Quantum transport through single alkanedithiol molecular junctions

Research Center for Applied Sciences, Academia Sinica

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September 11, 2009 The 4th Workshop on Quantum Science and Technology

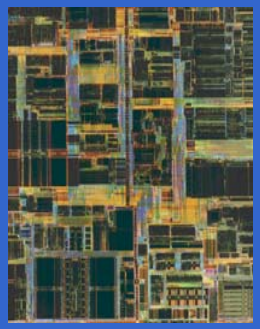
Outline:

1. Introduction
2. Comparison with experiments
   - A self-assembly monolayer (SAM)
   - A single molecule: High and low conductance
3. Summary

Acknowledgements:

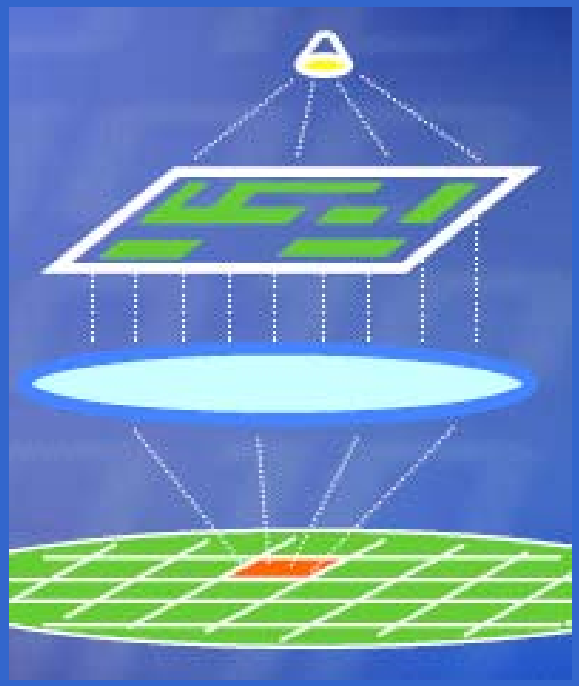
Dr. Arijit Sen

Introduction:



Transistors in Integrated Circuits

45 nm now



What's the problem?

Physical limit:
Diffraction of light.

Economical limitation:
Too expensive.

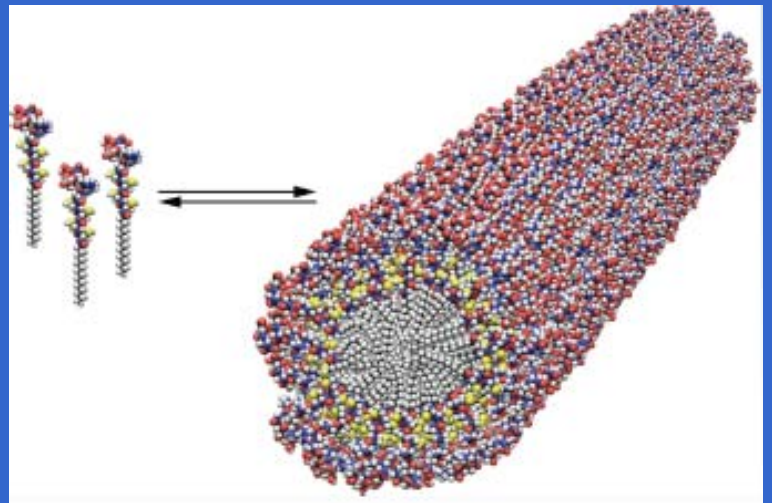
Molecular electronics: A solution

The main idea: use molecules to create analogues of today's IC chips.

Because molecules are small and can form structures by self-assembly.

Aviram & Ratner, (1974).

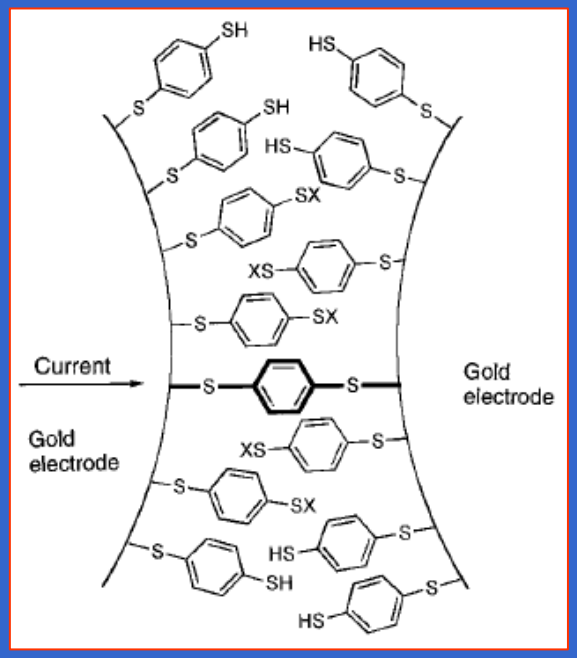
For example ..



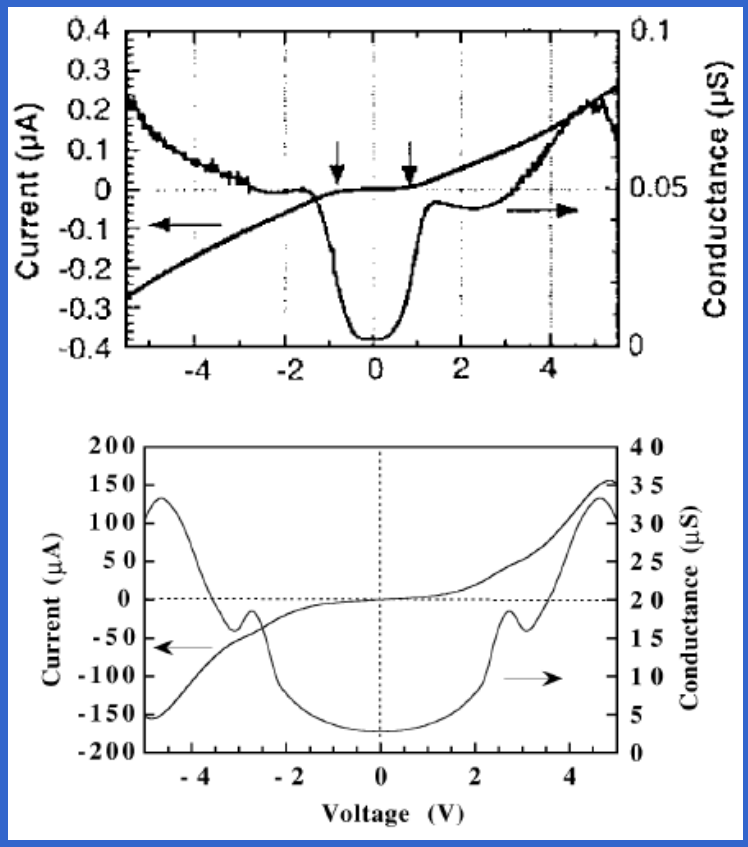
self-assembled
bioactive nanofiber

Science, 294, 1684 (2001)

