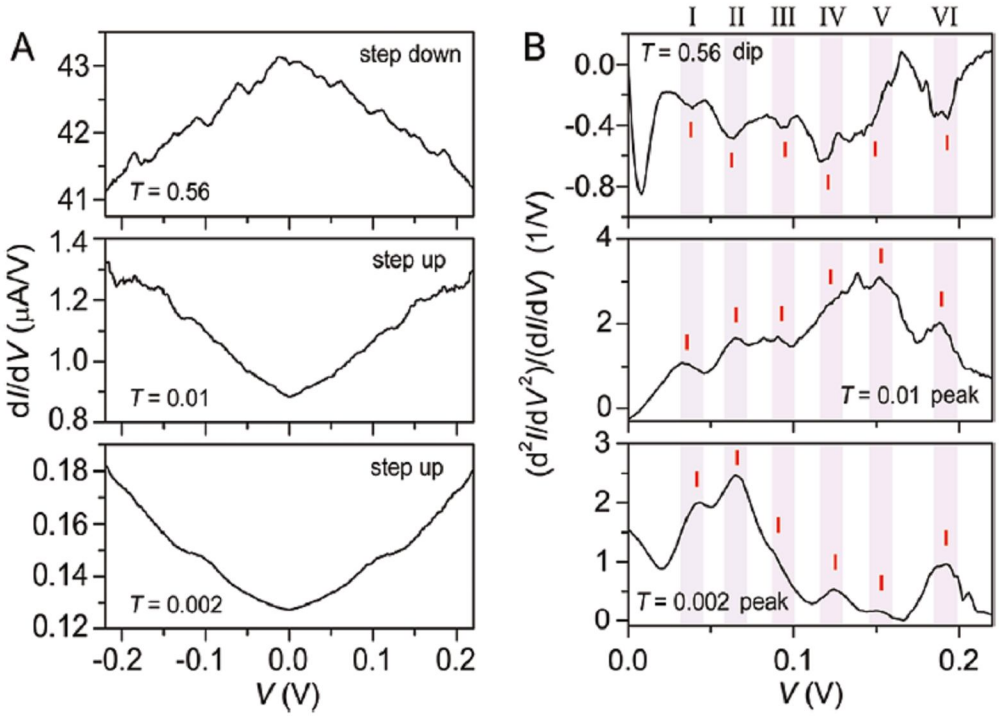
Nano Lett. 2011, 11, 3734–3738

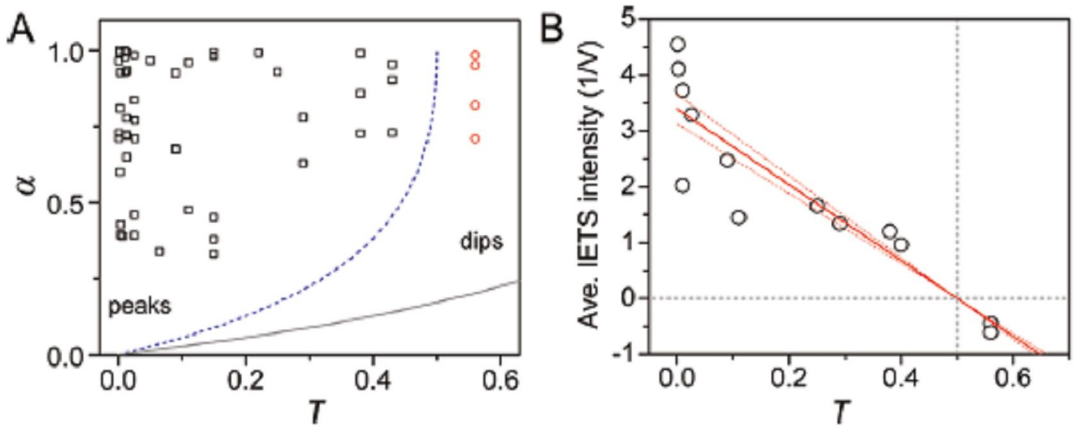
Results: Elke Scheer group – Konstanz

IETS-PCS transitions downscaled

PCS-IETS transition observed for symmetric G=0.5G0

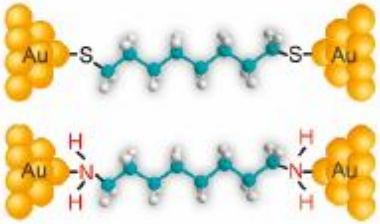
for asymmetric: at lower G0 also intensity scaling is seen as calculated



