Quantum properties of atomic-sized conductors

Nicolás Agraït[a], Alfredo Levy Yeyati[b], Jan M. van Ruitenbeek[c,*]

N. Agraït et al. / Physics Reports 377 (2003) 81–279

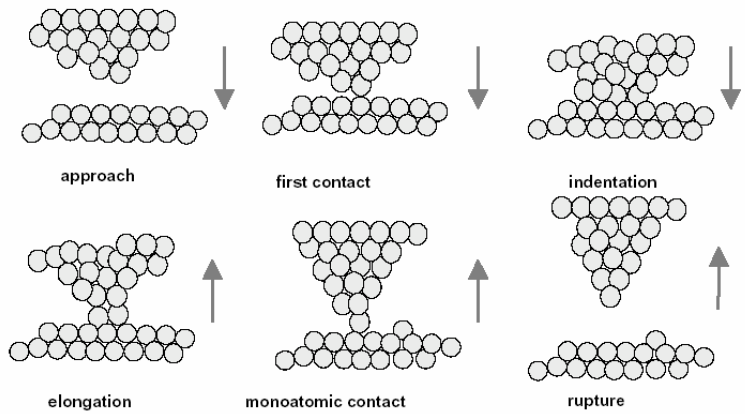
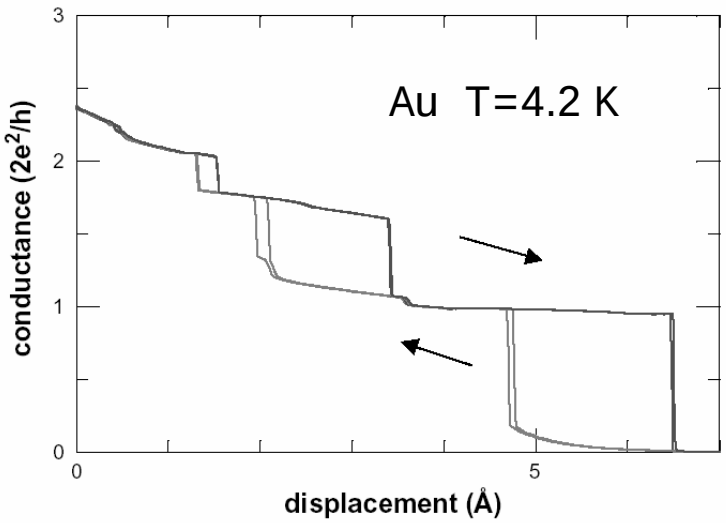


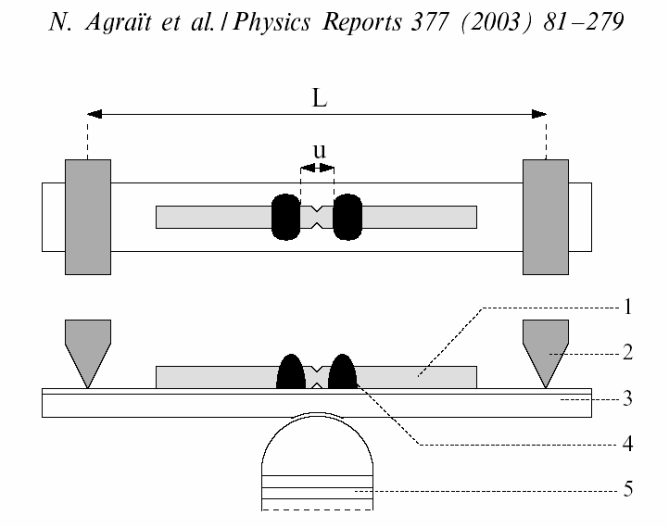
Fig. 3. Cartoon representation of contact fabrication using an STM.



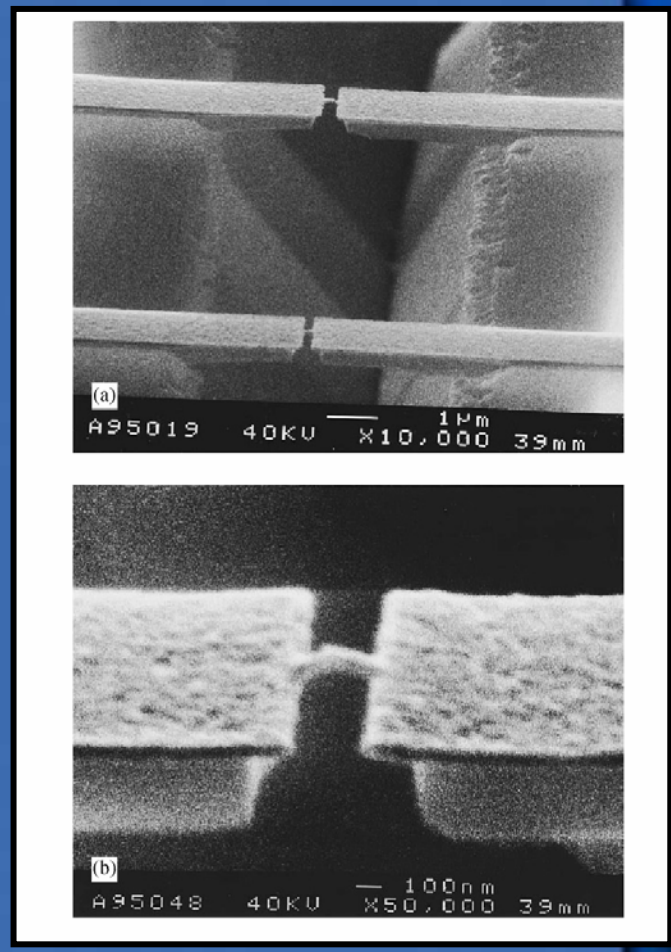
10 – 100 x
yield strength
cf. bulk material

Stable up to 2 V →
Sustain current
densities up to
2 x 10^15 A/m^2 !

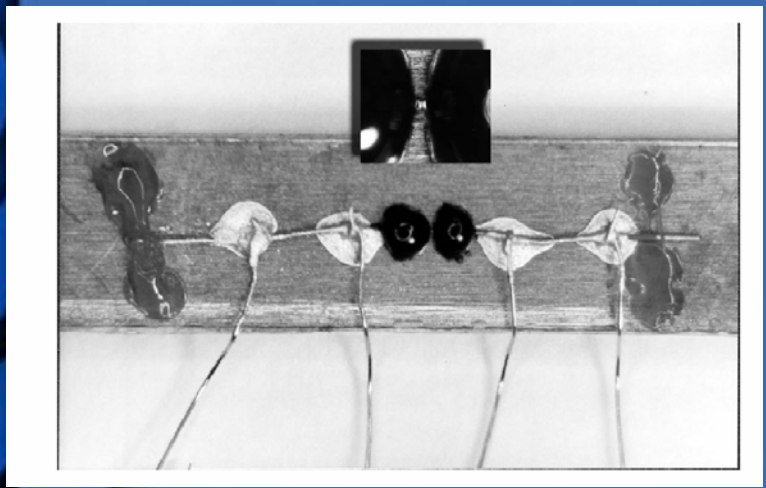
Mechanically controlled break junction (MCBJ) device



1. notched wire
2. fixed counter supports
3. bending beam
4. epoxy adhesive
5. stacked piezo element



Optical microscope image



4.5 mm

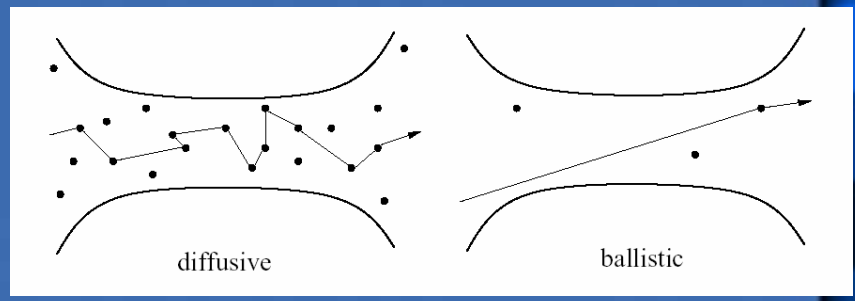
SEM image of Au/SiO2/Si microfabricated suspended bridge

Reed group Appl. Phys. Lett. 67, 1160 (95)

Do it yourself ! (Foley et al, AJP 67, 389 (99))

Ballistic contacts

Ohm's law $G = \sigma S/L$ does not hold!