Previous measurement and modeling:



Science **278**, 252 (1997)

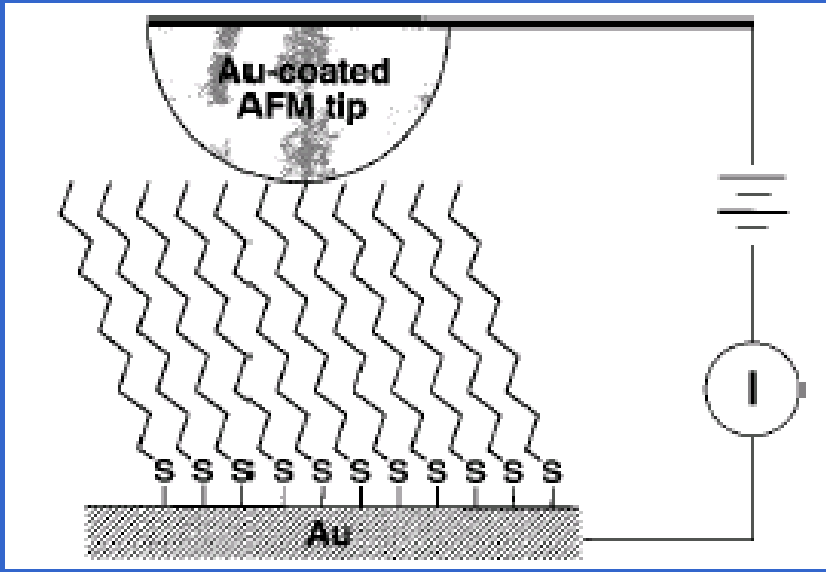


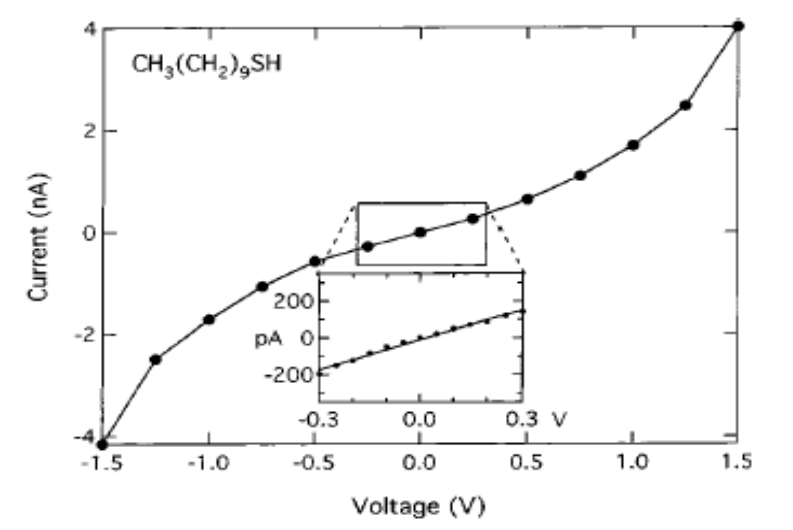
PRL **84**, 979 (2000)

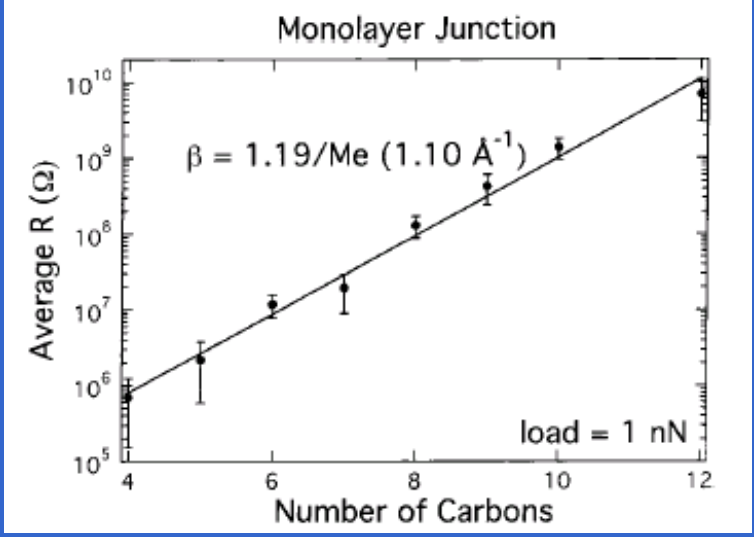
500 times of difference!

A SAM measurement: Alkanethiol molecular wires

Wold and Frisbie, JACS 123, 5549 (2001)



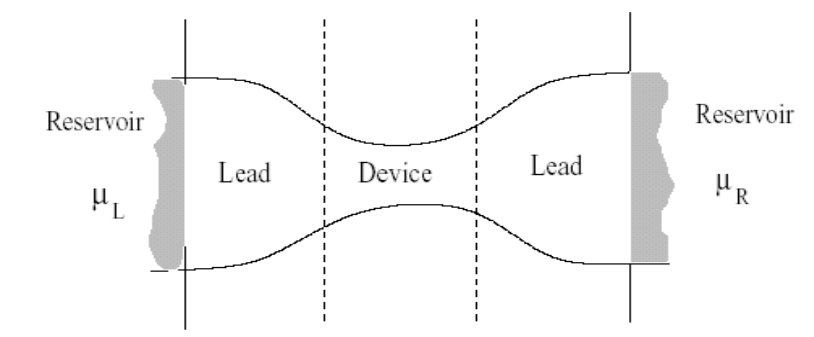




Rather similar results from other groups: M. Reed et al (2003); Lindsay et al, Nanotechnology, 13, 5 (2002).

Our method:

How to calculate current?



