Quantum transport in nanostructures

奈米結構中的量子輸運

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Outline:

1. Introduction

Why molecular electronics?

Quantum transport theory

2. Comparison with experiments

A self-assembly monolayer (SAM)
A single molecule: High and low conductance

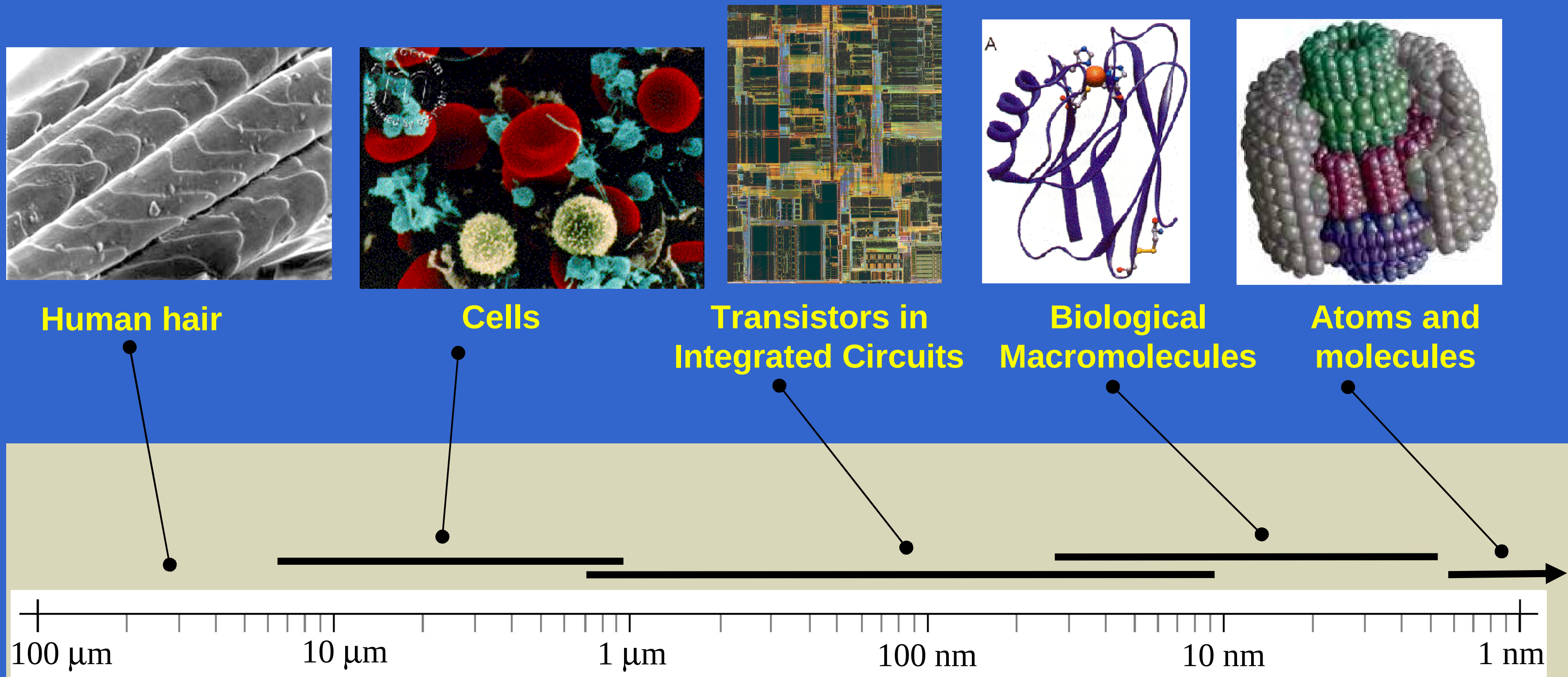
3. Spontaneous oscillation of current

A C_{60} molecule

4. Ongoing works

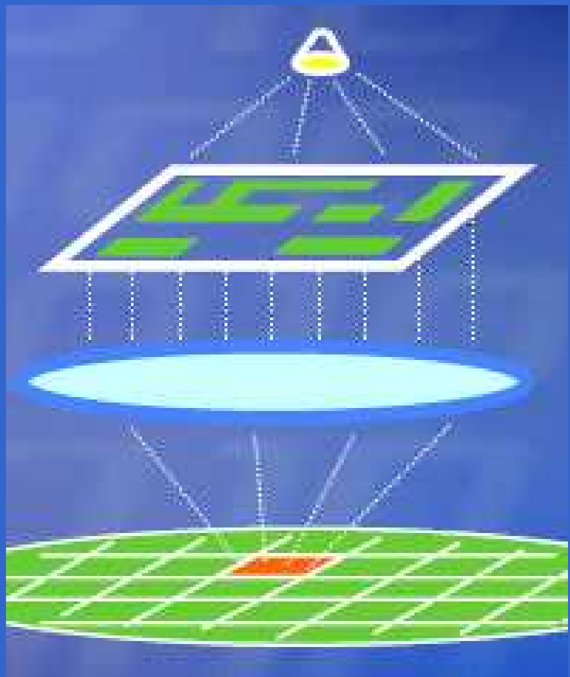
5. Summary

1. Introduction:



Nanotechnology: works at the atomic, molecular and supra-molecular levels, at the **0.1 – 100 nm scale**, with **fundamentally new properties.**

What's the problem?



45 nm now

Physical limit:
Diffraction of light.

Economical limitation:
Too expensive.

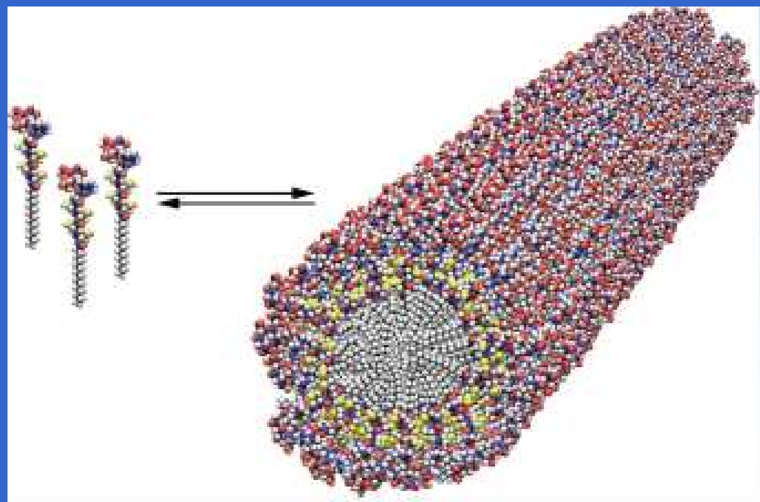
Molecular electronics: A solution

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).

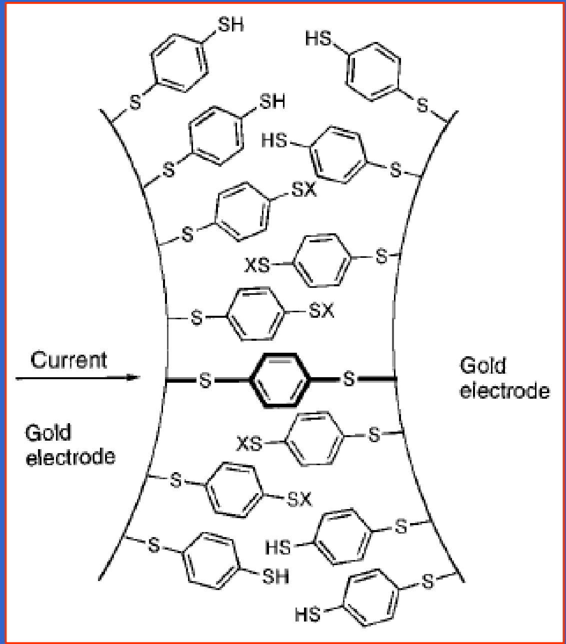
For example ..