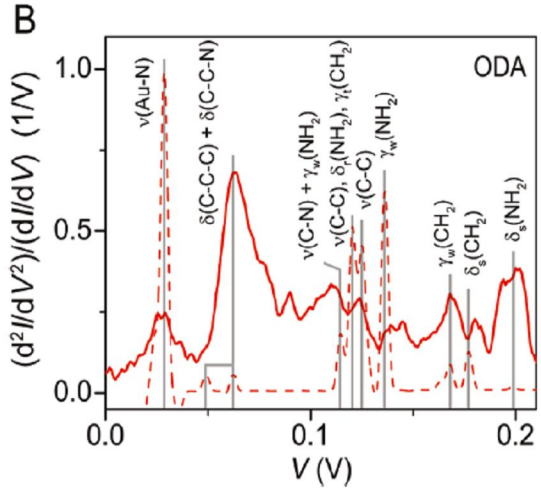


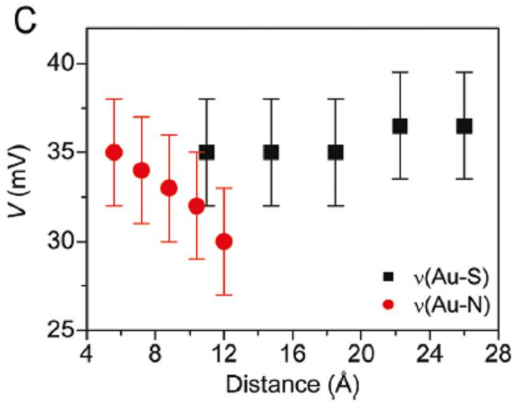
Nano Lett. 2011, 11, 3734–3738

Results: Elke Scheer group – Konstanz



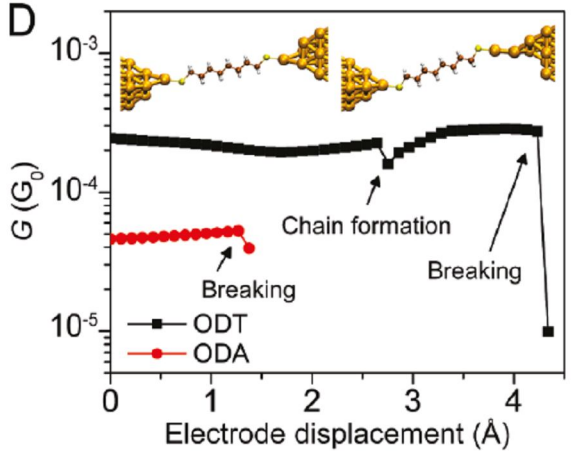
Thiol or Amin by IETS
IETS investigation of lowest peak





DFT for vibration modes fit well - IETS normalized by conductance
Anchoring group has influence on spectra

They find that thiol is stronger – Au chains can be pulled
- average breaking length much longer (histogram)
- kinks in the traces (new atom pulled)
- same in simulation
- investigate Au-S and Au-N mode, redshifts for amine (weakening of the bond)
- for thiol they see Au-Au mode



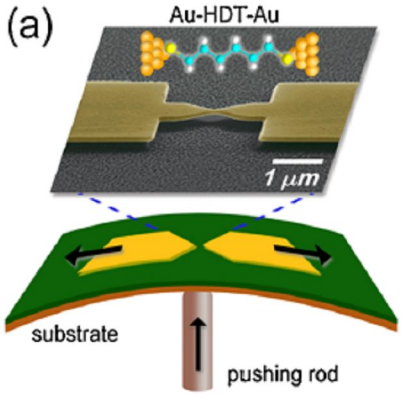
ACS Nano. 5, 4104 (2011)

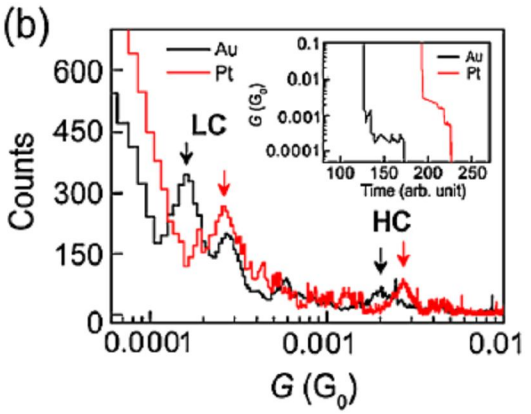
Results: Elke Scheer group – Konstanz

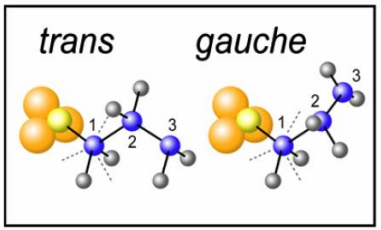
„Conductance and Vibrational States of Single-Molecule Junctions controlled by Mechanical Stretching and Material Variation”

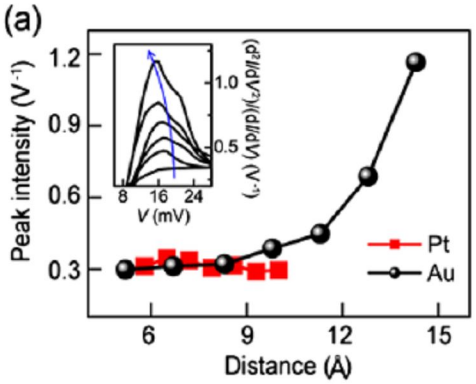
Pt and Au junctions with hexanedithiol

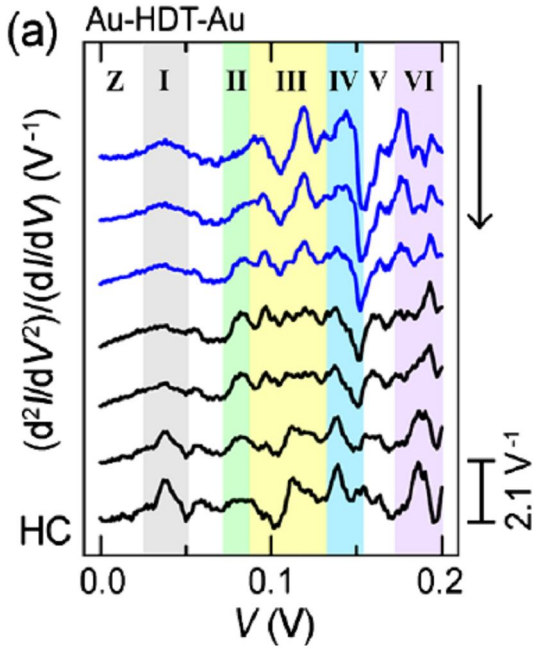
-IETS show change in molecular conformation during stretching (smaller jumps in cond.)
- stretching distance longer for Au (chain)
- Analyze Au-Au, Pt-Pt, and Au-S and Pt-S mode: the Au-Au gets stronger in stretching, as a result of chain formation, Pt-Pt not
- Au-S changes from HC to LC: sliding to different binding site of endgroup