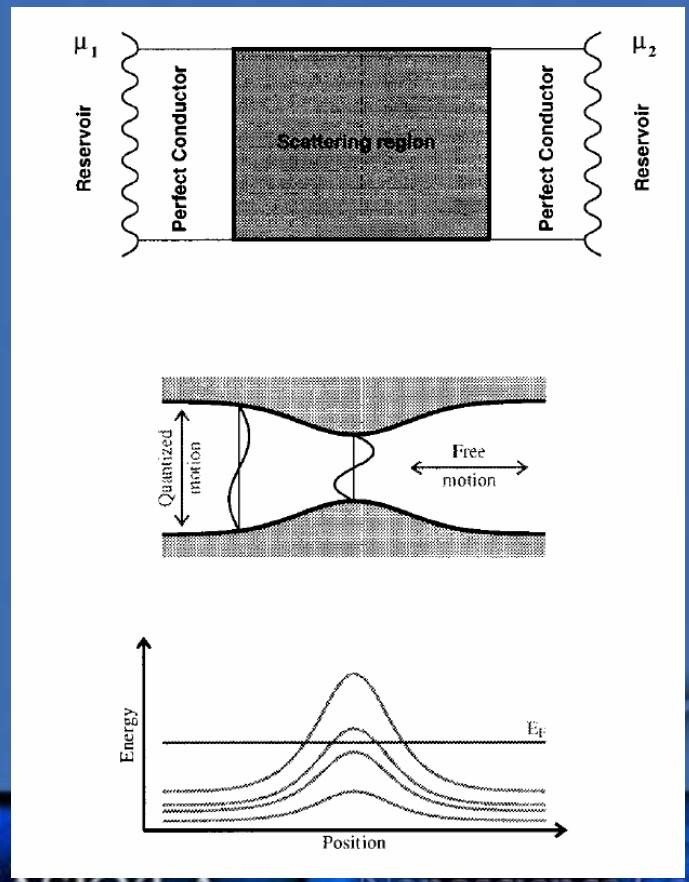
L << electron elastic mean free path
→Ballistic transport through the contact
(scattering only at boundaries)

Semiclassically (Sharvin)

$$\mathbf{j}(\mathbf{r}) = \frac{2e}{L^3} \sum_{\mathbf{k}} \mathbf{v}_{\mathbf{k}} f_{\mathbf{k}}(\mathbf{r})$$

→ $$G_S = \frac{2e^2}{h} \left(\frac{k_F a}{2} \right)^2$$

(a is the contact radius)



Conductance eigenchannels

Landauer-Büttiker

$$G = G_0 \mathrm{Tr}[\mathbf{t}^\dagger \mathbf{t}]$$

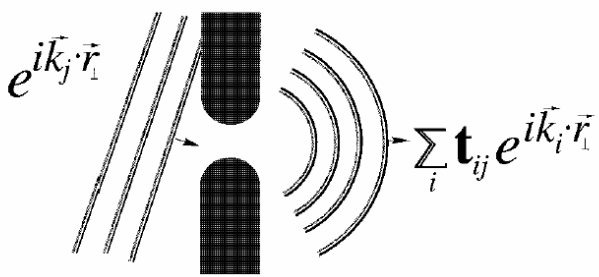
$G_0 = 2e^2/h$

$$\mathbf{U}_{\mathrm{out}}^\dagger \, \mathbf{t} \, \mathbf{U}_{\mathrm{in}} = \mathrm{diag}\{\sqrt{T_i}\}$$

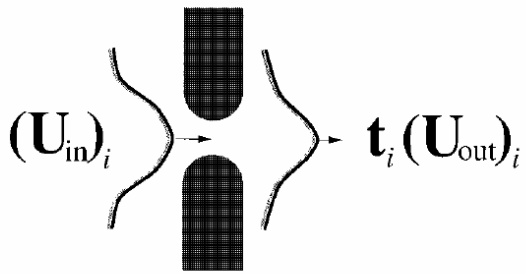
$$\mathbf{U}_{\mathrm{in}}^\dagger \, \mathbf{t}^\dagger \mathbf{t} \, \mathbf{U}_{\mathrm{in}} = \mathrm{diag}\{T_i\}$$

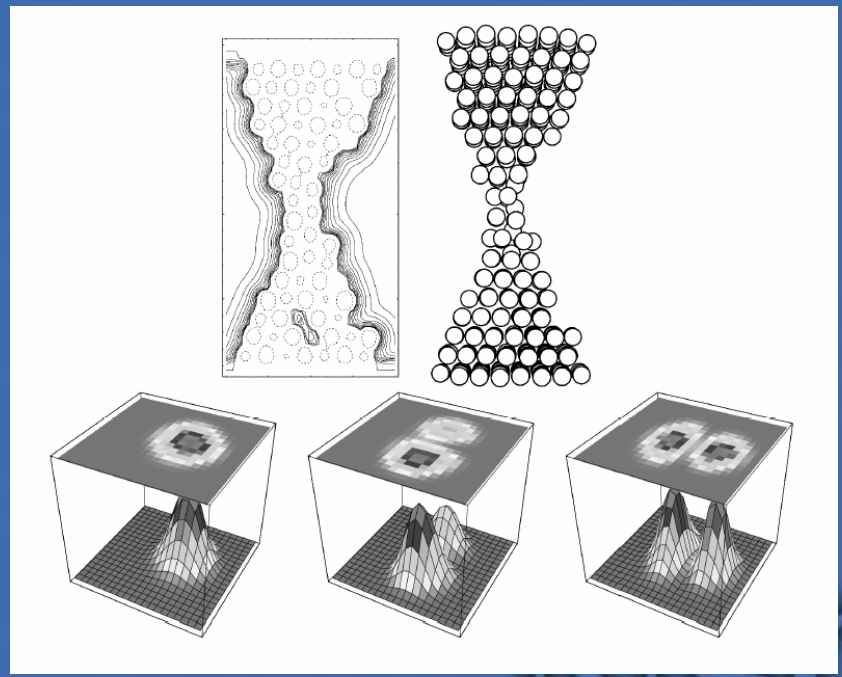
$$\mathbf{U}_{\mathrm{out}} = \mathbf{t}\mathbf{U}_{\mathrm{in}} \, \mathrm{diag}\{1/\sqrt{T_i}\}$$

Plane-wave Basis:



Eigenchannel Basis:

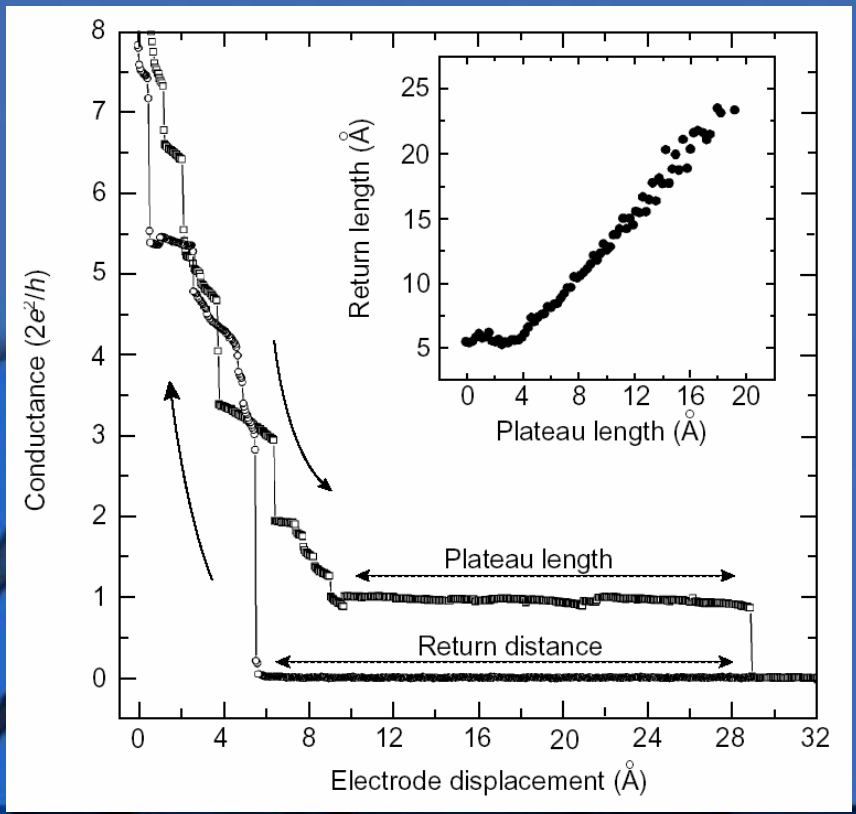




Brandbyge et al, PRB 55, 2637 (97); PRB 56, 14956 (97)