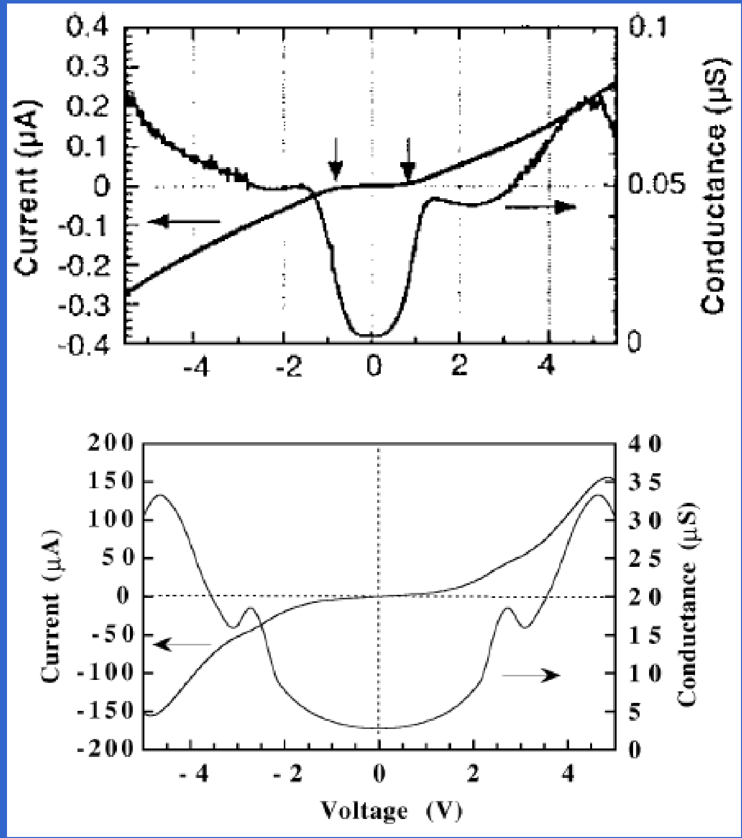
self-assembled bioactive nanofiber

Science, 294, 1684 (2001)

Previous measurement and modeling:



Science **278**, 252 (1997)

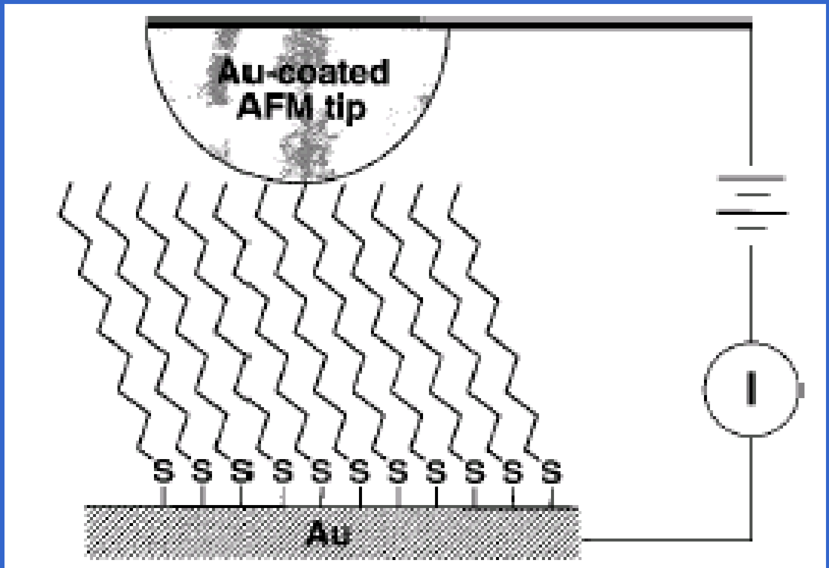


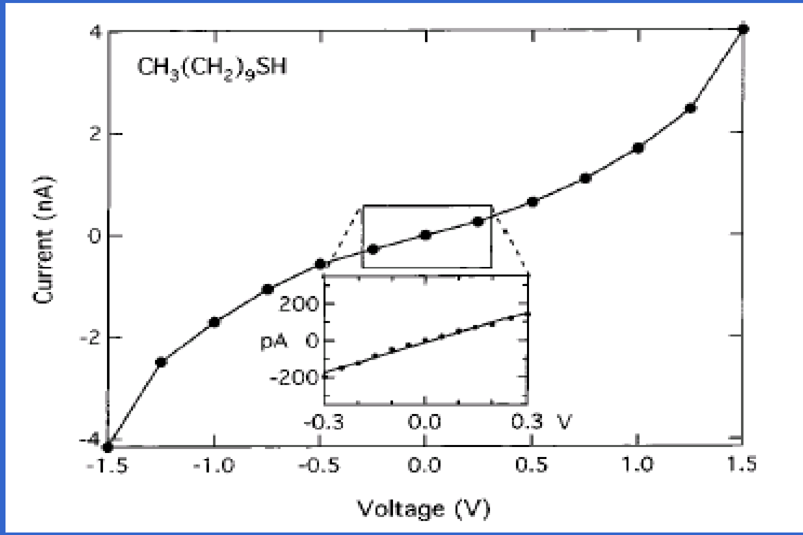
PRL **84**, 979 (2000)

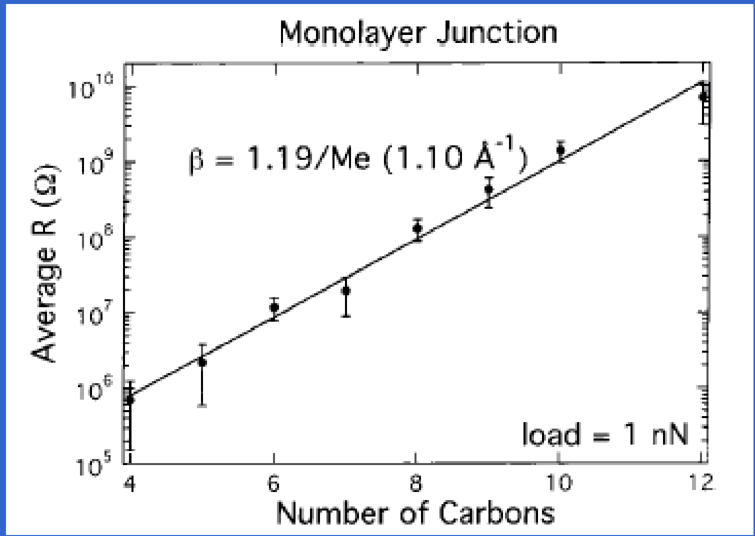
500 times of difference!

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).

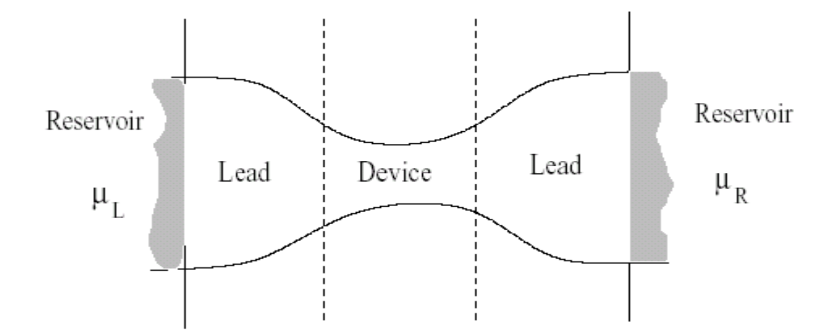
Quantum transport theory:

Ohm's law: $$R = \frac{L}{\sigma A}$$ **?**

Coherence length: l_ϕ

Elastic mean free path: l_m

Ballistic regime: $$L < l_m < l_\phi$$



The resistance of a conductor:

$$R = G^{-1} = \frac{h}{2e^2 M} \approx \frac{12.9k\Omega}{M}$$

The origin of resistance : Contact

When not ideal, a scattering region appears:

$$R_i = 1 - T_i$$

$$G = \frac{2e^2}{h}\sum_{i=1}^{M} T_i = \frac{2e^2}{h} MT$$

(Landauer formula)

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:

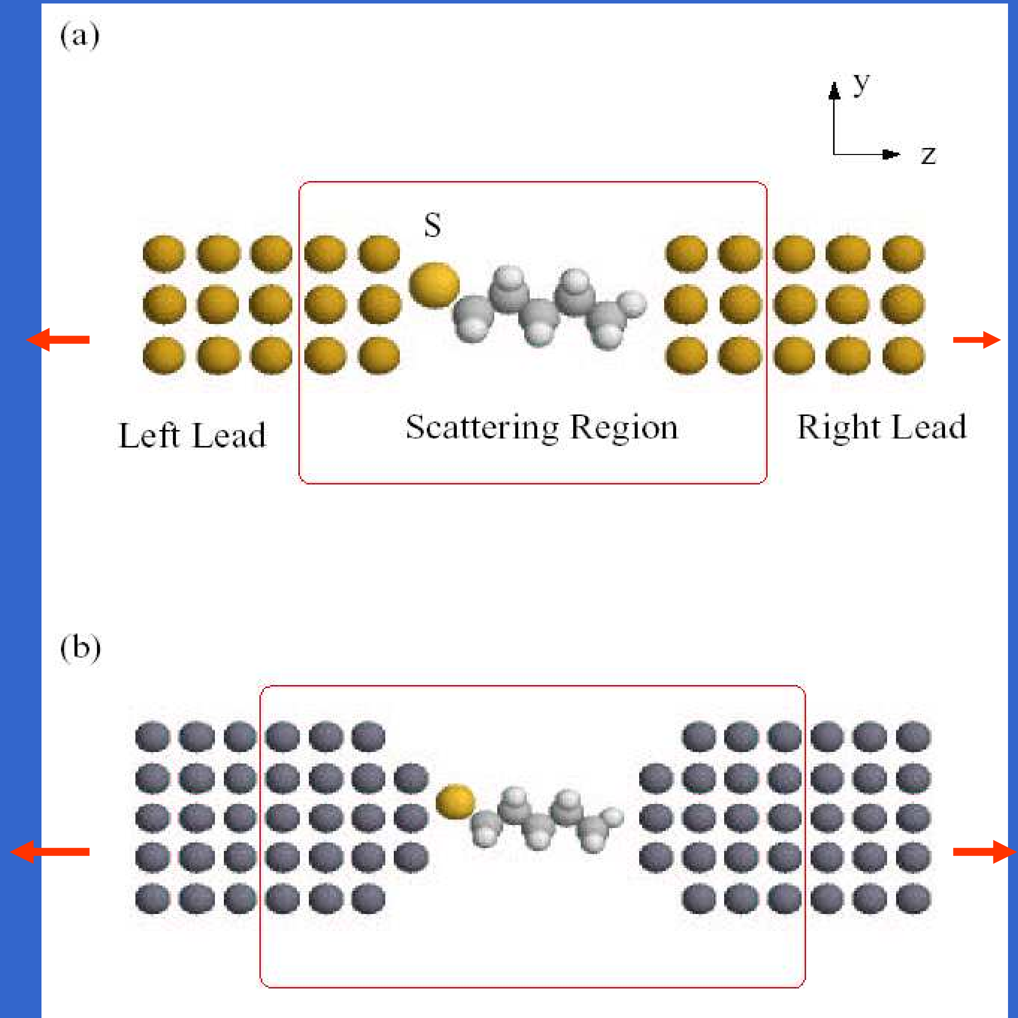
Taylor, Guo, Wang, PRB 63, 245407(2001)-----McGill-Device-CALculator (McDCAL); Brandbyge, et al, PRB 65, 165401(2002)---Transiesta.