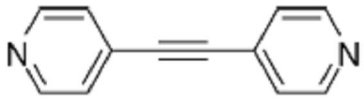




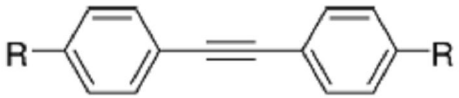


PRL. ***106****, 196804 (2011)*

Wandlowski group
Anchoring groups

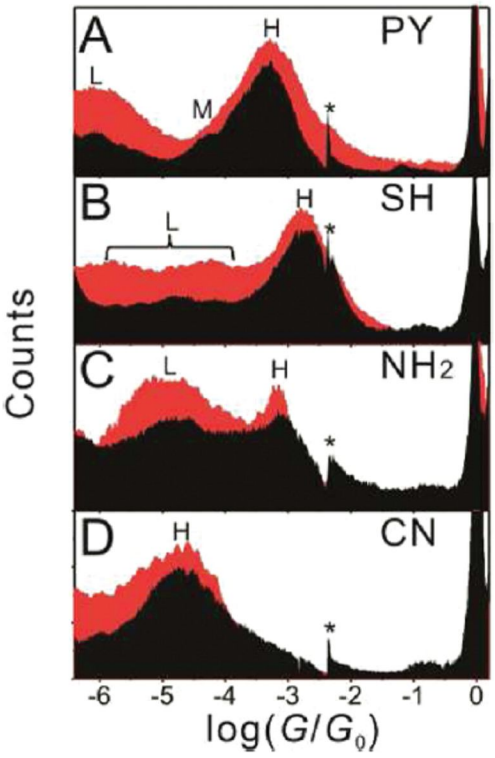


1a Py

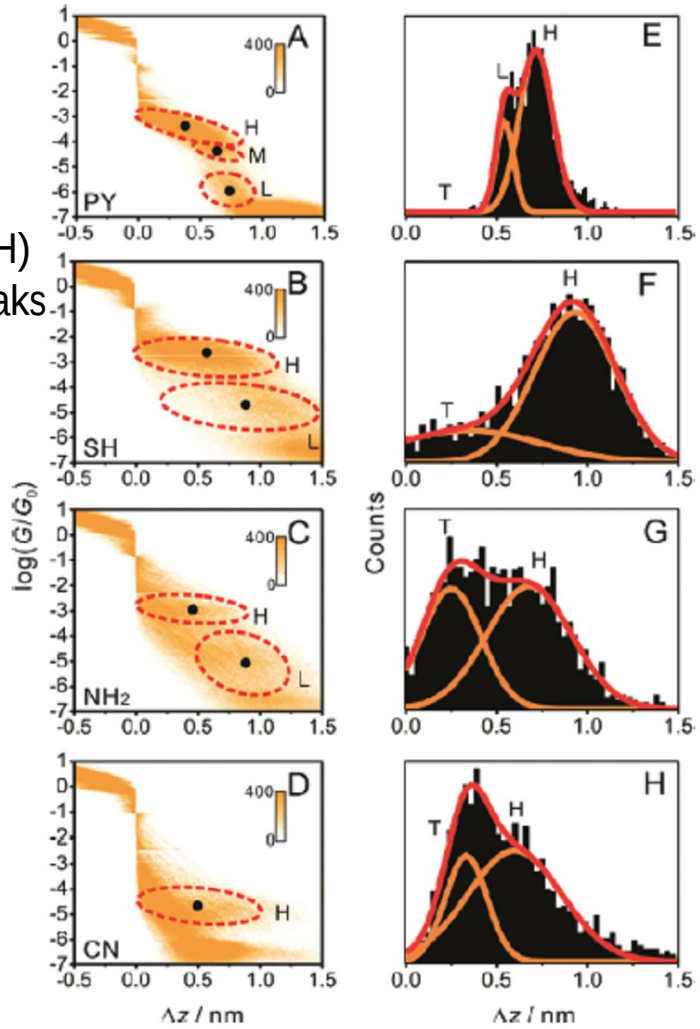


1b R=SH
1c R=NH_2
1d R=CN

MCBJ+STM-BJ measurements



- 2 or 3 configurations for every group
- 2D trace histograms
- relative displacement histograms (PLH) display peaks corresponding to diff.peaks

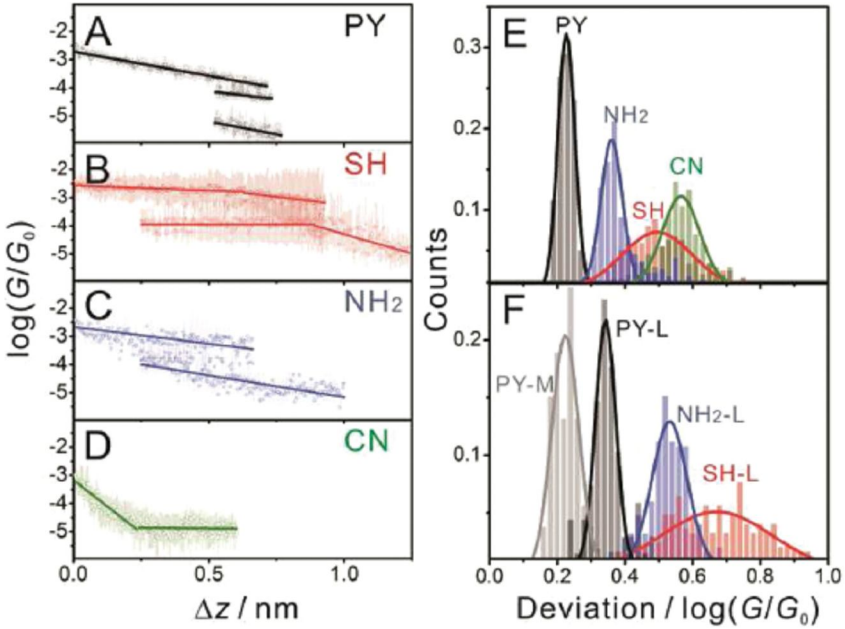


Wenjing Hong et al., JACS (2011), dx.doi.org/10.1021/ja209844r

Wandlowski group
Anchoring groups

- Analyze the average of the 2d histogram, show trends
-Also possible to analyze width at a defined Δz, and look az the distribution: this gives info about the variability of binding conductance
- Measure I-V: correspond to calculations