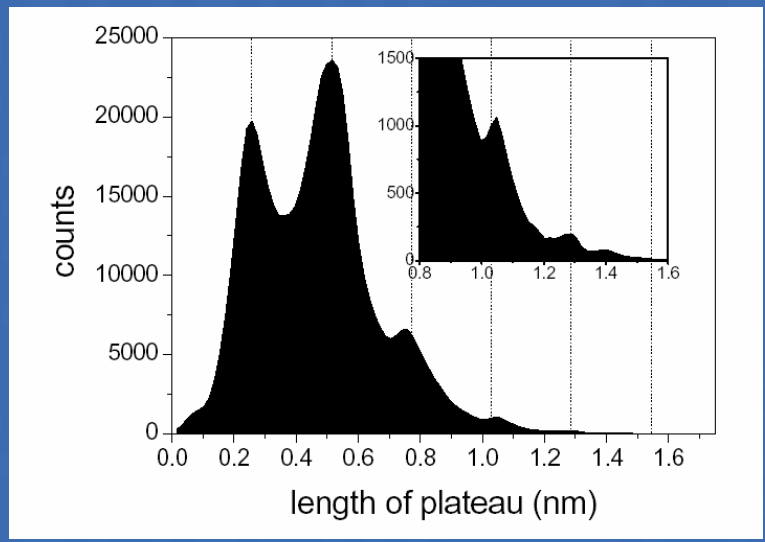
Formation and manipulation of a metallic wire of single gold atoms

A. I. Yanson*, G. Rubio Bollinger†, H. E. van den Brom*, N. Agraït† & J. M. van Ruitenbeek*



Distribution of (calibrated)
1 g0 plateau lengths
About 10 000 traces

PRB 66, 085418 (02)



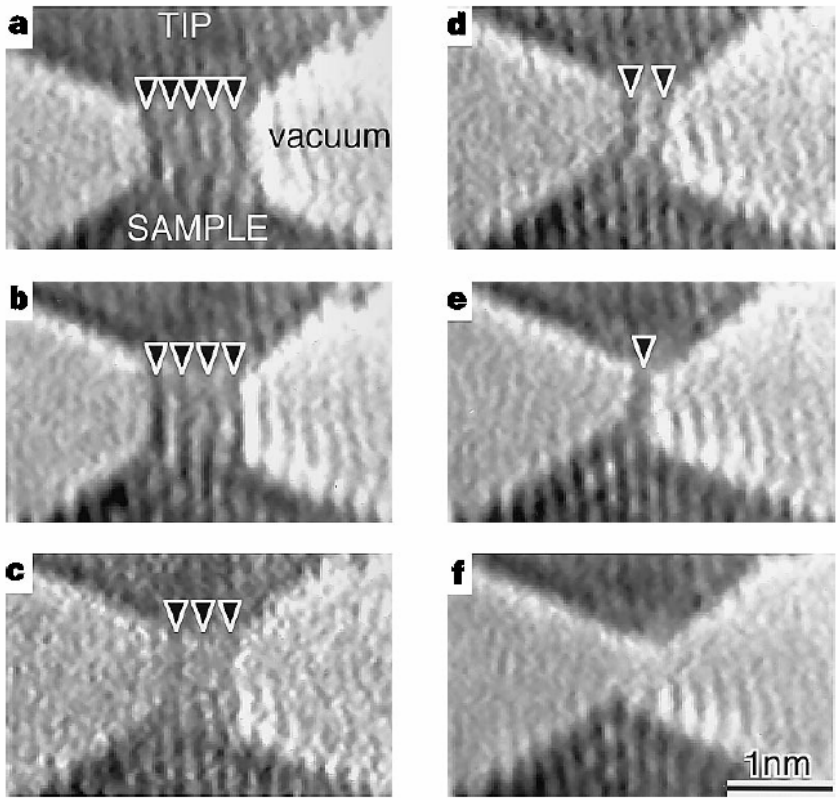
Chains of up to least 5-6 Au atoms
Au-Au distance about 2.6 A

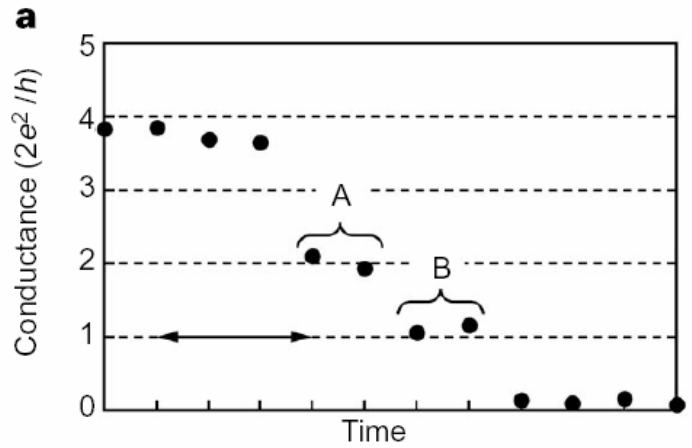
NATURE | VOL 395 | 22 OCTOBER 1998 | www.nature.com

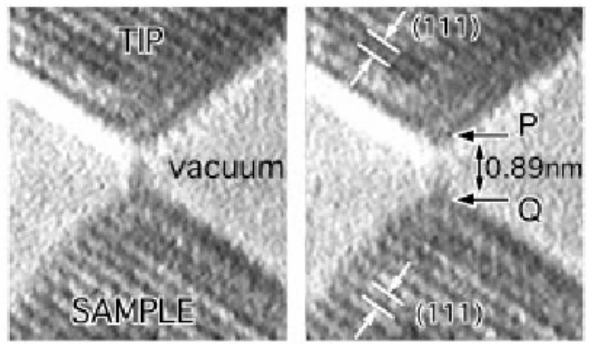
Quantized conductance through individual rows of suspended gold atoms