2. Comparison with experiments: Alkanethiol molecules

Our model:

Au electrodes

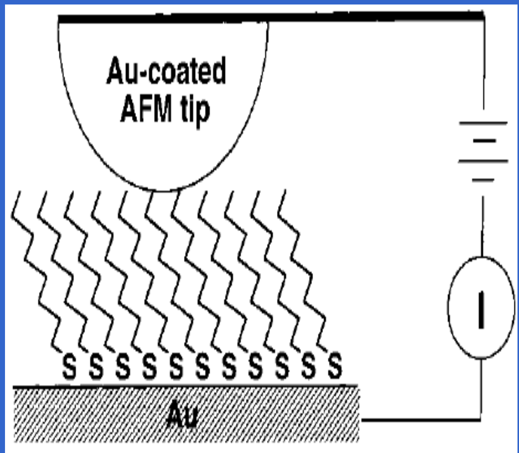
Al electrodes

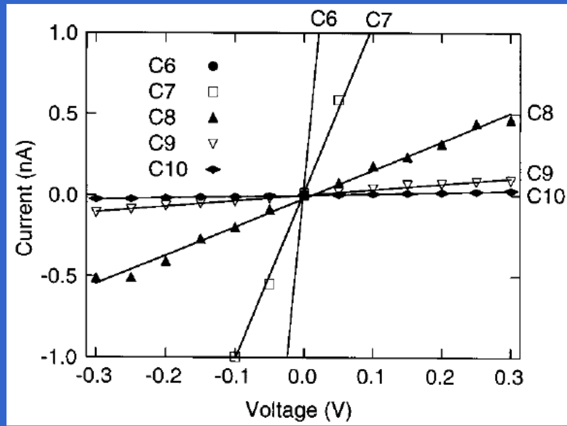


Kaun & Guo, Nano Lett. 3, 1521 (2003)

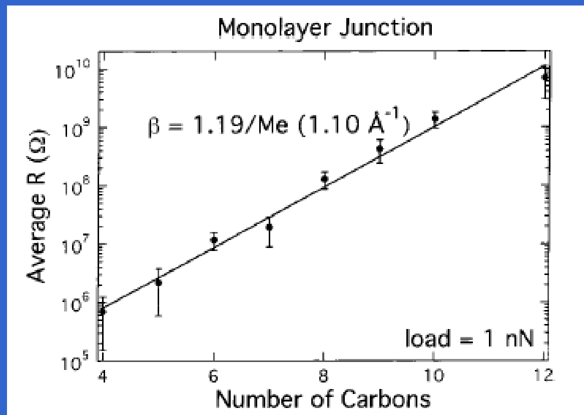
Comparison with experiments

Experiment



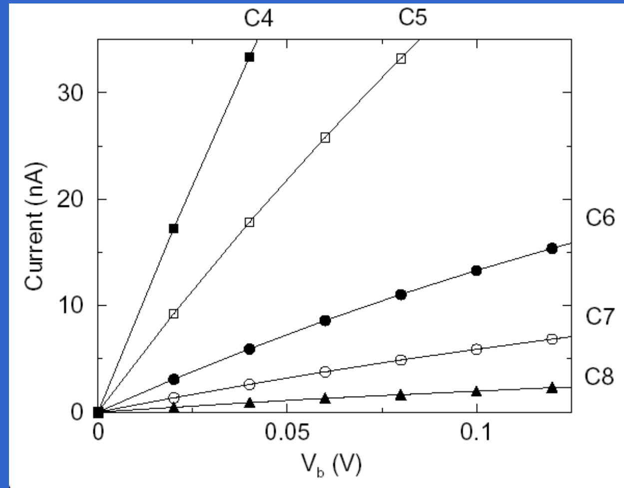


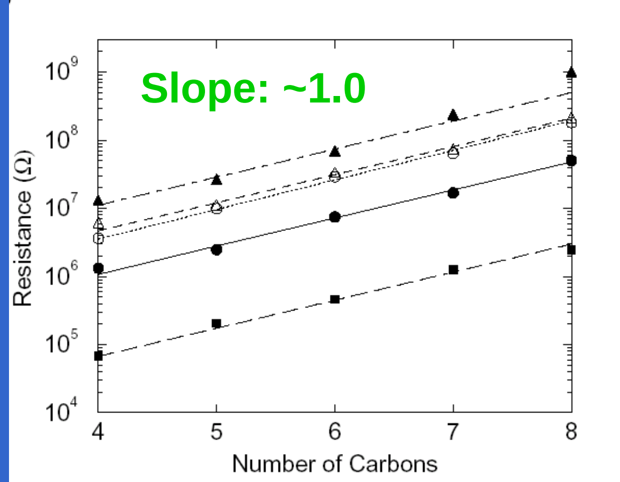
$$R_n = R_o \exp(\beta n)$$



JACS 123, 5549 (2001)

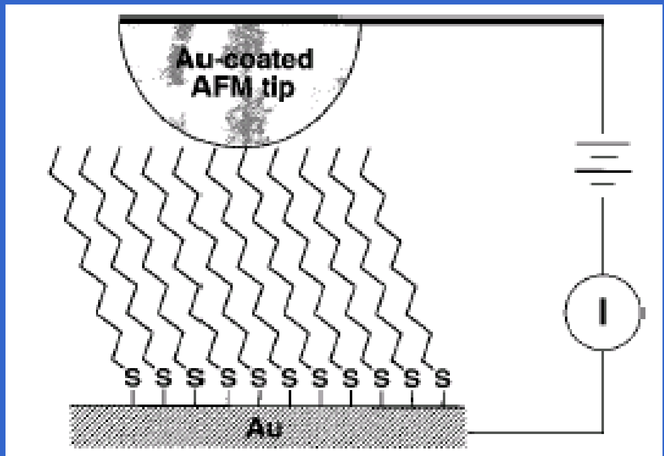
Our modeling

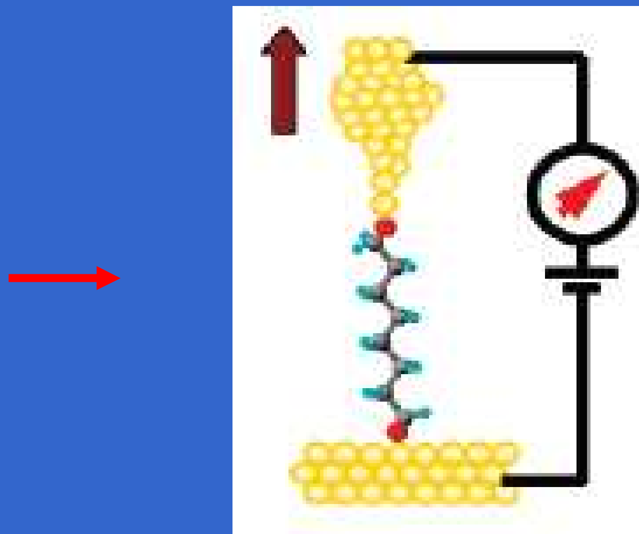




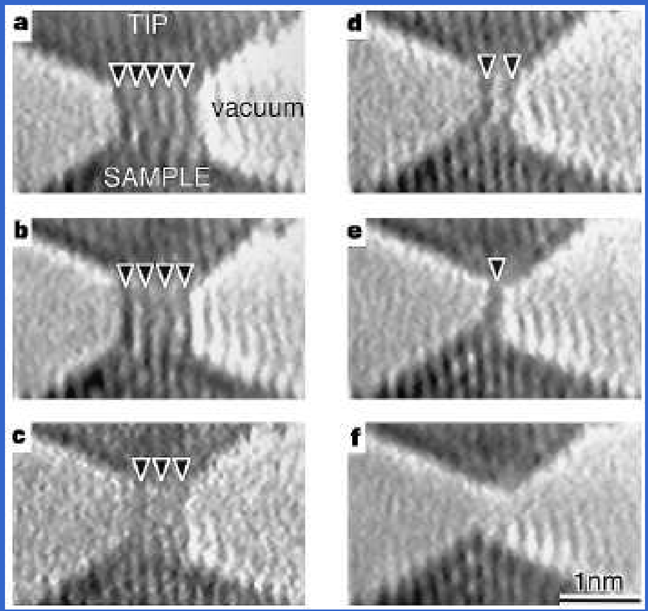
Nano Lett. 3, 1521 (2003)

What is the single-molecule conductance?