- Py is the best, high cond, narrow distribution, no deprotection needed

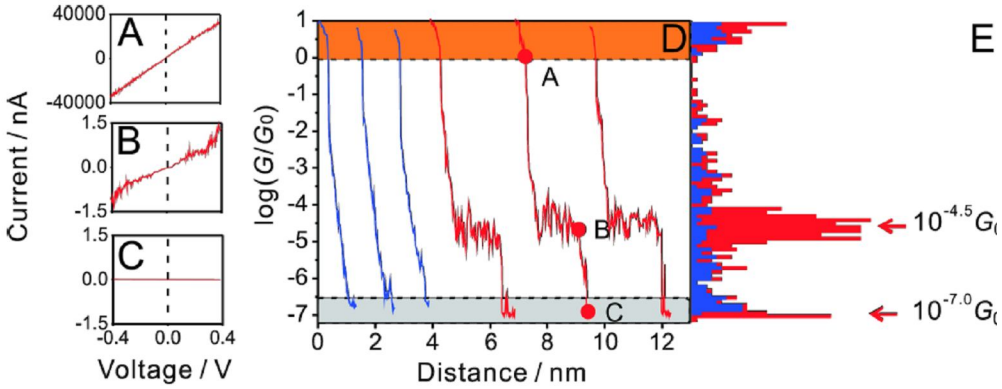


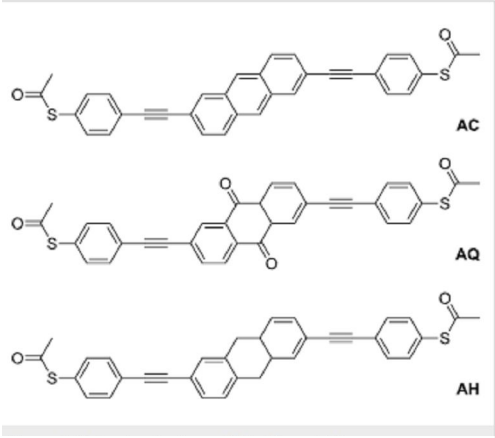
Wenjing Hong et al., JACS (2011), dx.doi.org/10.1021/ja209844r

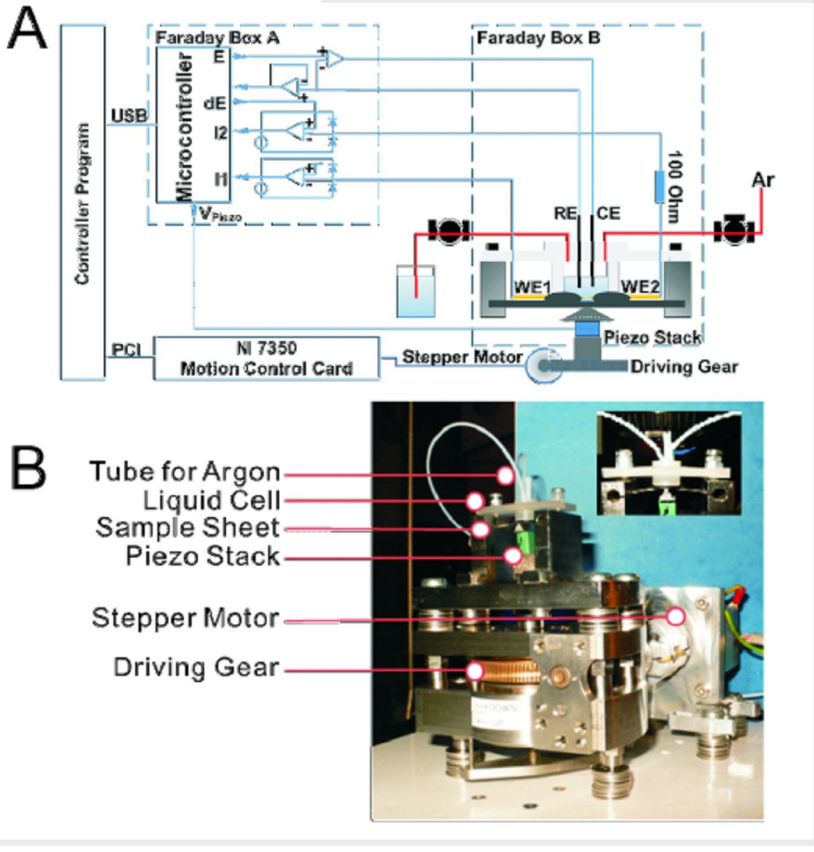
Wandlowski group

study of conjugation (same molecules as v.d. Molen)

- lot of details about setup, electronics etc.
- can really measure down to low conductance (10fA)
- possible to measure IV-s
- histogram with STM, MCBJ, and from I-Vs: the same ☺
 - 0.5 nm·s−1 stretching speed, *V*bias from −0.4 V to +0.4 V at a rate of 25 V·s−1