Landauer formula:

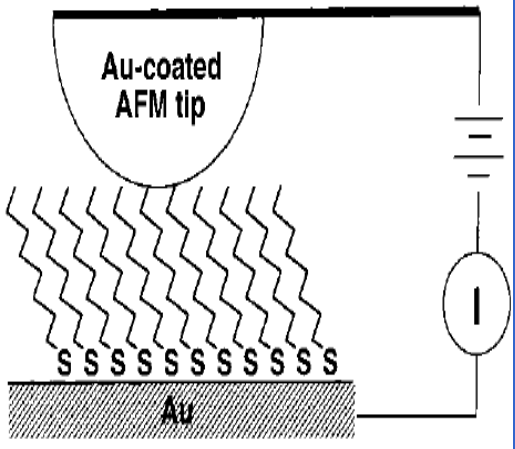
$$I(V_b) = \frac{2e^2}{h} \int_{-\infty}^{+\infty} T(E, V_b)\left(f_l - f_r\right) dE$$

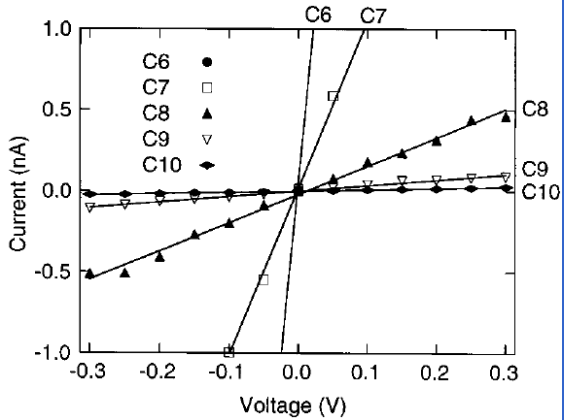
DFT plus non-equilibrium Green's functions:

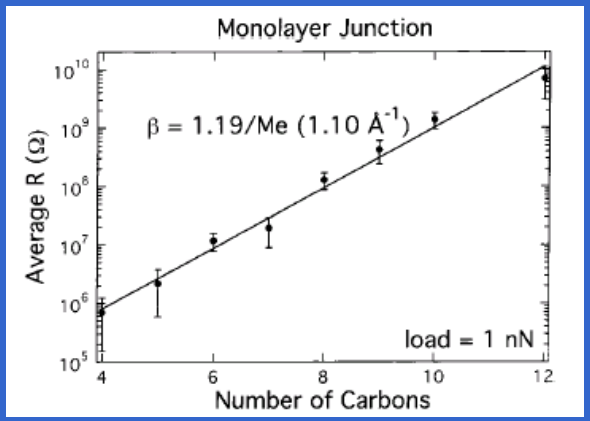
Taylor, Guo, Wang, PRB 63, 245407(2001)-----McGill-Device-CALculator (McDCAL); Brandbyge, et al, PRB 65, 165401(2002)---Transiesta.

Comparison with experiments

Experiment



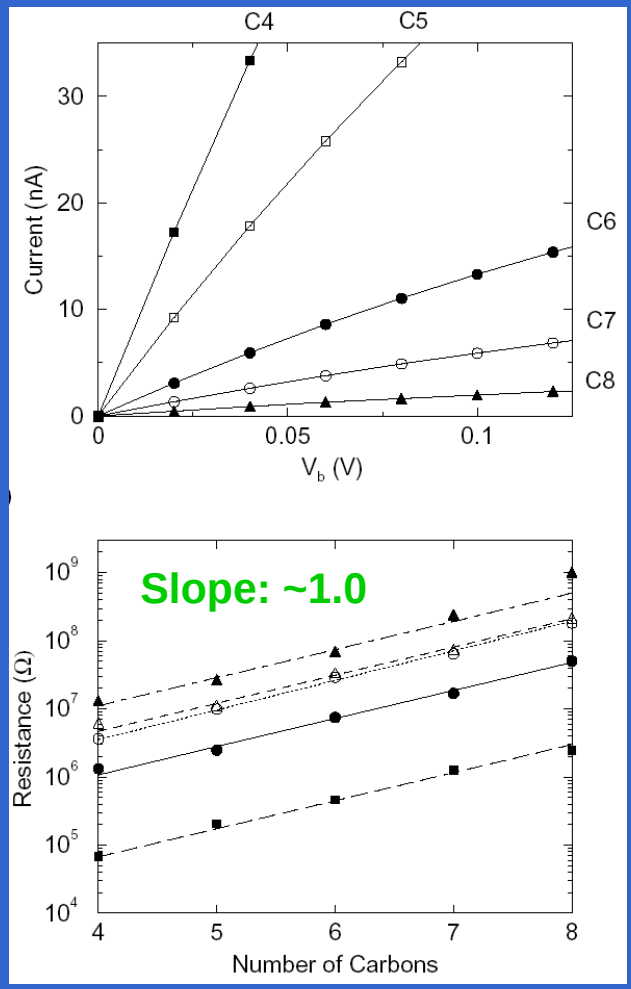




$$R_n = R_o \exp(\beta n)$$

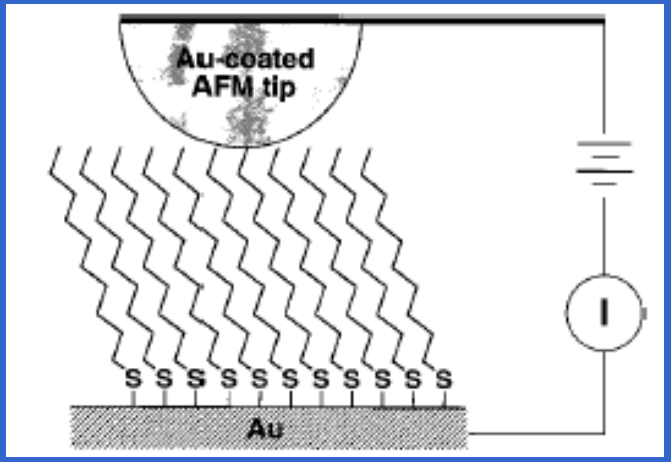
JACS 123, 5549 (2001)