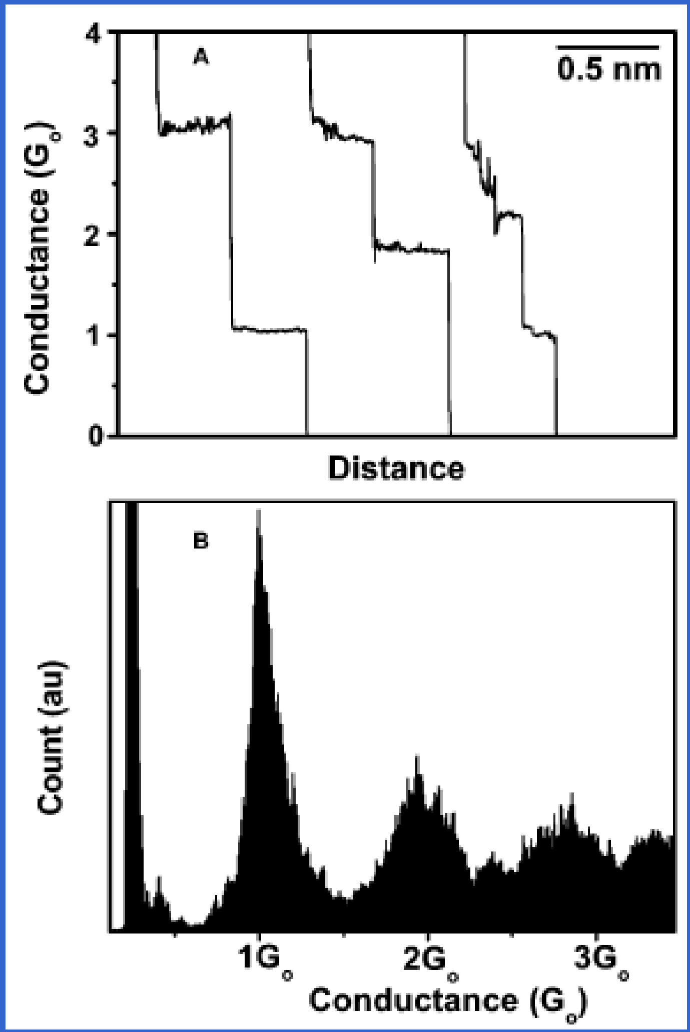




Conductance of a Au nanowire:

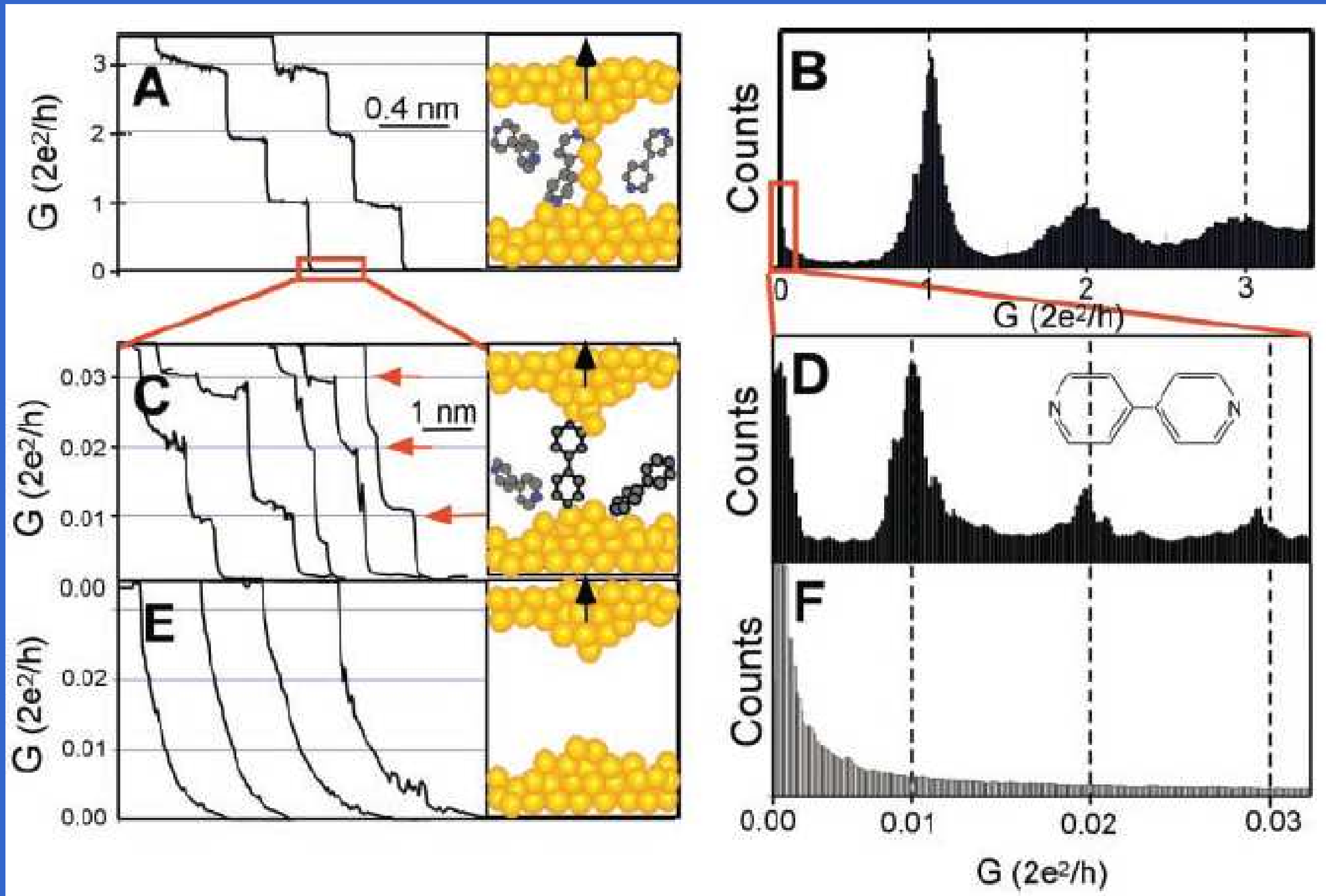


Nature 395, 780 (1998)



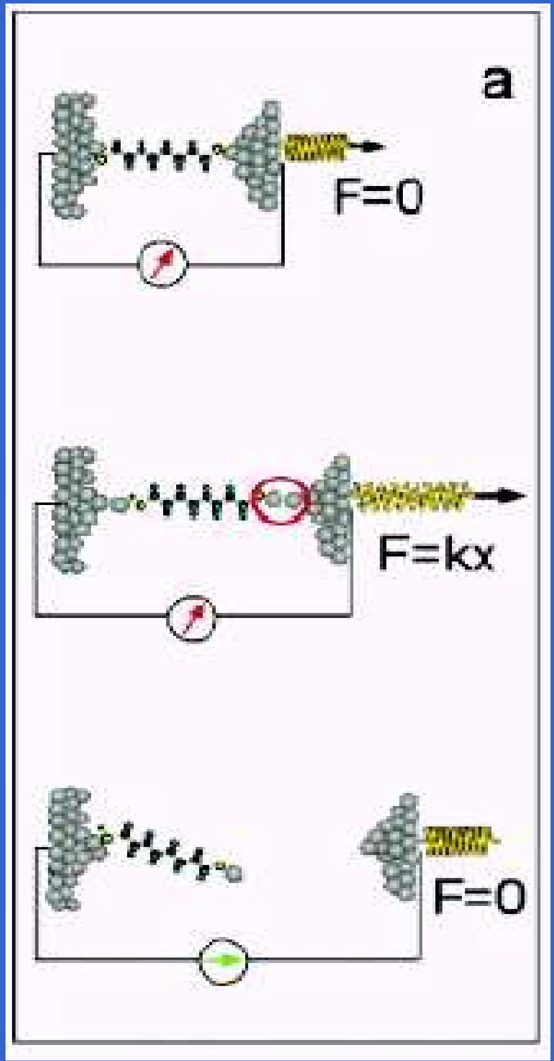
Nano Lett. 6, 2362 (2006)