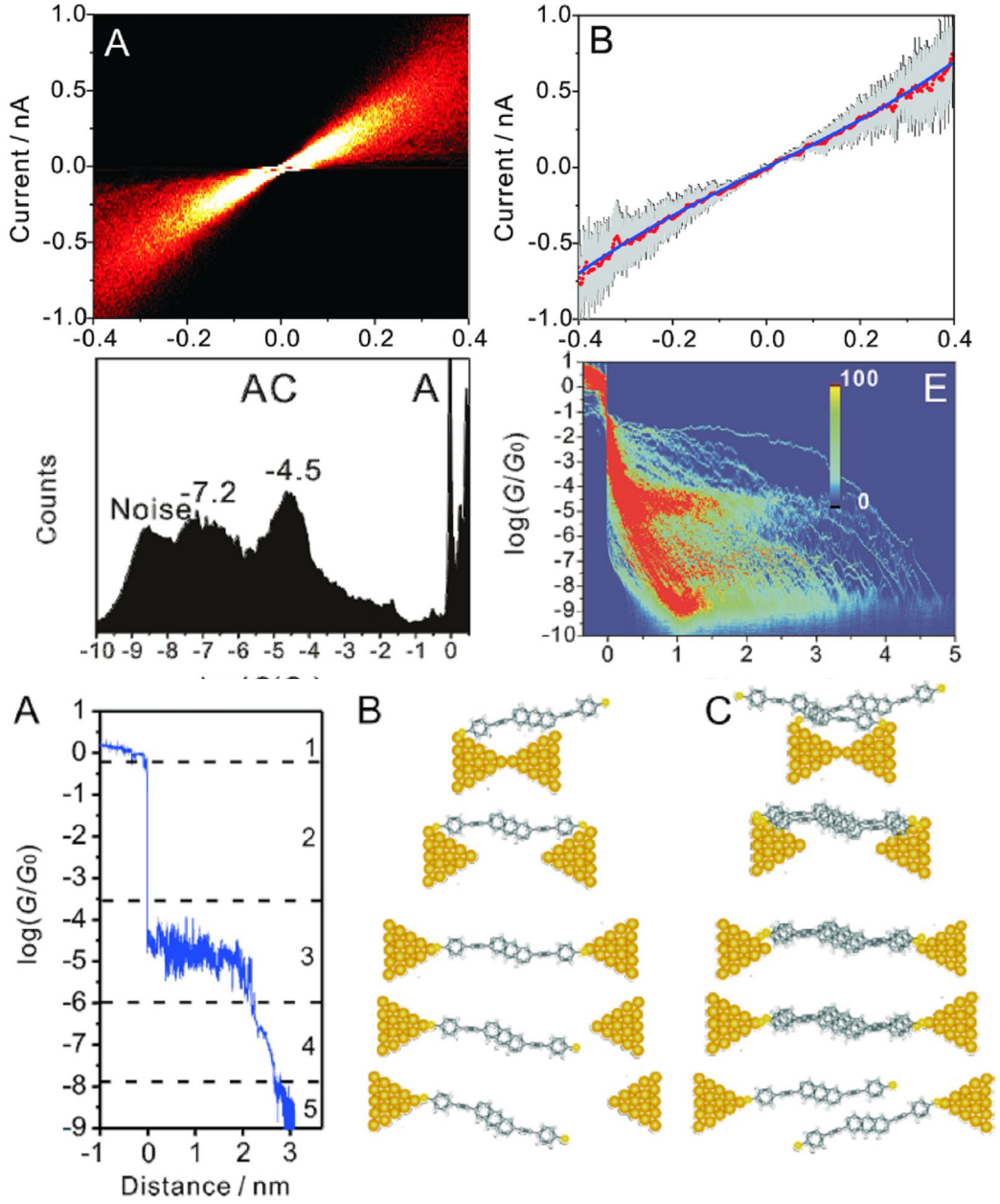


W. Hong et al., Beilstein J. Nanotechnol. ***2011,*** *2, 699–713.*

Wandlowski group

measure I-Vs, average and fit, close the parameters to DFT
relation is similar as for Molen
(AC -4.5, AQ -7; AH -6.3 qinterference)
for AC the lower is possibly pi-pi stacking

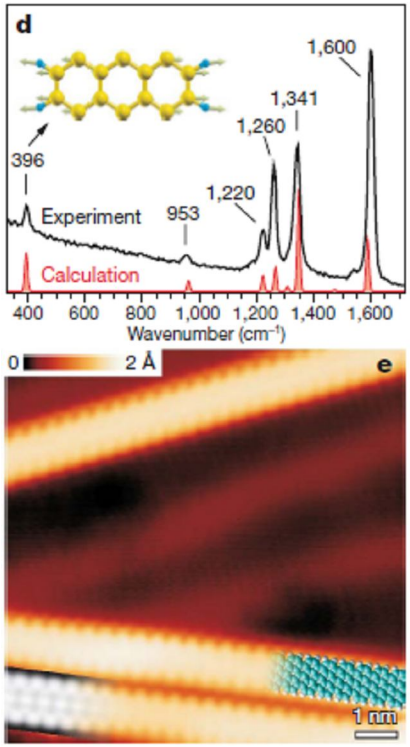
also create length histograms
- scale tunnel calibration from STM, use the same for MCBJ