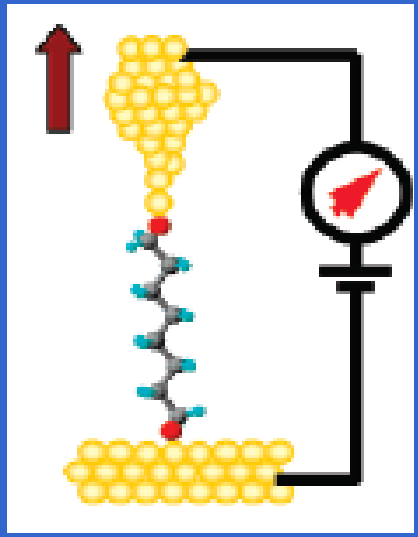
Our modeling



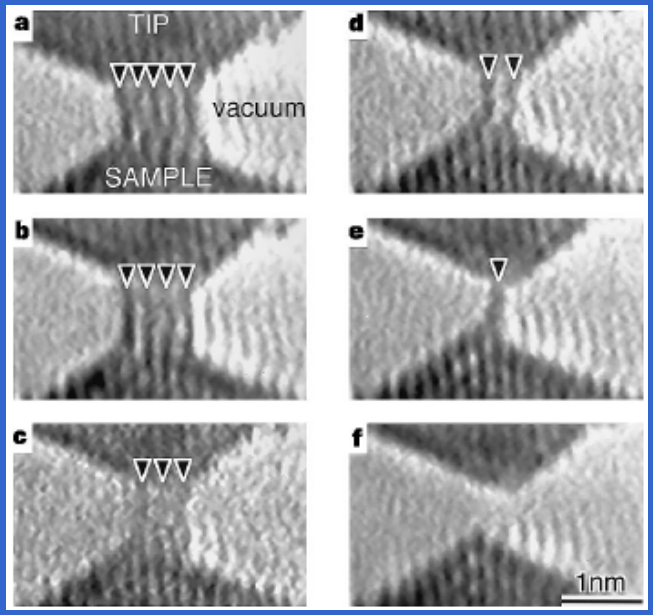
Nano Lett. 3, 1521 (2003)

What is the single-molecule conductance?

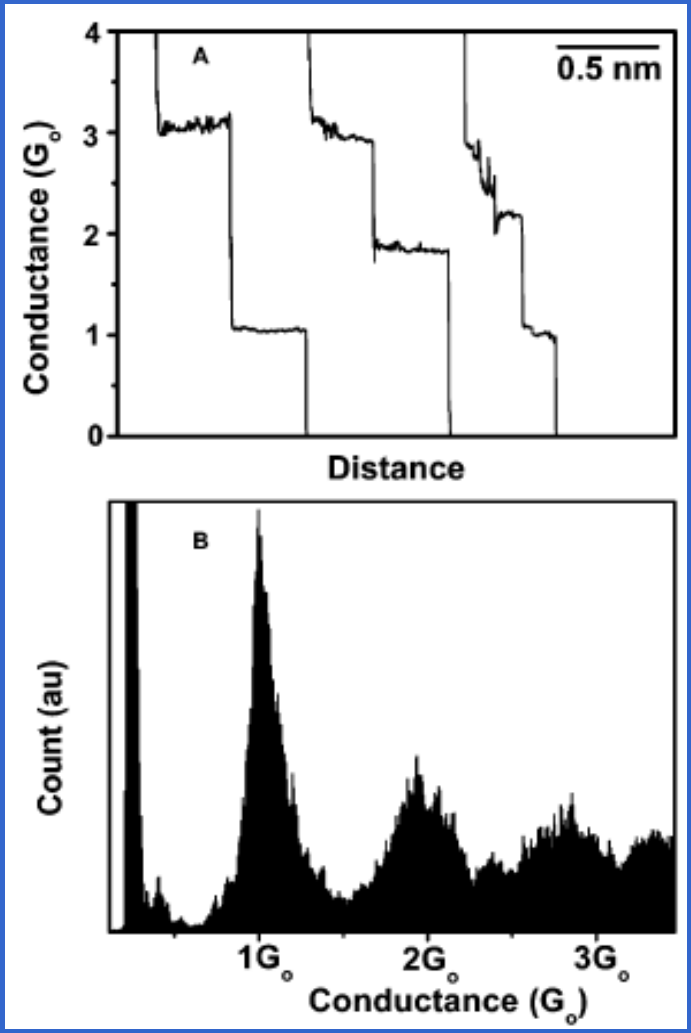




Conductance of a Au nanowire:

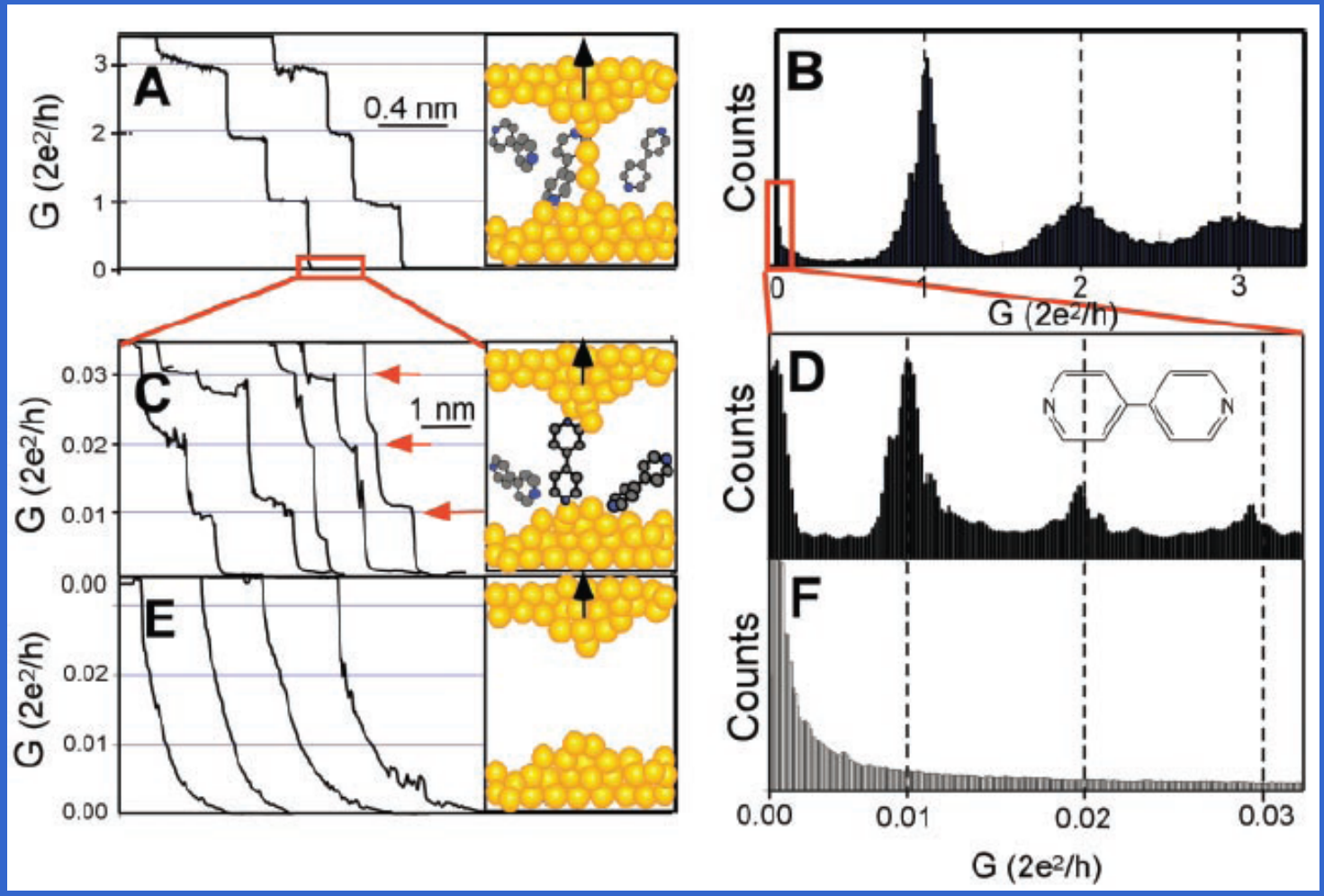


Nature 395, 780 (1998)



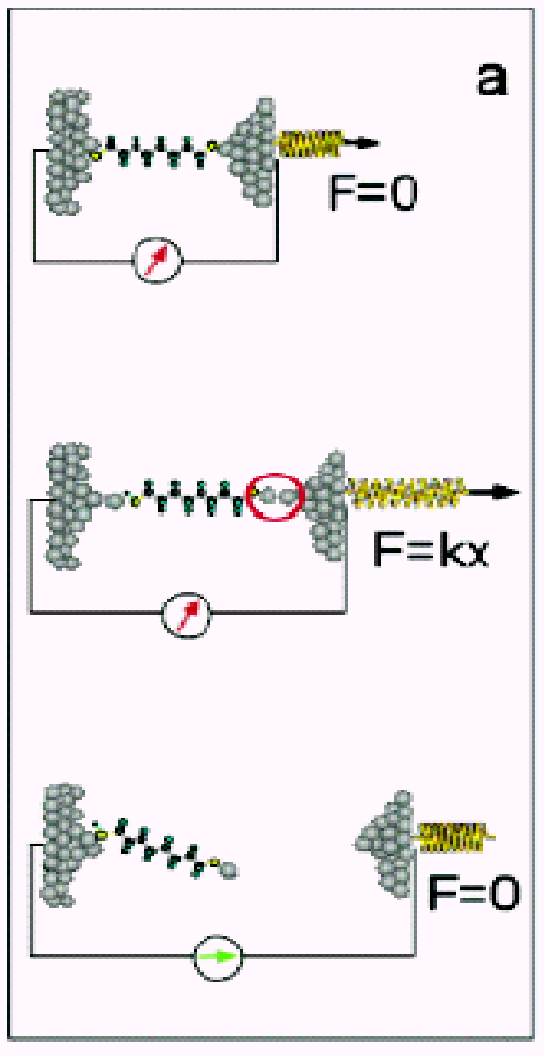
Nano Lett. 6, 2362 (2006)

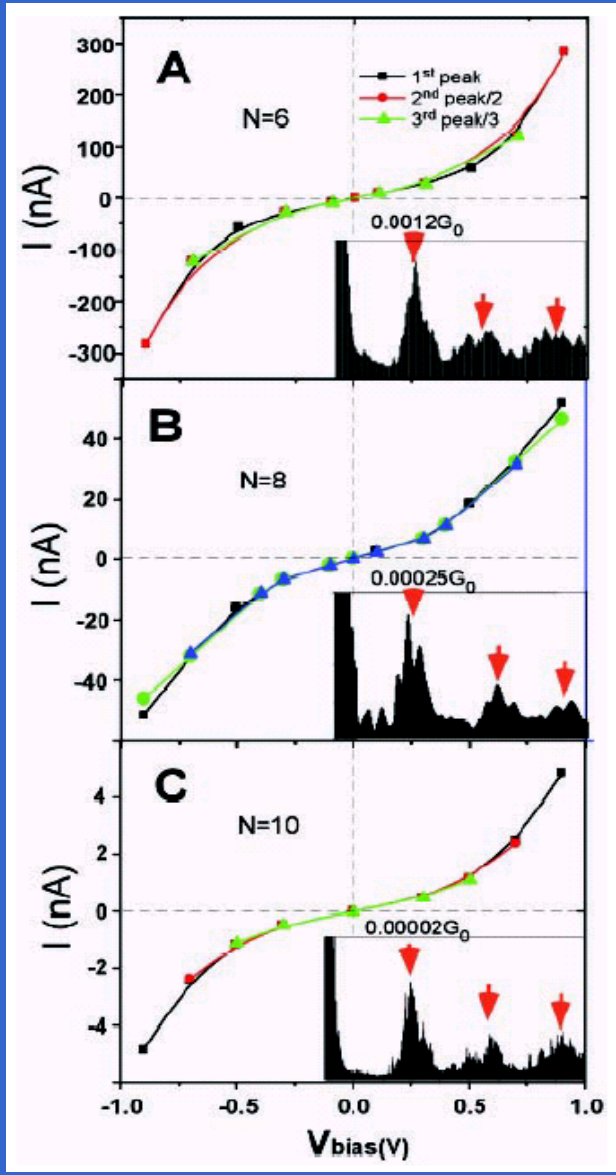
Conductance of a single molecule



J. Tao et al, Science (2003)

Measurement on single alkanedithiol molecules





$$R_n = R_o \exp(\beta n)$$

$$\beta = 1.05$$

J. Tao et al, JACS (2003); Science (2003)

Previous modeling:

PRL 95, 156803 (2005) PHYSICAL REVIEW LETTERS week ending 7 OCTOBER 2005

Conductance of an Ensemble of Molecular Wires: A Statistical Analysis

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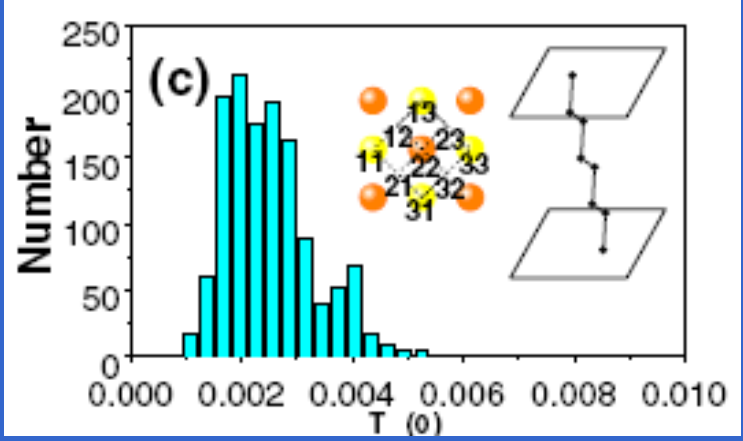
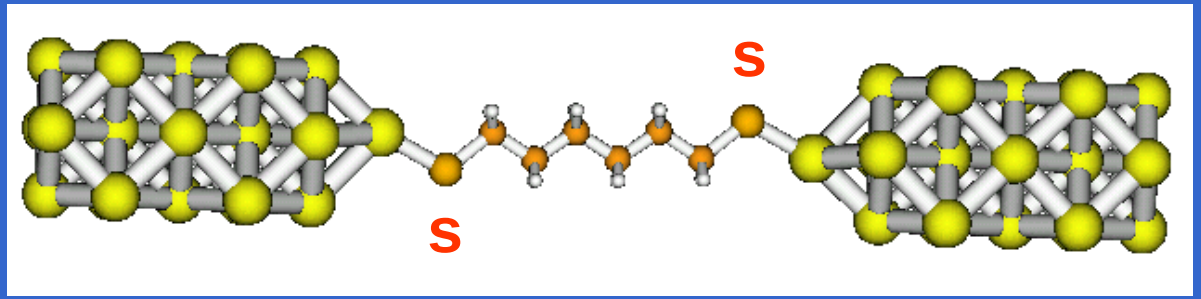
(Received 21 April 2005; published 3 October 2005)



	Calculation	Experiment
N = 6	G = 0.0025	0.0012

Unit: G_0

Our model:



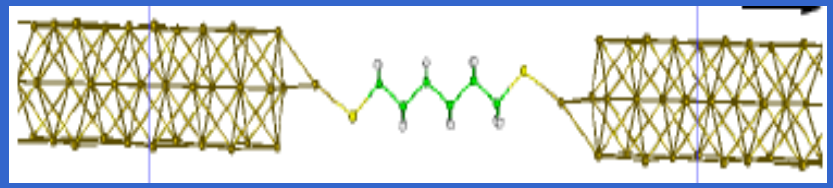
		Calculation	Experiment
N = 6	G =	0.0010	0.0012
N = 8	G =	0.000 13	0.000 25
N = 10	G =	0.000 02	0.000 02

Unit: G_0

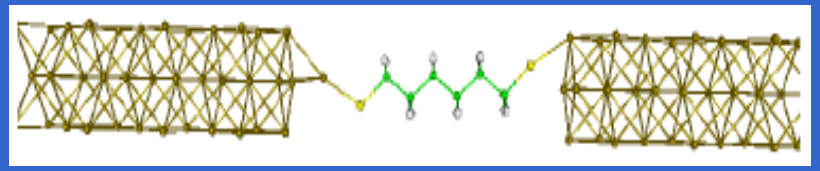
Kaun & Seideman, Phys. Rev. B 77, 033414 (2008)

Contact effect (N=6):