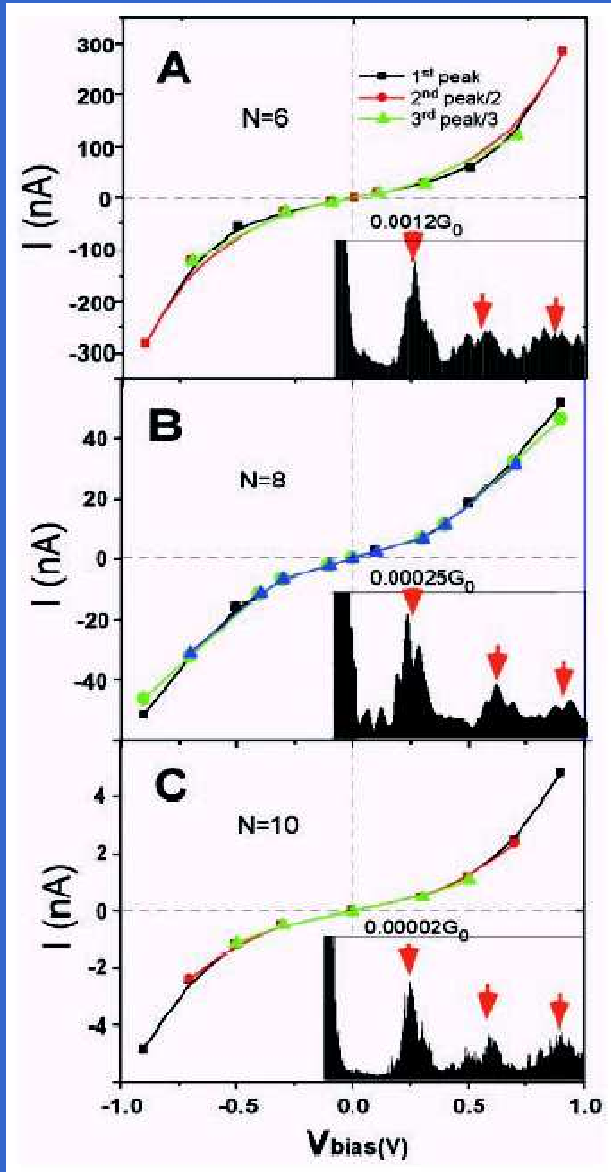
Conductance of a single molecule



J. Tao et al, Science (2003)

New measurement on single alkanedithiol molecule





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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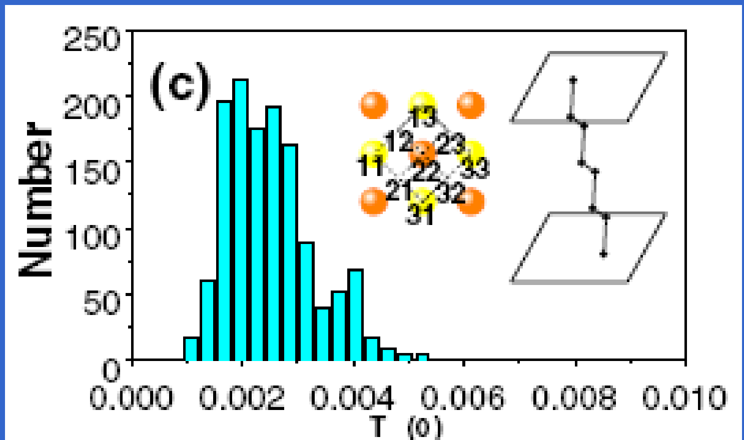
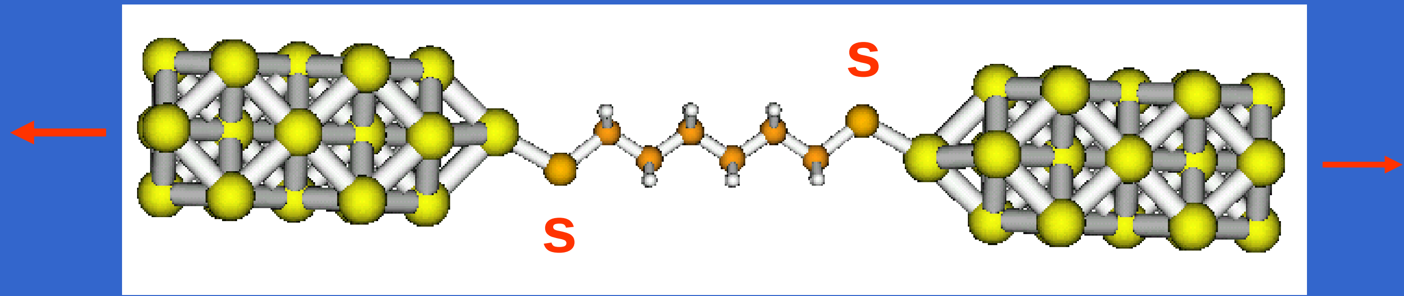
(Received 21 April 2005; published 3 October 2005)



	Calculation	Experiment
N = 6 G =	0.0025	0.0012

Unit: G_0

Our model:



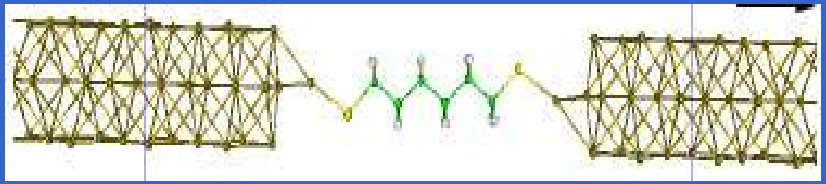
		Calculation	Experiment
N = 6	G =	0.001 0	0.001 2
N = 8	G =	0.000 13	0.000 25
N = 10	G =	0.000 02	0.000 02

Unit: G_0

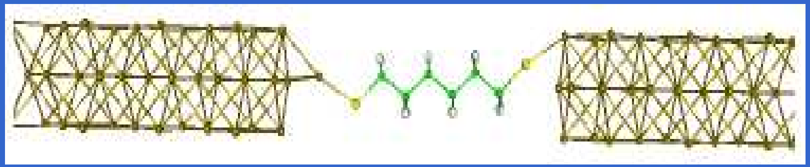
Kaun & Seideman, Phys. Rev. B 77, 033414 (2008)

Contact effect (N=6):