Hideaki Ohnishi*, Yukihito Kondo* & Kunio Takayanagi*†

STM tip in UHV with HRTEM

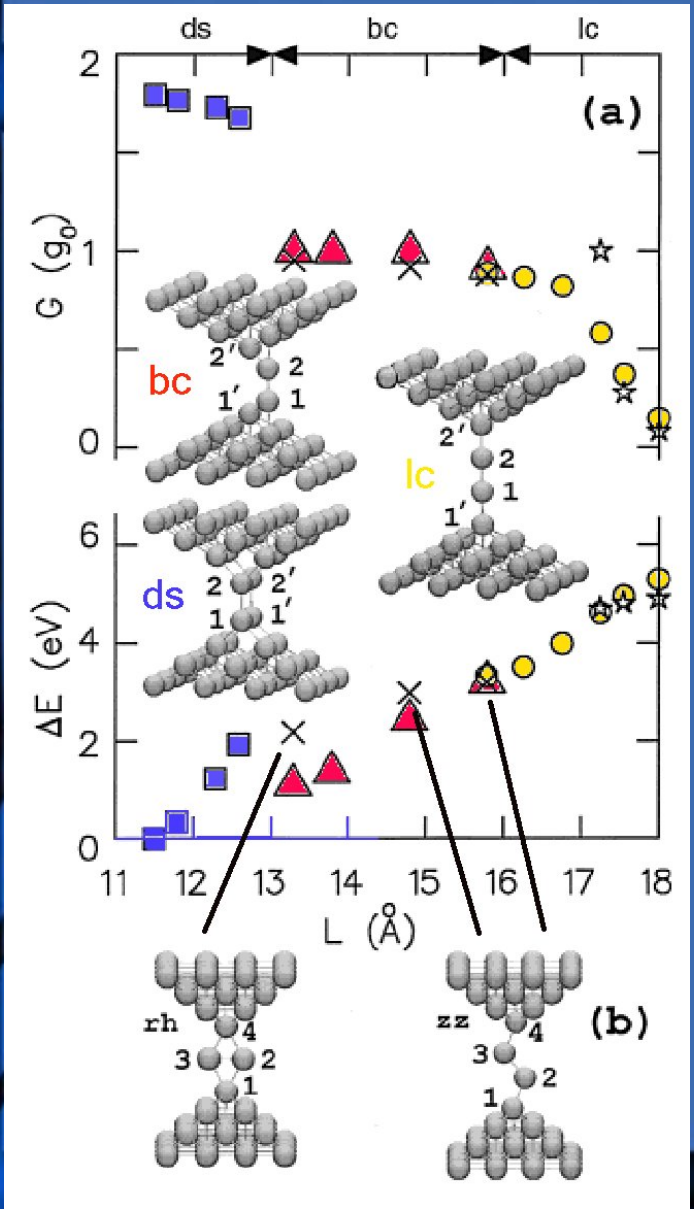






NATURE | VOL 395 | 22 OCTOBER 1998 | www.nature.com

Variety of possible pathways from double strands to rupture

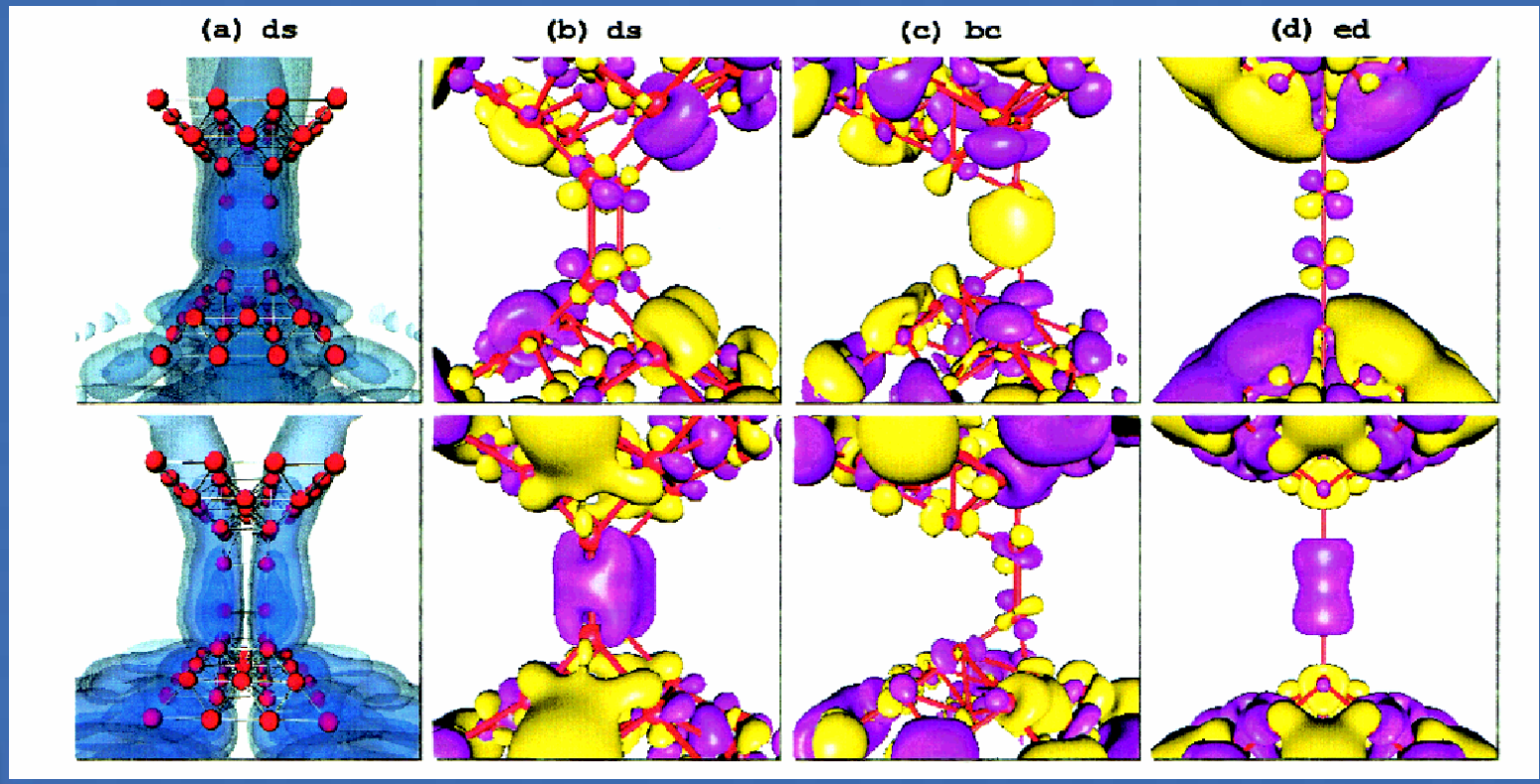


ds – double strand
bc – bent chain
rh – rhombus
zz – zigzag
lc – linear chain, dimerization in the middle or at the ends

pulling force about 4 nN for ds,
1 nN for bc and lc

Hakkinen et al, JPCB 104, 9063 (2000)

Conductance channels and orbitals



Ch1: 0.97 g0	Homo	Homo	Homo
Ch2: 0.7 g0	Homo-1	Homo-1	Homo-2

How stiff are gold chains?

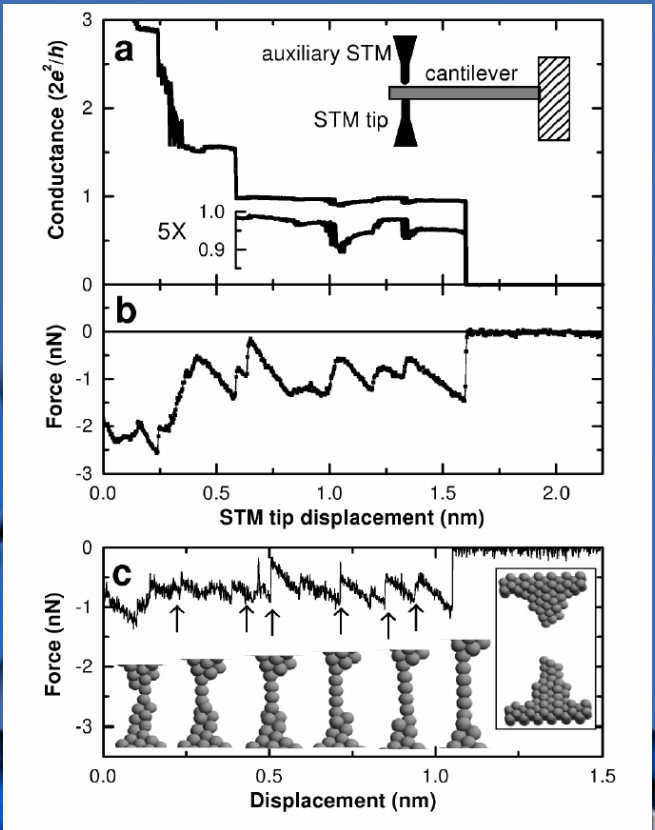
Rubio-Bollinger et al, PRL 87, 026101 (01)
(calculations Jacobsen group)