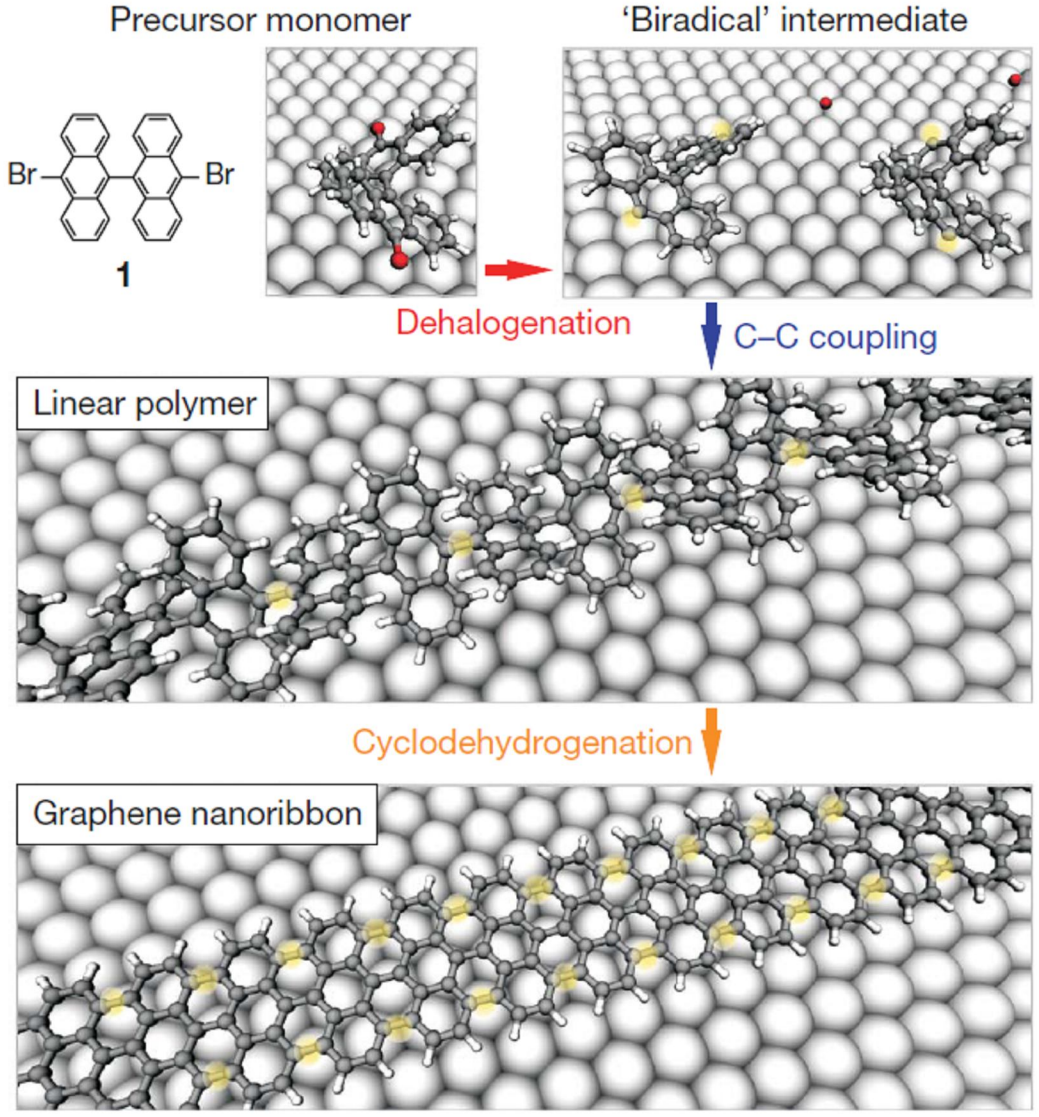


W. Hong et al., Beilstein J. Nanotechnol. ***2011,*** *2, 699–713.*

Roman Fasel – EMPA
Graphene growth on surfaces

- On-surface forming of graphene ribbons
- Confirm with STM
- Raman measurement
- Simulation (STM, Raman)



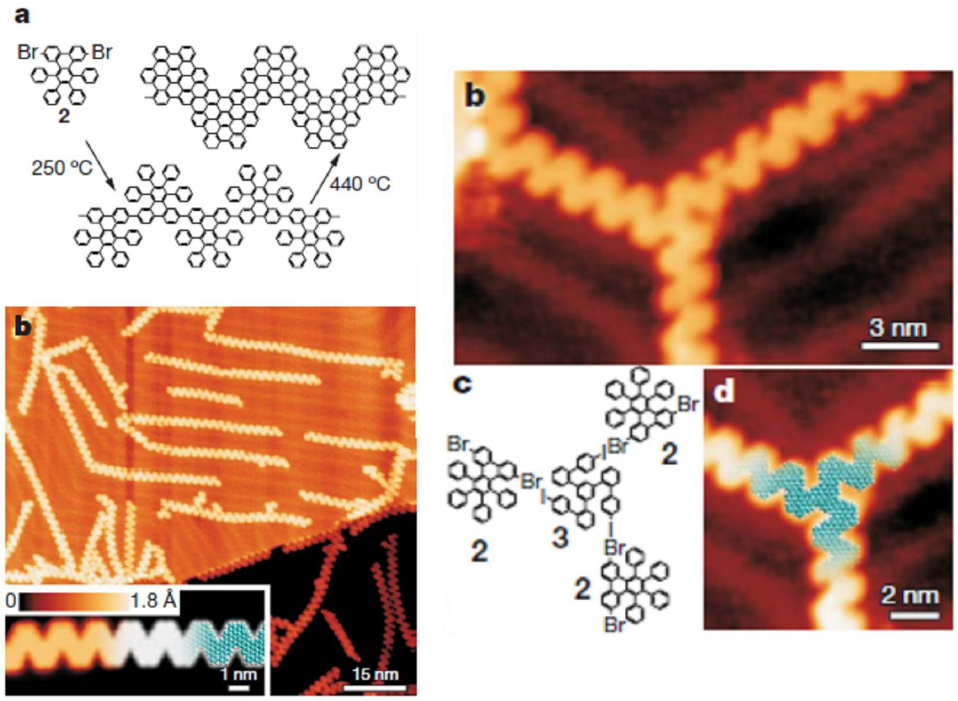


Jinming Cai et al., Nature 466, 470 (2010)

Roman Fasel – EMPA
Graphene growth on surfaces

- well defined boundary
- possibly gap depends strongly on width (heterojunctions possible: ribbons with different width)
- several forms are possible
- only possible on metal surface

need to transfer to Si/SiO_2
they contacted it, yet Shottky barrier

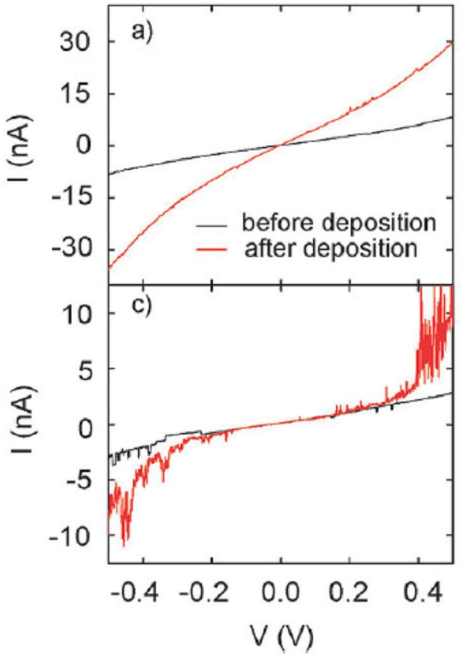


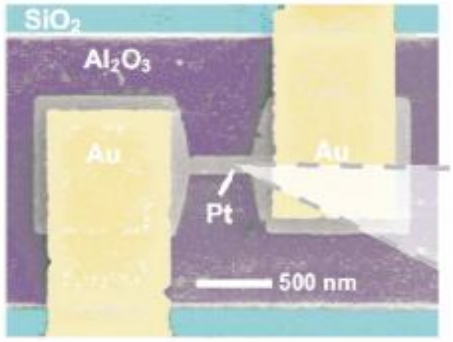
Jinming Cai et al., Nature 466, 470 (2010)