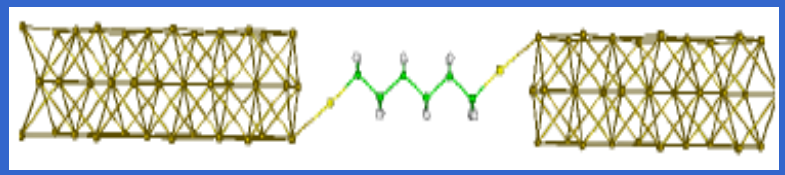
a

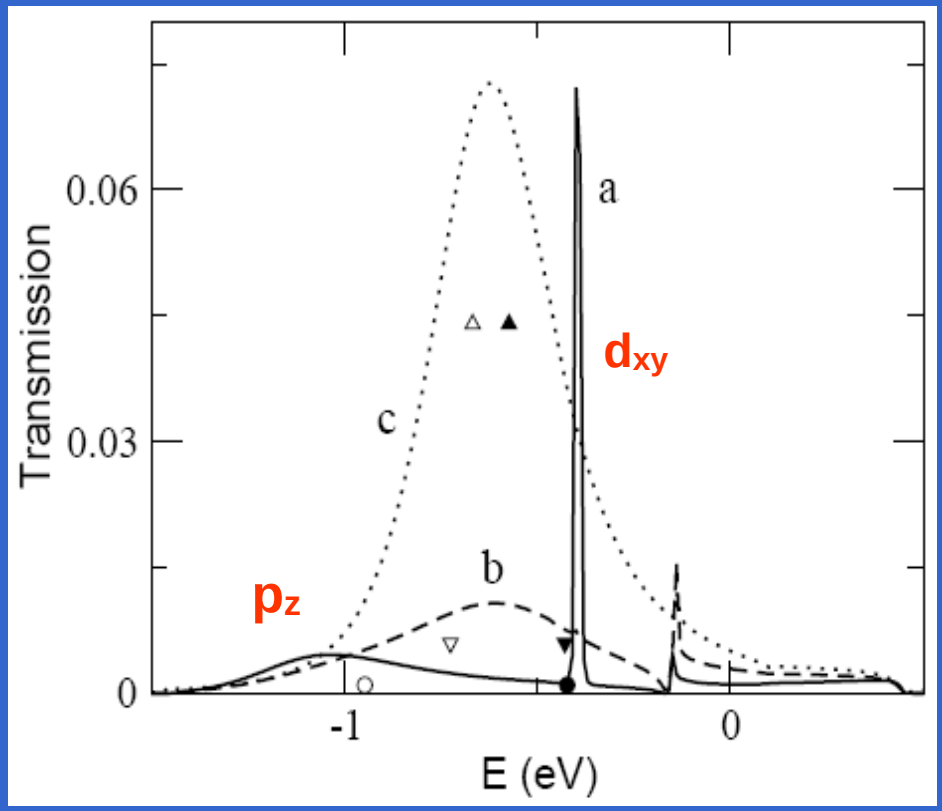


b



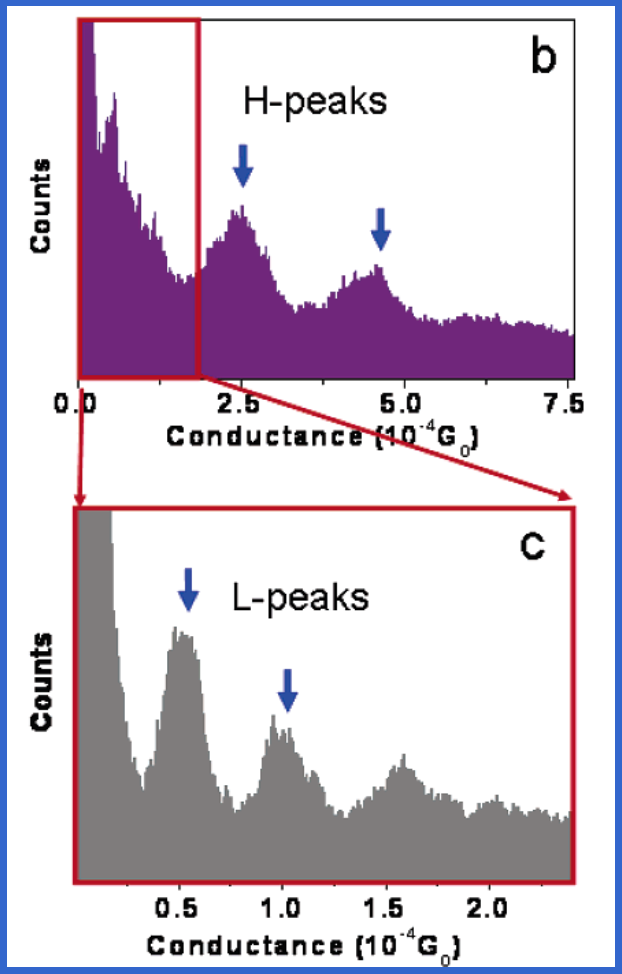
c

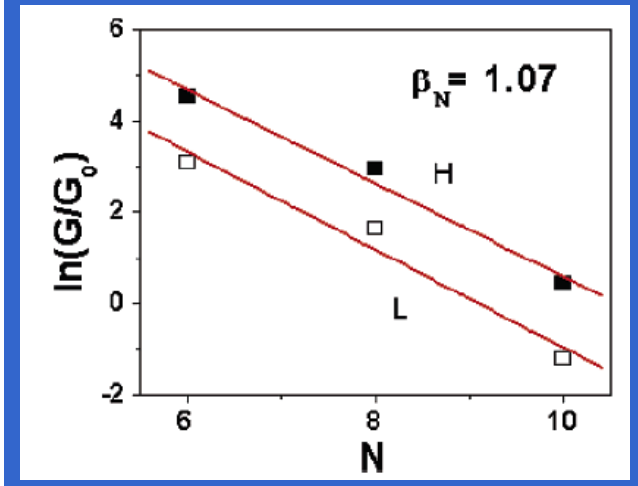




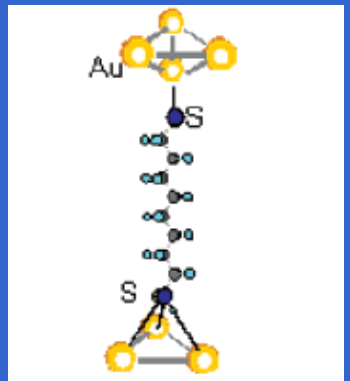
Kaun & Seideman, Phys. Rev. B 77, 033414 (2008)

New experimental results:

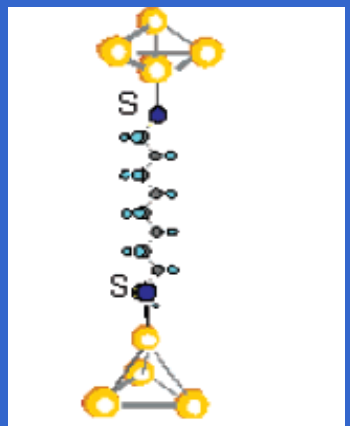




JACS, 128, 2135 (2006)