Breaking force of the (1 g_0) chain :

- 1.5 nN (STM)
- 1 nN (classical simulation)
- 1.5-1.6 nN (DFT) cf. max force per bulk bond 0.7 nN

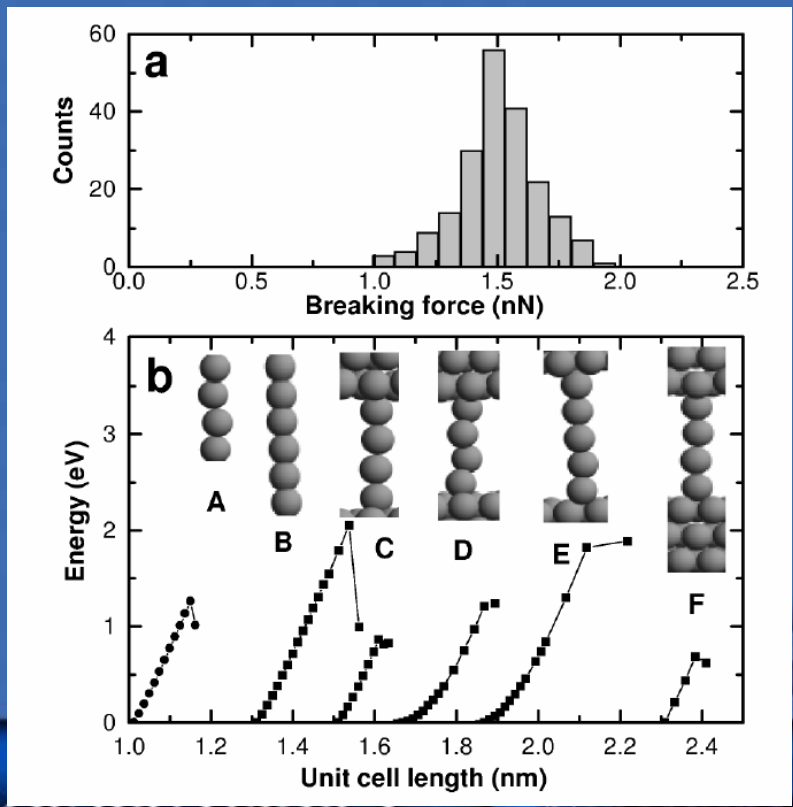
STM

EMT



STM

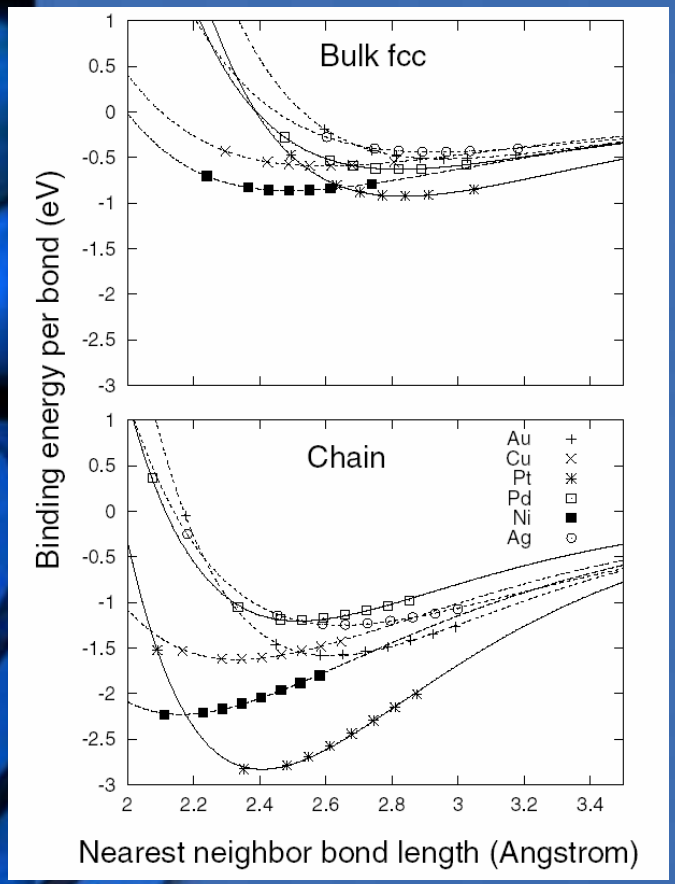
DFT



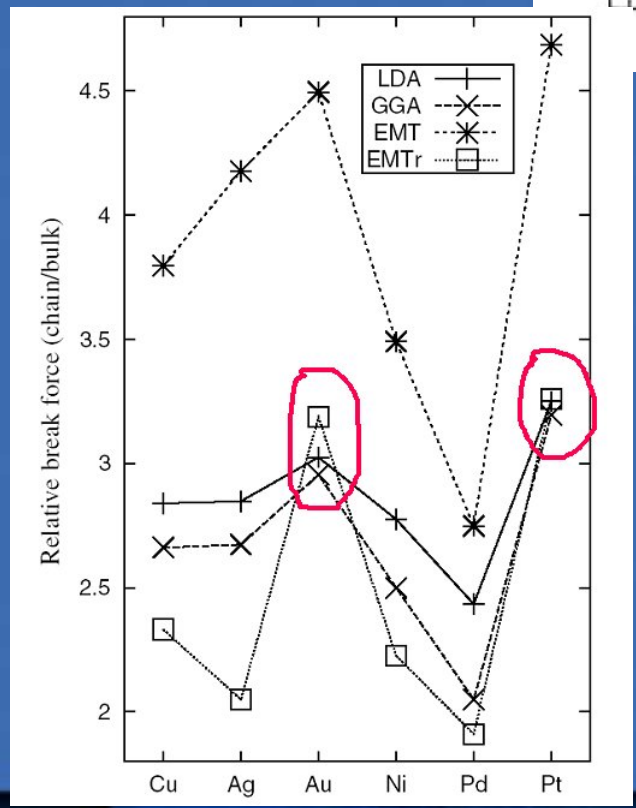
Anomalously stiff chains of Au and Pt

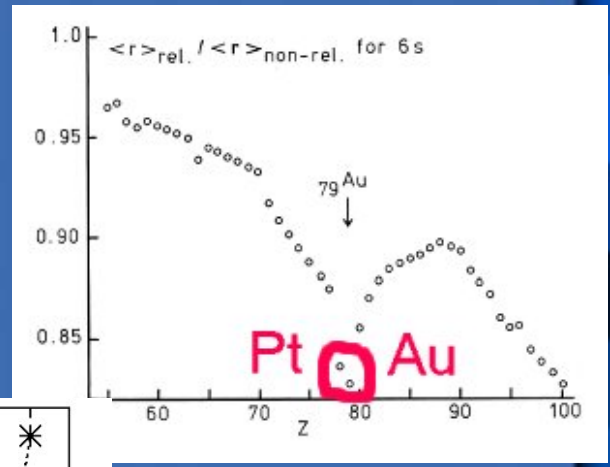
(←Relativistic bonding effects?)

(← surface reconstruction?)