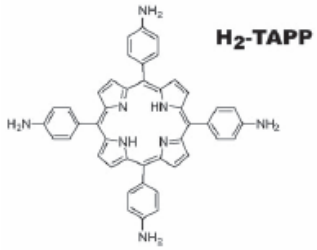
Ferry Prins – Delft
Migration & Graphene electroburning

graphene electroburning: under ambient conditions, multilayer, 1-2nm gap formed
extended molecules to use pi-pi stacking
migration did not work

Prins et al., APL 94, 123101 (2009): Pt electromigration under ambient conditions
Prins et al., PCCP 13, 14297 (2011)
B Gao *et al* 2011 *Nanotechnology* **22** 205705

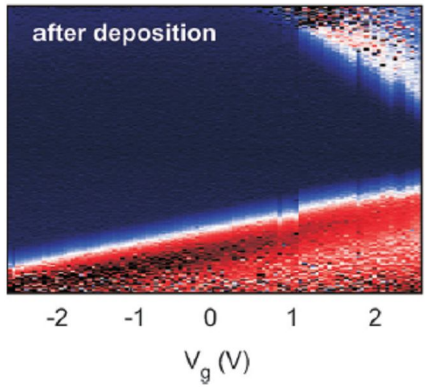






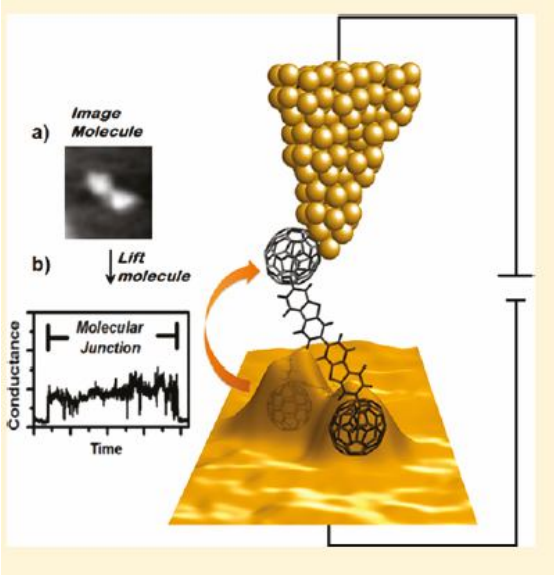
Molecules admitted to the Pt electrodes
Characterize before after
- for most devices higher current (lowering the tunnel barrier), and no gate response
- for one device strong gate response and double barrier structure

- strongly hybridized molecules are hard to gate



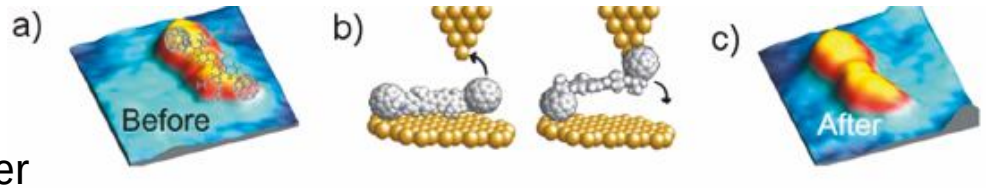
Prins et al., PCCP 13, 14297 (2011)

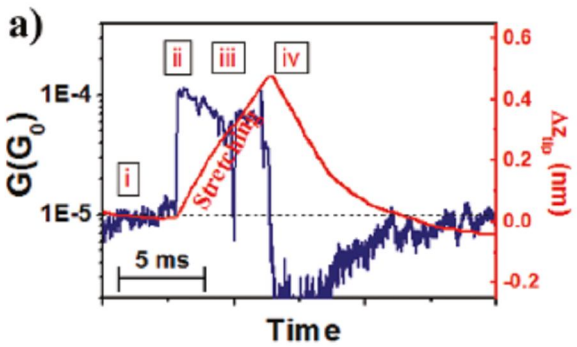
Agrait Group

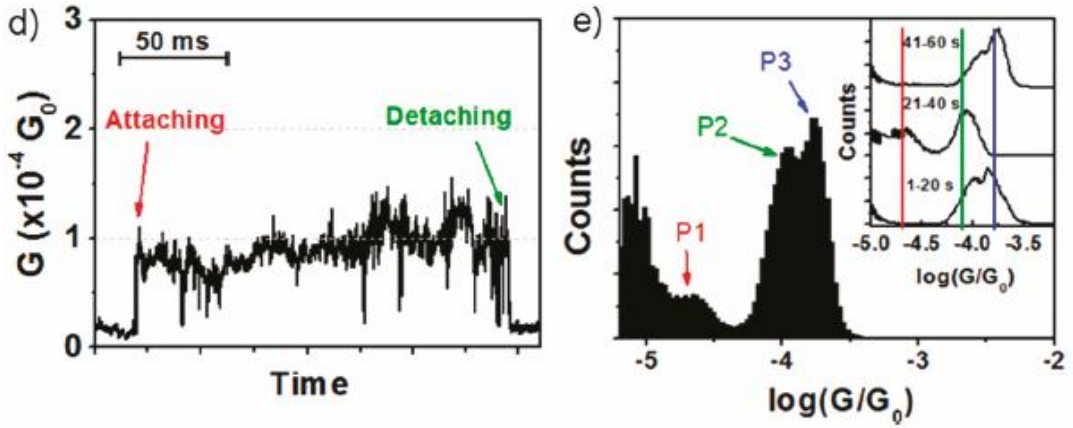


-„standard STM-BJ experiments" (e.g. show that thiols strong, but also modifies the gold electrodes)
- **STM characterization measurements on dumbbell molecules**