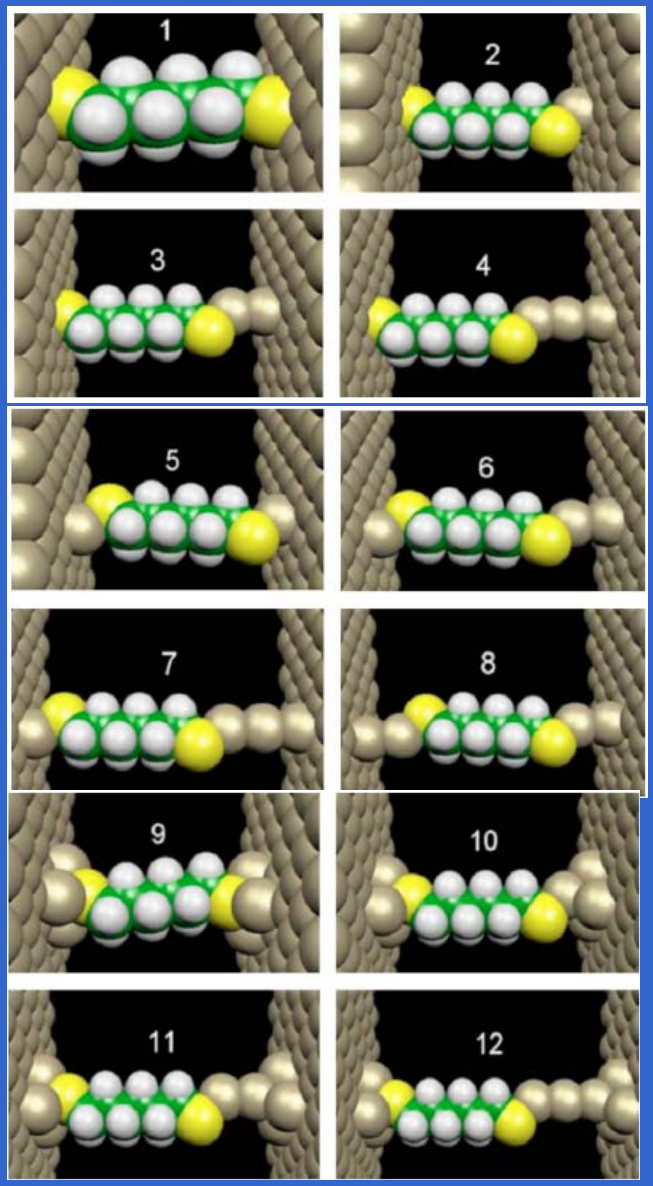
Top-Molecule-Hollow

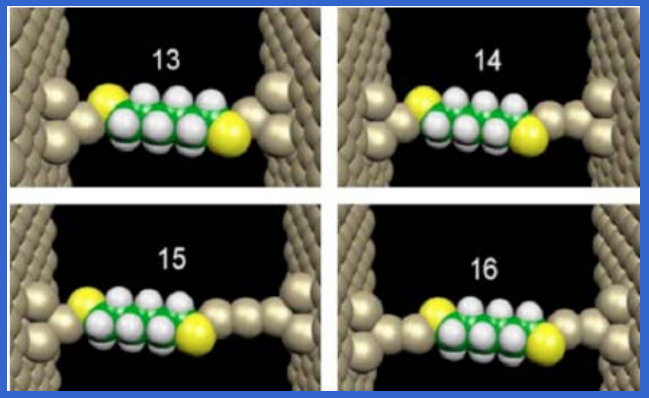


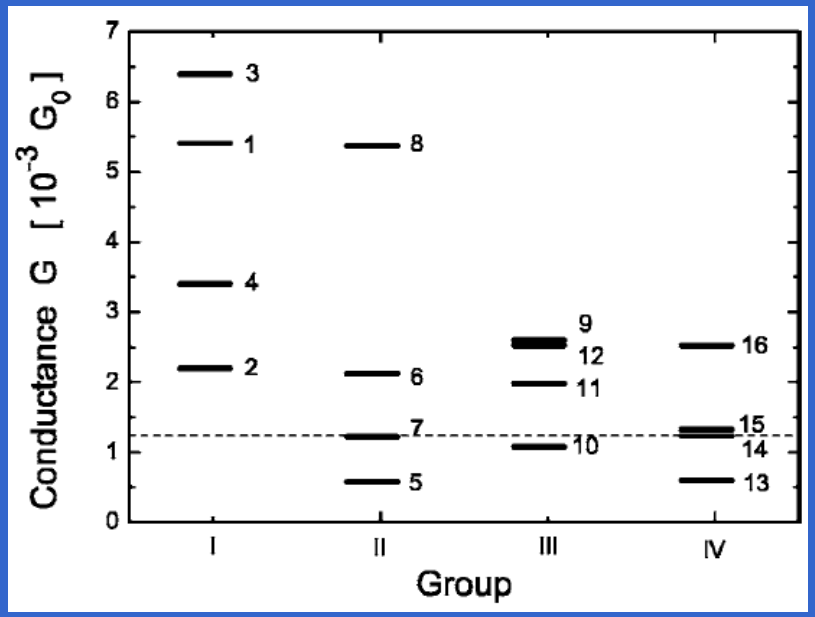
Top-Molecule-Top

?

Quantitative agreement?







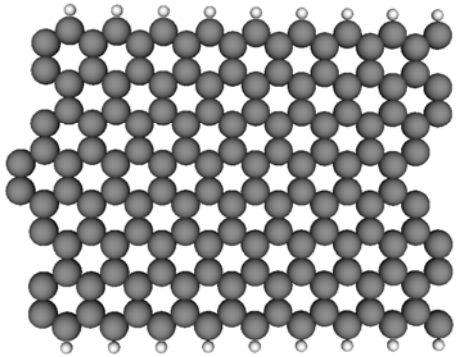
Muller *et al*, Phys. Rev. B, 73, 045403 (2006)

Sumary:

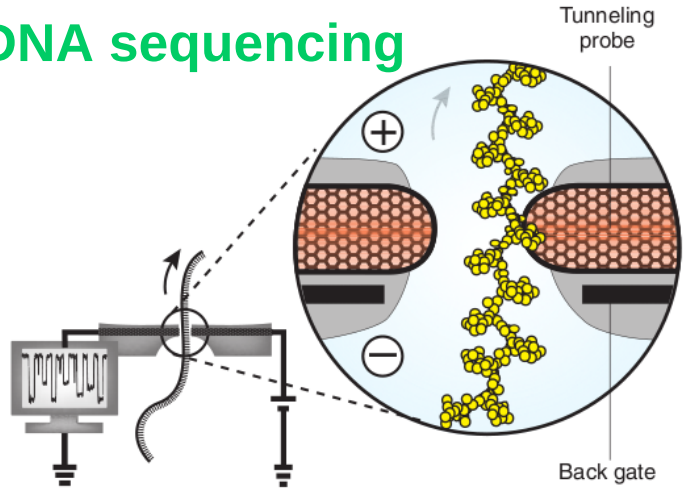
- Conductance are quantitative consistent to experimental data
- Au-S hybridization states dominates the conduction in junctions
- The structure of electrodes plays an important role.

Ongoing works:

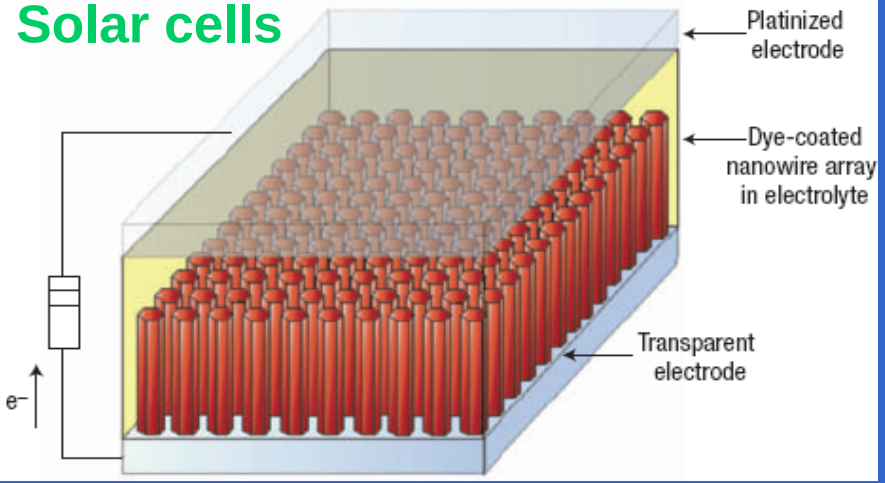
Graphene nanoribbons



DNA sequencing



Solar cells



Thermoelectricity