Bahn and Jacobsen, PRL 87, 266101 (01)

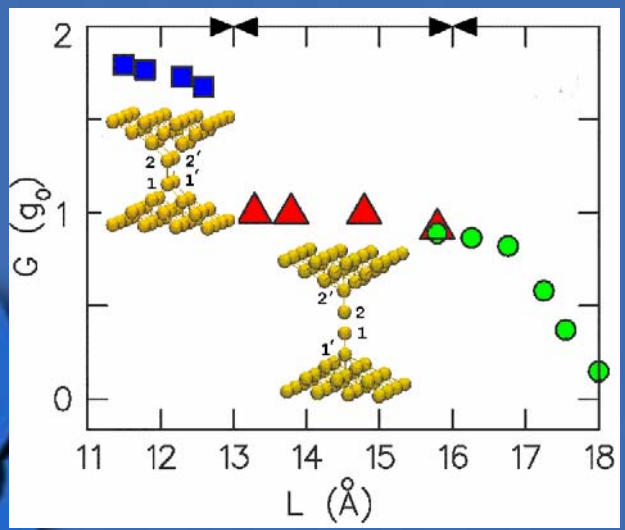


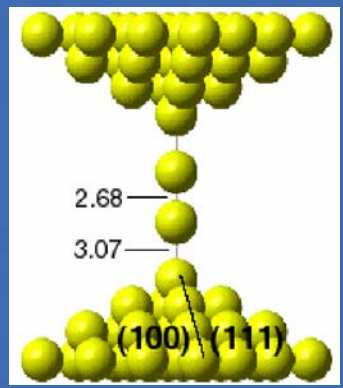


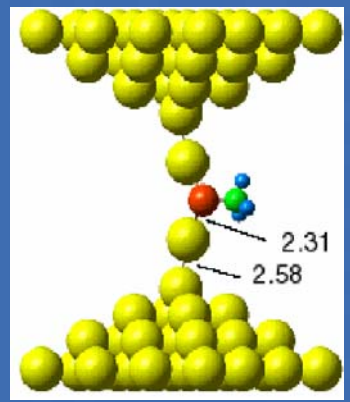
Pyykko et al

Gold nanowire chemistry

- reduced dimensions → changes in electronic structure
- modified chemical activity
- nanosensors



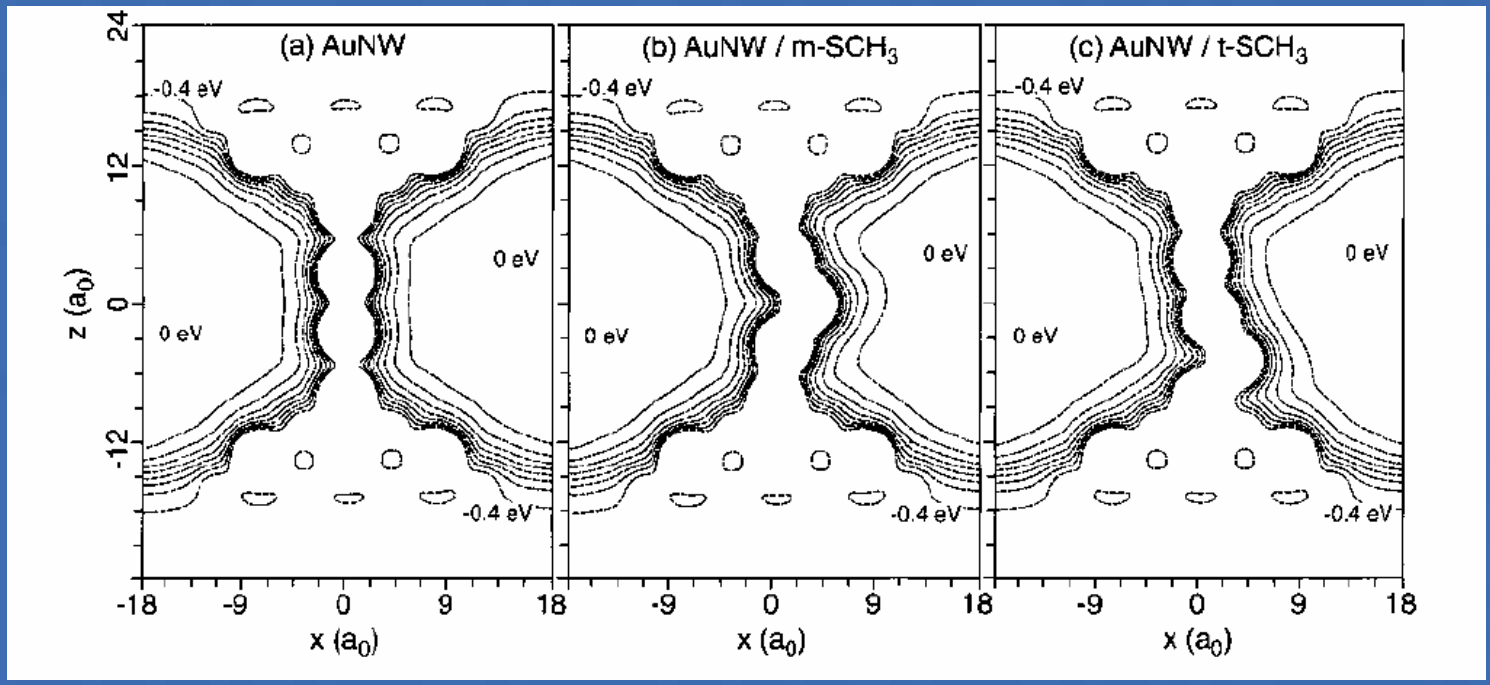


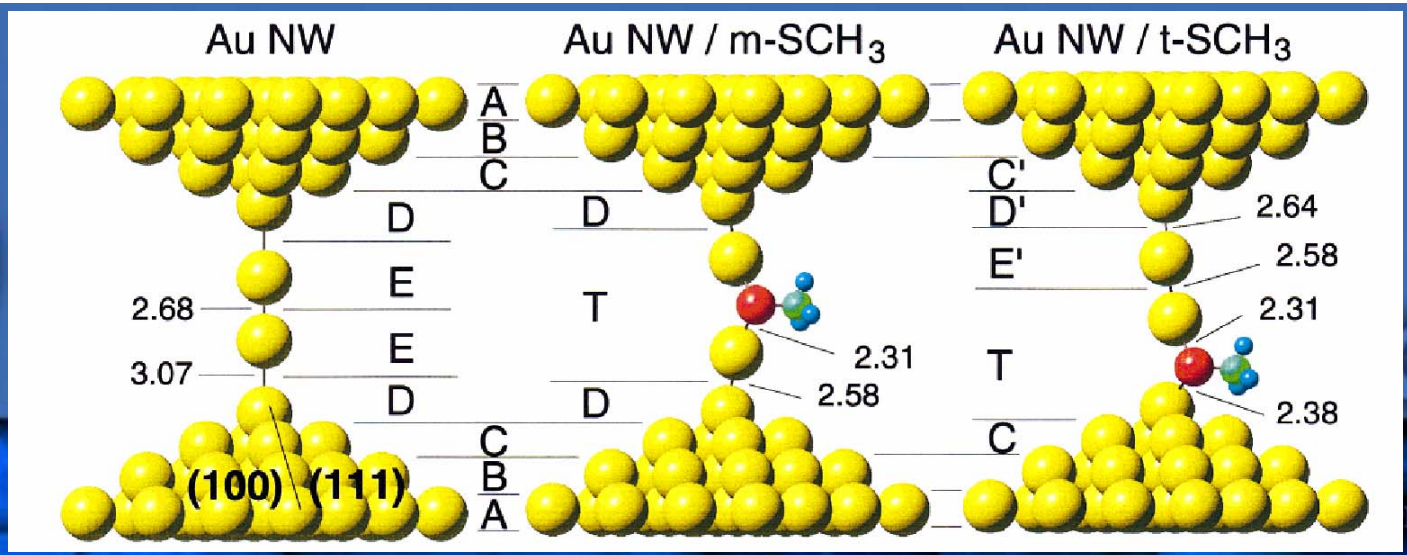


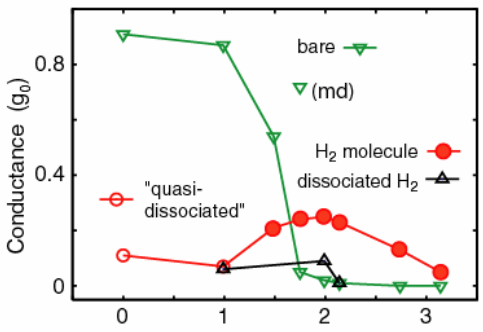
Hakkinen et al, J. Phys. Chem. B **103**, 8814 (99); **104**, 9063 (2000)