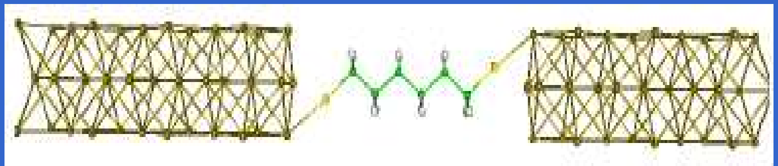
a

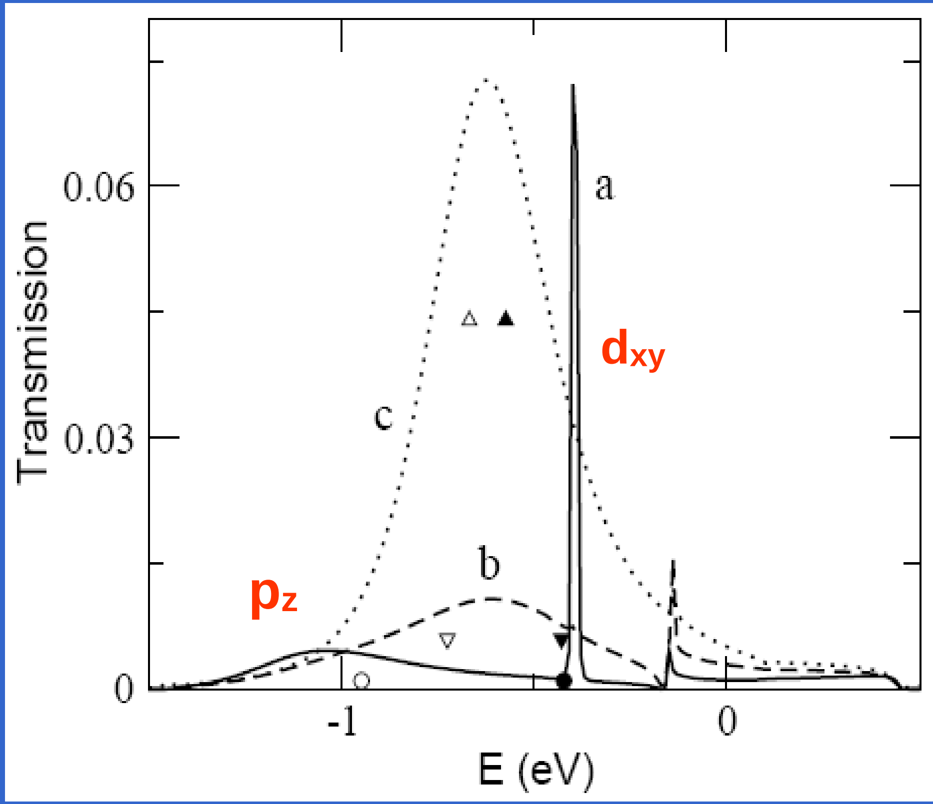


b



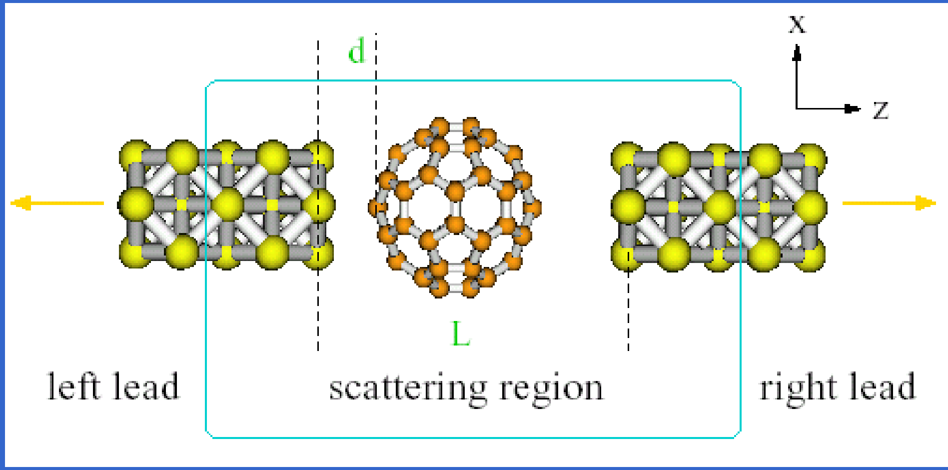
c



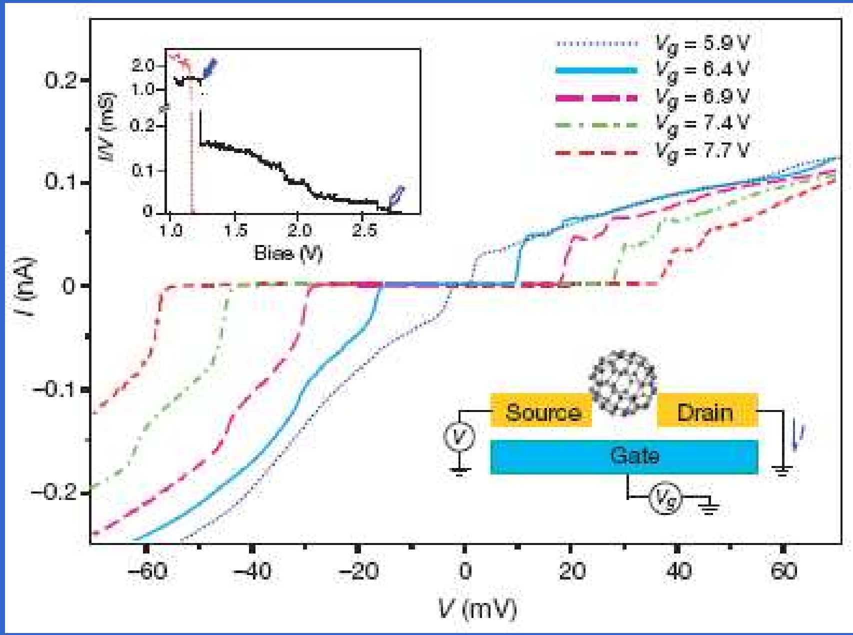


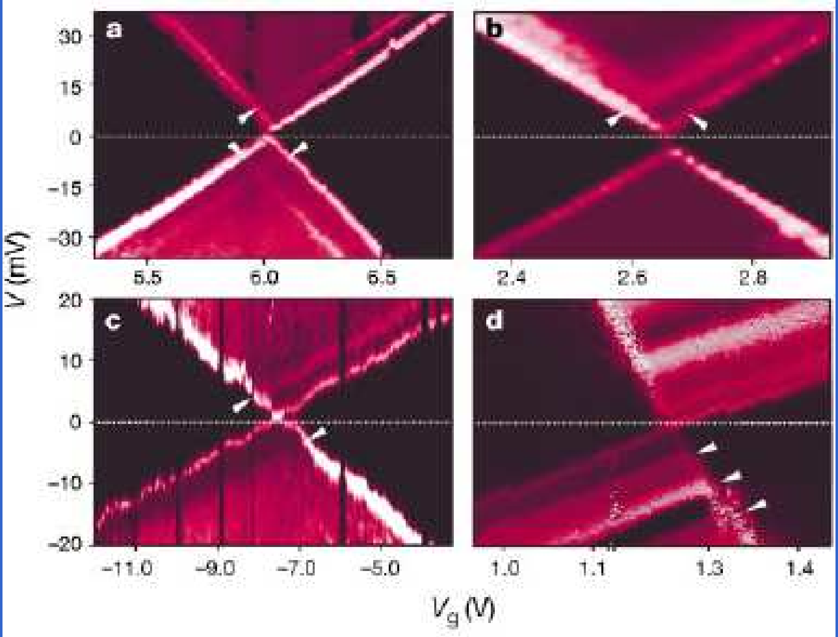
Kaun & Seideman, Phys. Rev. B 77, 033414 (2008)

4. Spontaneous oscillation of current



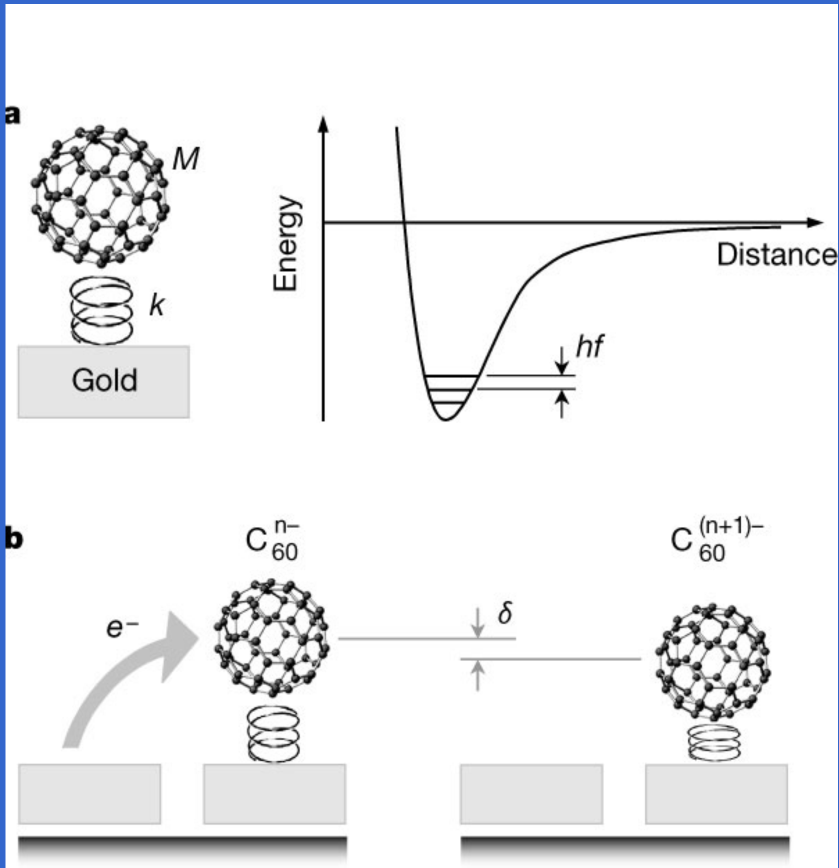
Nanomechanical oscillations in a single-C_{60} transistor

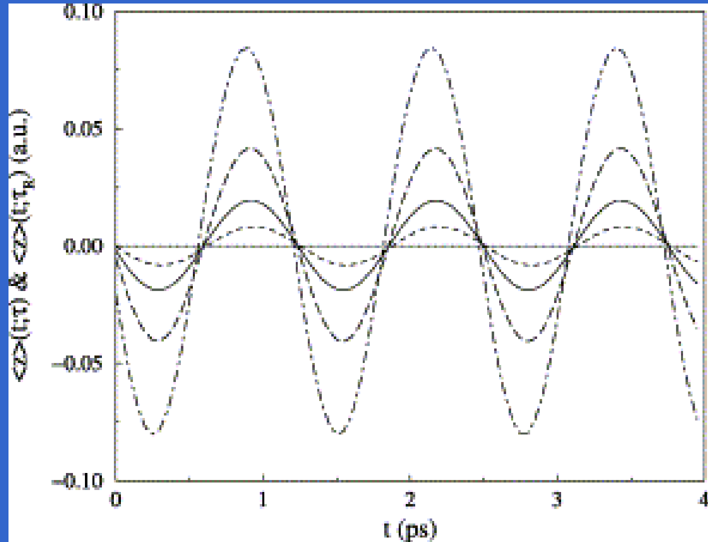




H. Park, et al, Nature (2000)

Current-driven oscillations:





Predictions from calculations

T. Seideman, et al, Chem. Phys. (2002)

<Z> ⟵ the lifetime of resonance

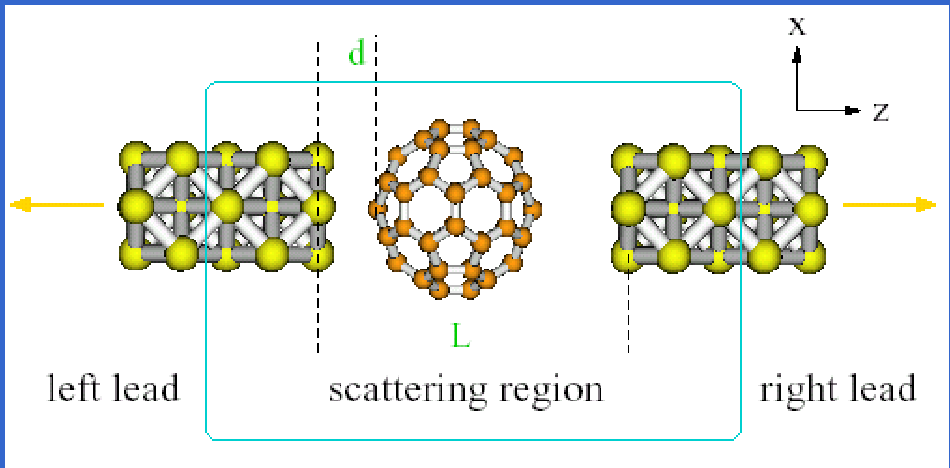
f ⟵ the C_{60} mass

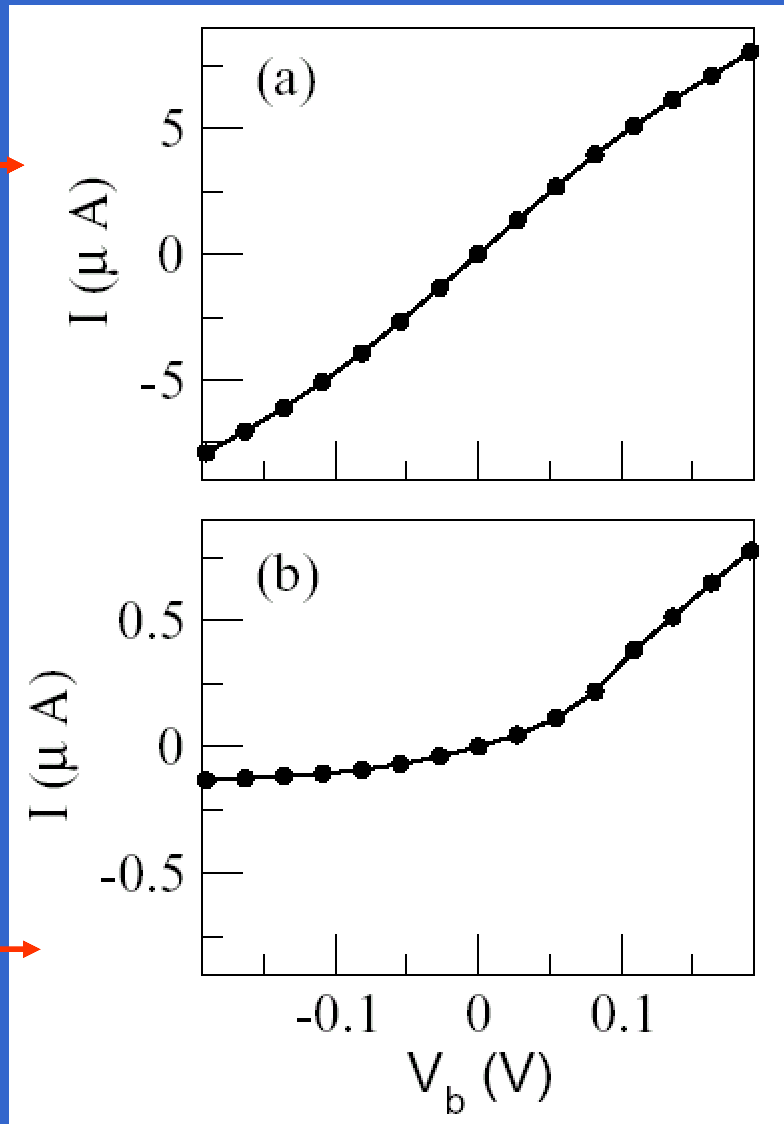
The bouncing Bucky ball

H. Park, et al, Nature (2000)

Our model:

Symmetric coupling

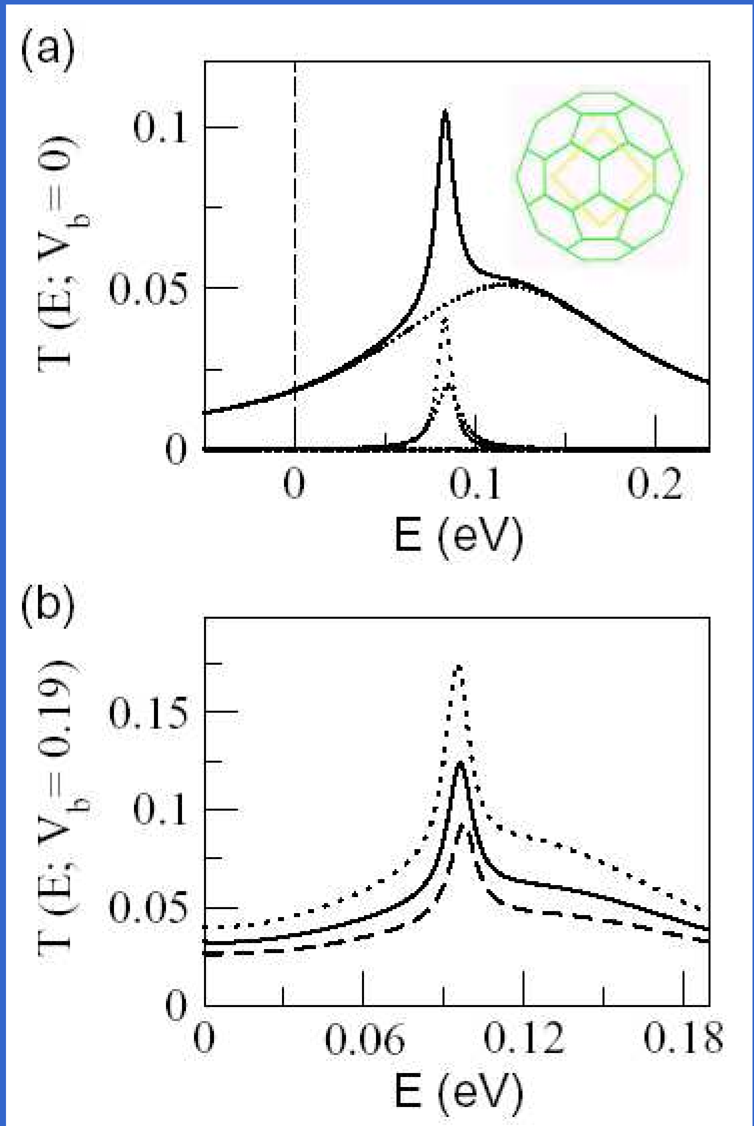




Asymmetric coupling

(L = 26.42 a.u.)

Transmission spectra:

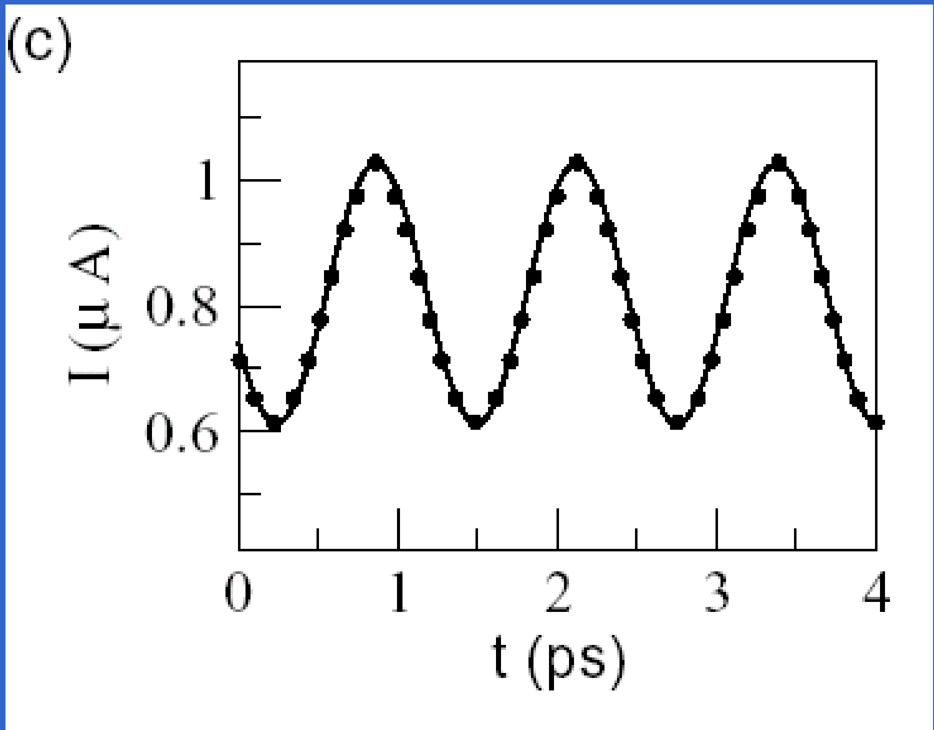


Three channels

One induces the motion; the other probes it.