- RoomT measurement
- First image, find separate one (C60 easy), go above with a tip,
- For right height (open loop), the molecule is bouncing up-down
- only 60 s long meas.
- Changes in conductance – conductance histogram
- measure I-V (hard) – offresonant tunneling
- Also stretch the molecule (close the loop)
- Measure STM-BJ histogram: less pronounced multiple molecules, multiple directions etc.
- imaging with C60, push C60 away with another







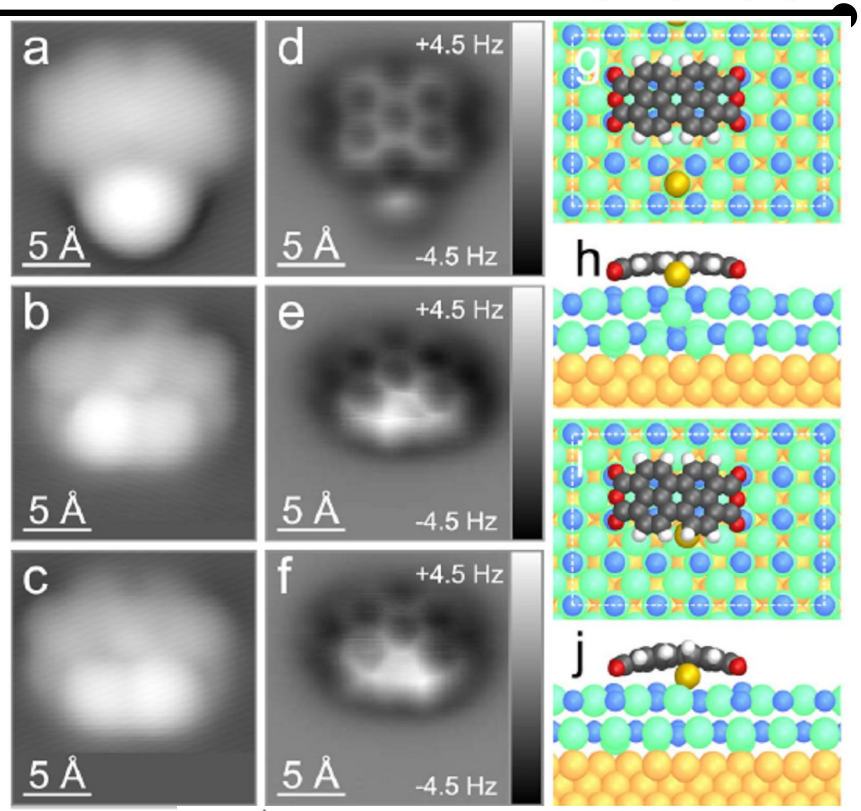
E. Leary et al., Nano Lett. ***11****, 2236 (2011)*

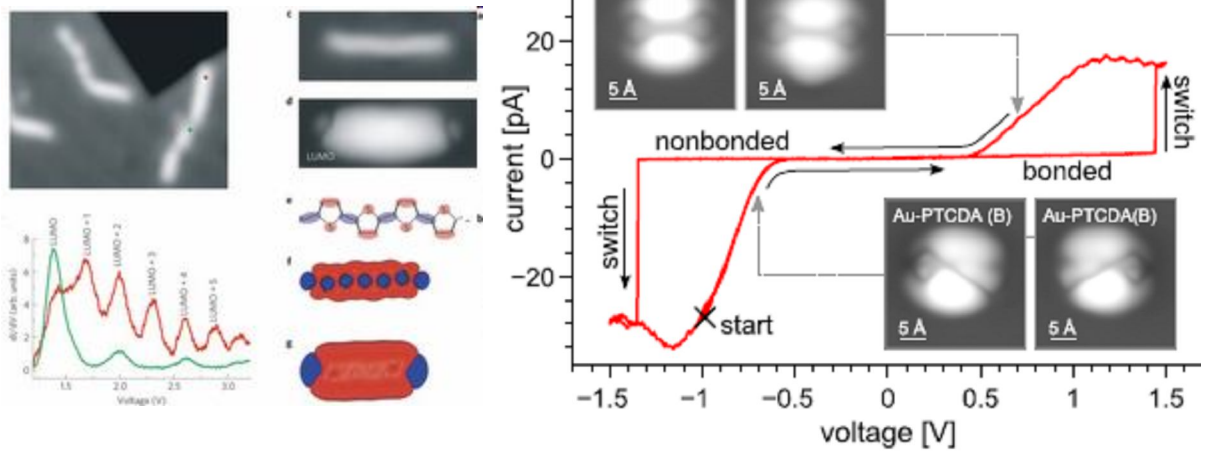
Jasha Repp

STM on ultrathin insulating substrates

E.g.: molecule (PTCDA) + gold adatom
- switching between bonded and nonbonded states
- orbital imaging
- combined with atomic precision AFM (qplus tuning fork), UHV, functionalized AFM tip (CO)

- more articles swicthing molecule (study different charge states, and difference STM images)
make wires from molecules, study standing waves and vibration modes, and the coupling of electronic and phonon modes (Nature Physics 6, 975–979 (2010))





Fabian Mohn, et al., PRL 105, 266102 (2010)

Conclusion?

-Kell vegyészkapcsolat

Alacsony hőmérséklet

- Kis molekulák log tartományban/érdekes elektródákkal
- Vagy beeresztés, esetleg kifűtés
- Nagy molekulákkal kell gate +BJ vagy más elektróda egyébként már nem érdekes
- STM – BJ rendszert arannyal tudnánk használni
- Grafén elektródák – (idővel ide is kell vegyész)

Szobán:

- 1-2 fémet megnézni, esetleg folyadékban
- Molekulák rácsöppentés/cella – kell jó ötlet a molekulára/mérésre, különben érdektelen
- I-V mérés működhet
- STM-BJ rendszer

-STM manipulálás/ultravékony szigetelő film - érdekes, de nem játszik

- Kellene valami más módszer a molekuláris kontaktusok létrehozására