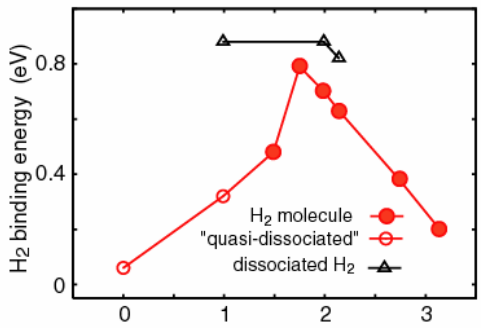
Self-consistent local potential and conductance

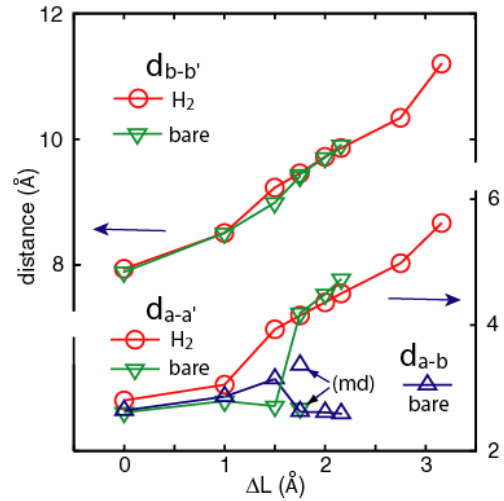
G = 0.58 g0 0.82 g0 0.88 g0











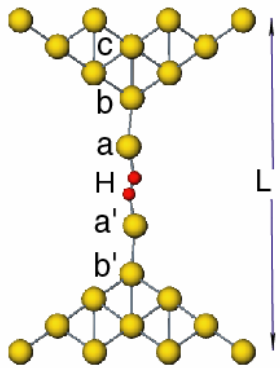


figure 4

NANO LETTERS
2004
Vol. 4, No. 10
1845−1852

Hydrogen Welding and Hydrogen Switches in a Monatomic Gold Nanowire

Robert N. Barnett, Hannu Häkkinen,† Andrew G. Scherbakov, and Uzi Landman*

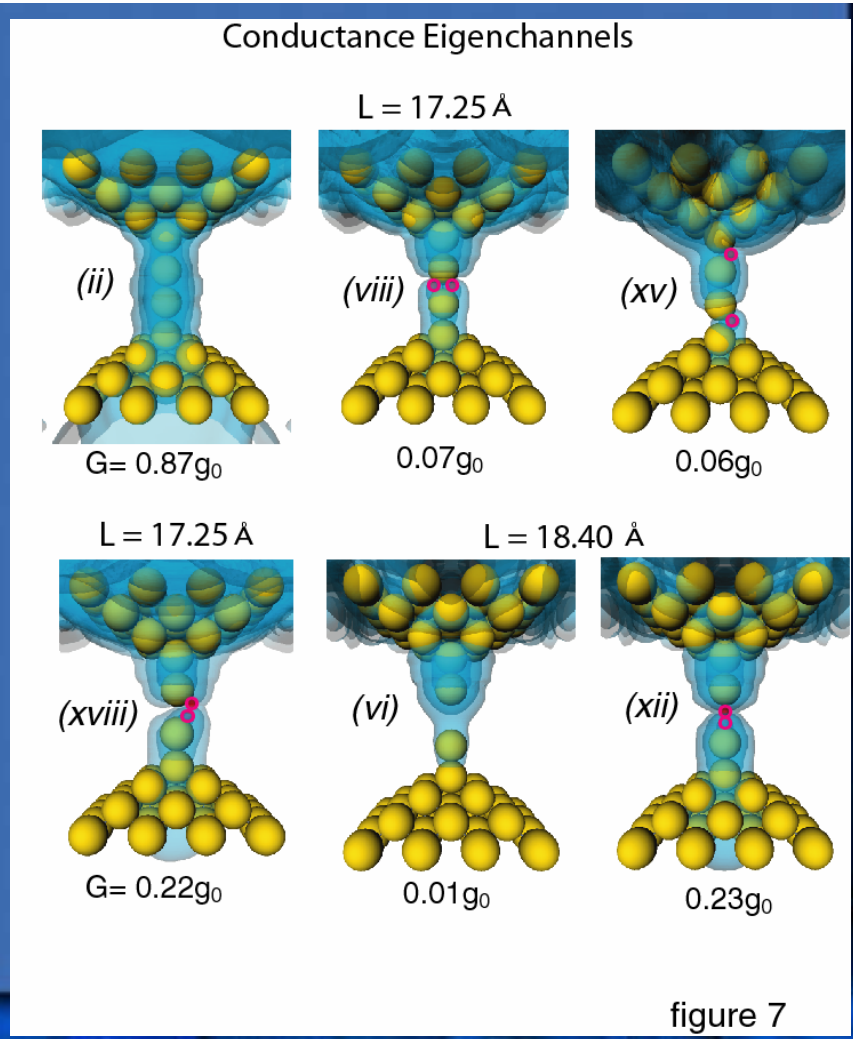
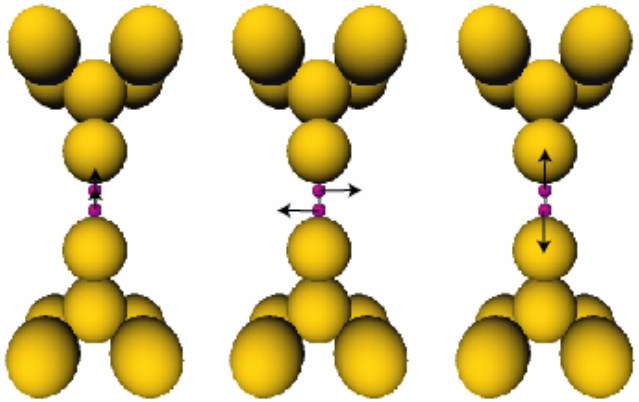


figure 7

H_2 frequencies

L = 18.40 (xii)

ω_1 = 130 meV
ω_2 = 58 meV
ω_3 = 308 meV



ω_1 "shuttle" ω_2 "wobble" ω_3 "stretch"

L = 19.00 (xiii)

ω_1 = 64 meV
ω_2 = 71 meV
ω_3 = 292 meV

(H_2 stretch 537 meV)

L = 17.25 (viii)

ω_1 = 148 meV
ω_2 = 104 meV
ω_3 = 205 meV

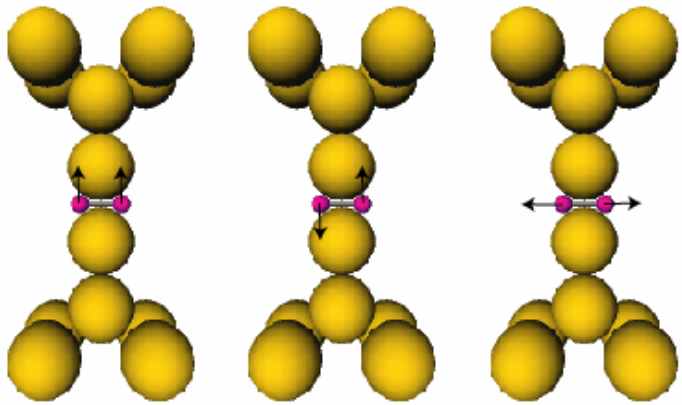
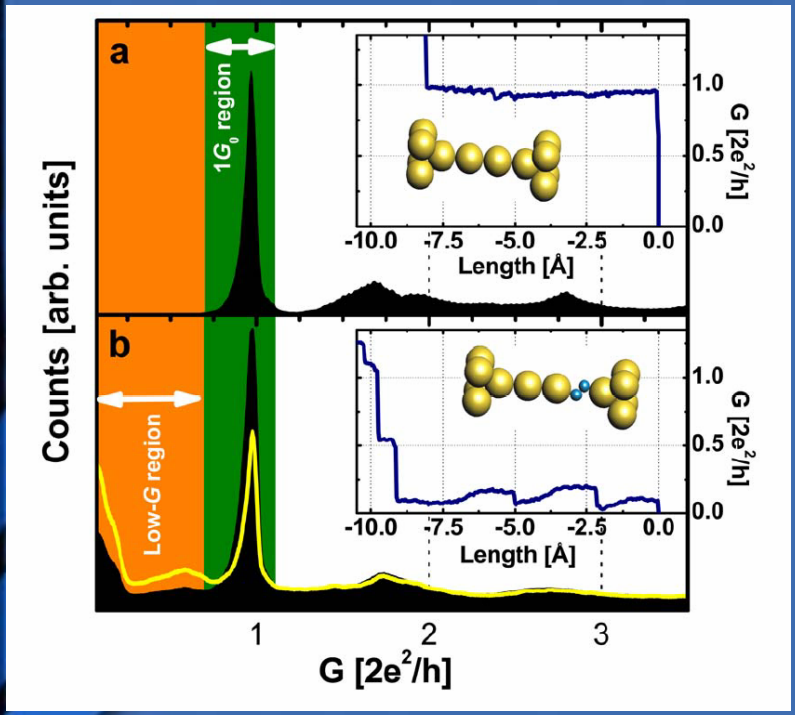


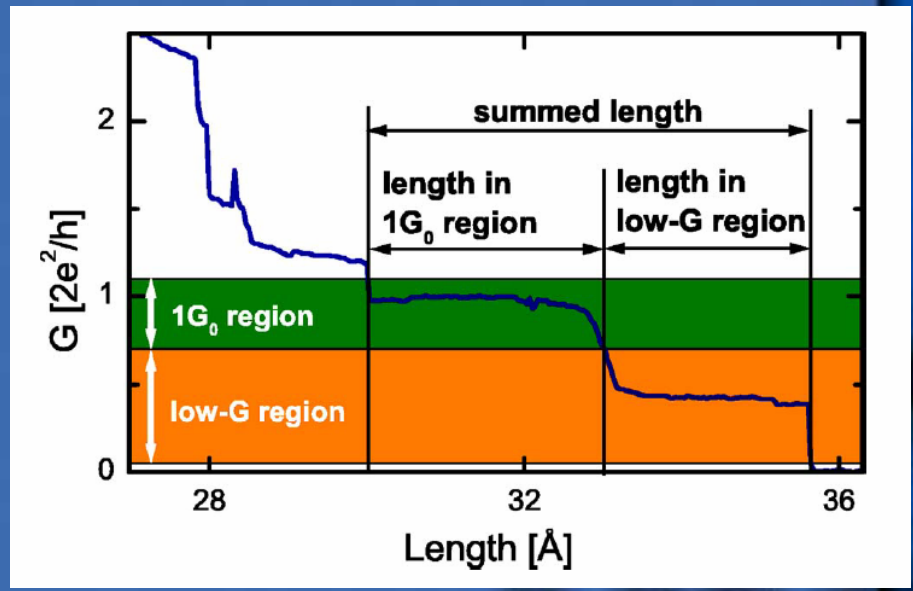
figure 8

PHYSICAL REVIEW B **73**, 075405 (2006)

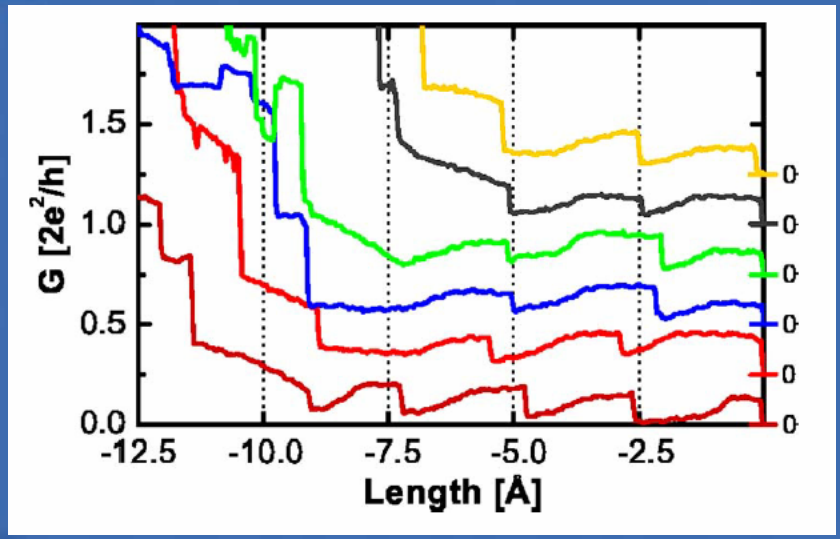
Pulling gold nanowires with a hydrogen clamp: Strong interactions of hydrogen molecules with gold nanojunctions

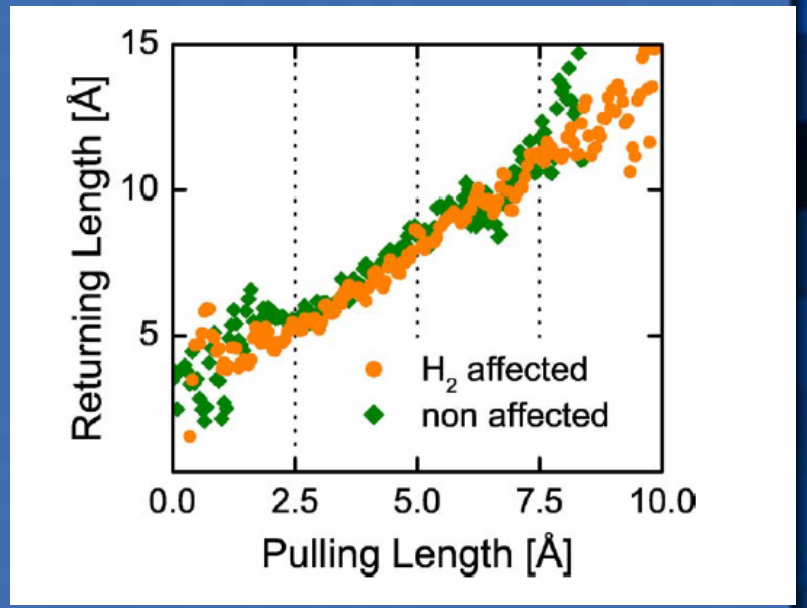
Sz. Csonka, A. Halbritter, and G. Mihály
Electron Transport Research Group of the Hungarian Academy of Sciences and Department of Physics, Budapest University of Technology and Economics, 1111 Budapest, Hungary
(Received 20 October 2005; revised manuscript received 29 November 2005; published 2 February 2006)



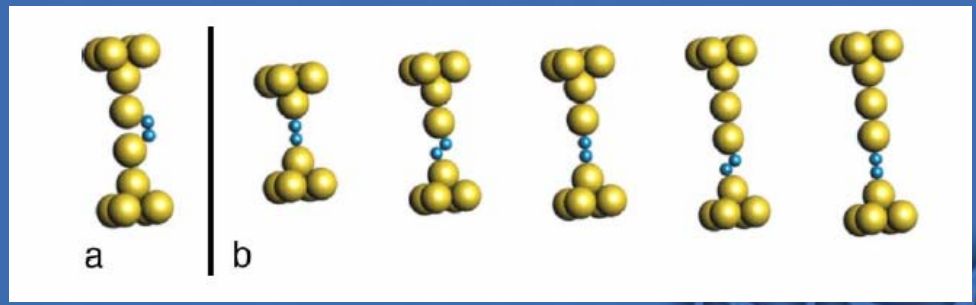


‘hydrogen-affected traces’





Interpretation!



Summary

- Au nanowires and quantum point contacts offer many possibilities to study quantum phenomena up to room-T
- stiff atomic chains with near-perfect conductance of 1 unit
- structure determination: interplay between theory & exp
- contact region (<100 atoms) manageable via DFT calculations
- tendency of ~ 1nm gold structures to prefer low-D & open structures partially due to relativistic bonding effects
- surprising chemistry by Au nanowires
- "sensor function" : changes in conductance upon adsorption