Different locations

Current oscillates as the molecule vibrates



The ac/dc ratio, the power output efficiency, is 0.26 (L = 26.42 a.u.)

When L = 25.42 a.u., the ratio is 0.07

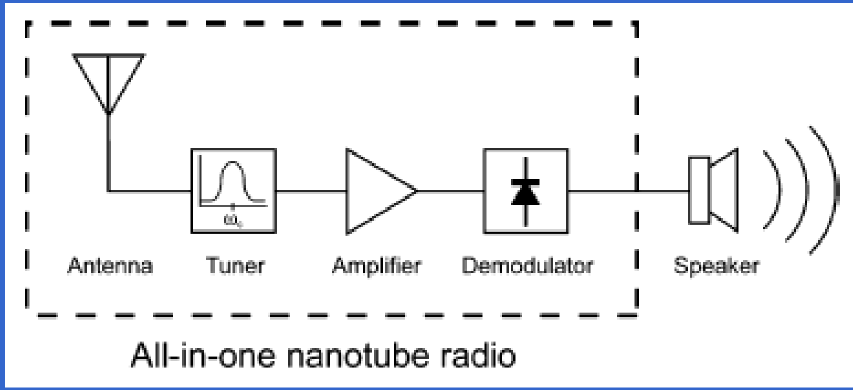
Only a range of L permits both a large ratio and high average conductance

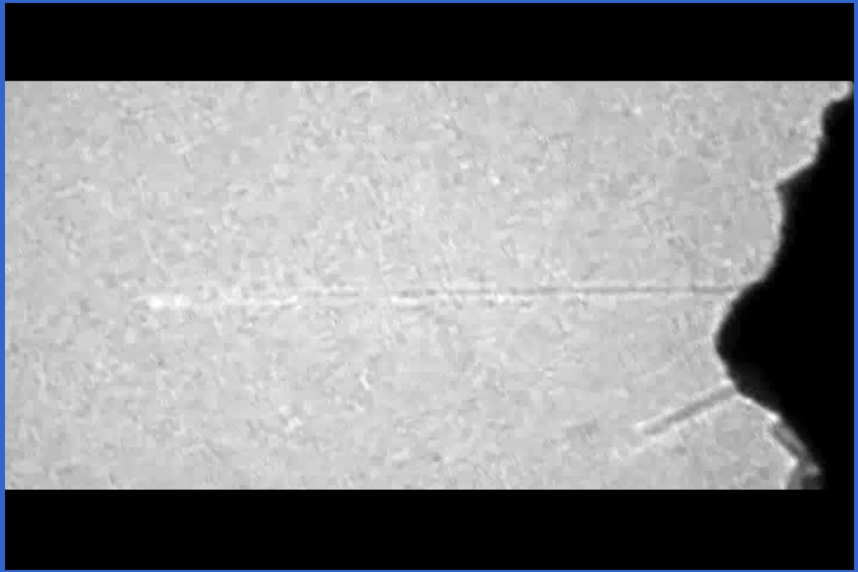
Kaun and Seideman, PRL 94, 226801 (2005)

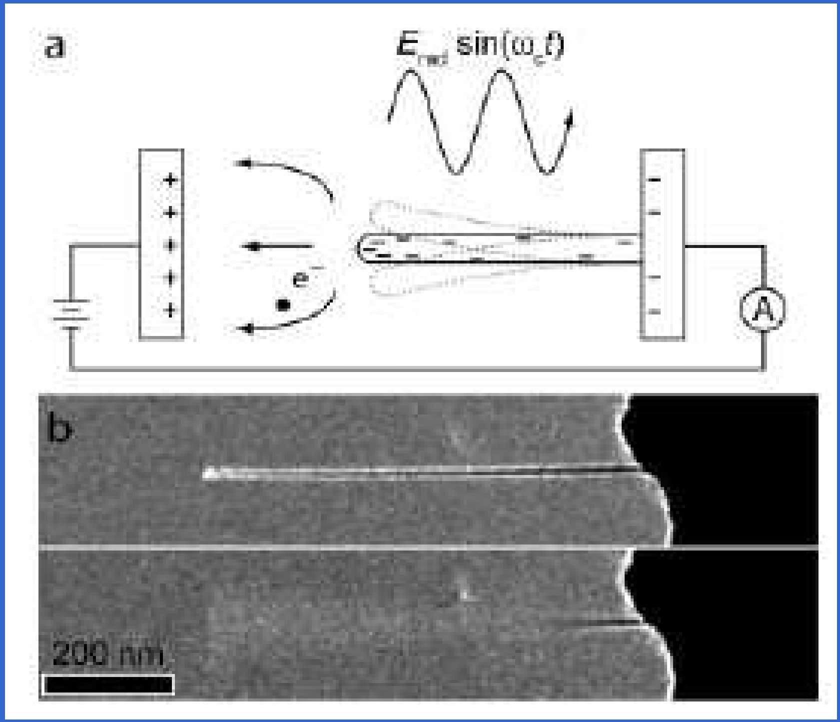
Applications:

- A nanoscale generator of a radiation field, thus a THz optoelectronic device.
- A miniature mass spectrometry.
- The direct, time-domain probing of the current-driven dynamics in nanojunctions.

Experimentally …. Nanotube radio



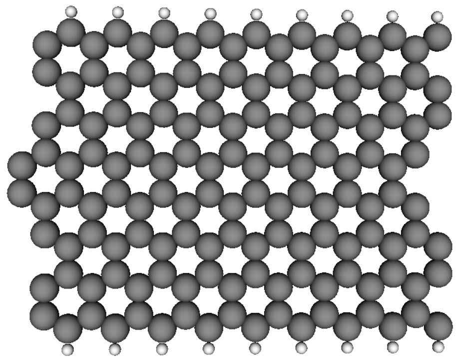




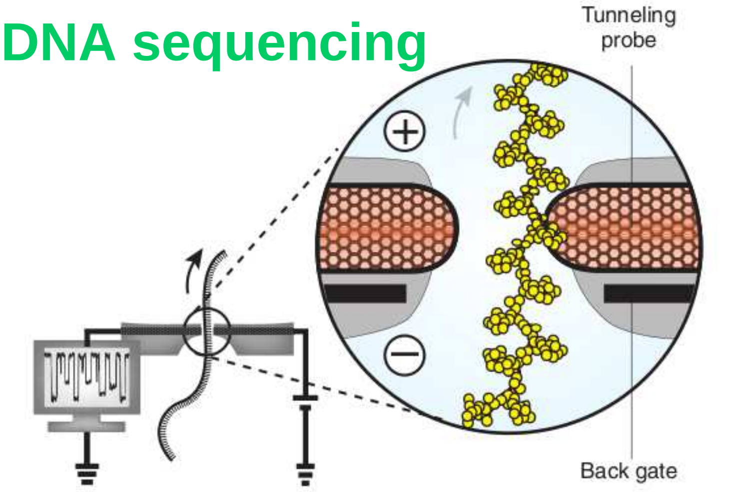
A. Zettl et al, Nano Lett. 7, 3508 (2007)

Ongoing works:

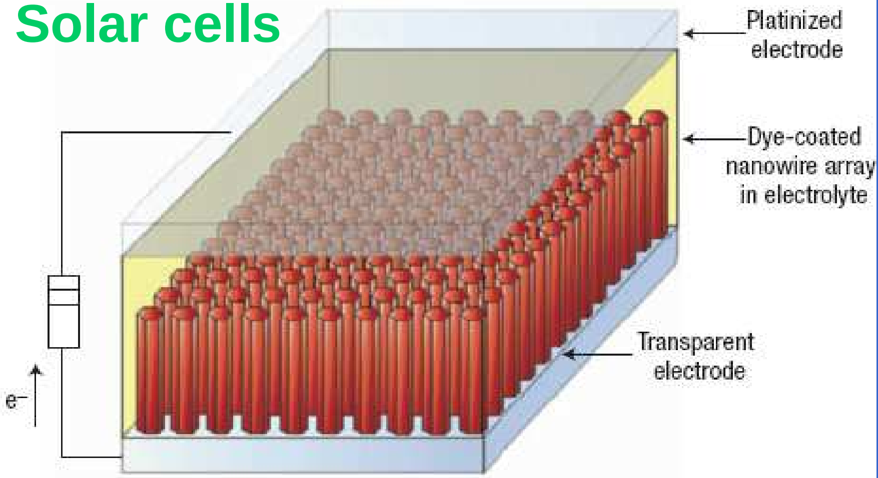
Graphene nanoribbons



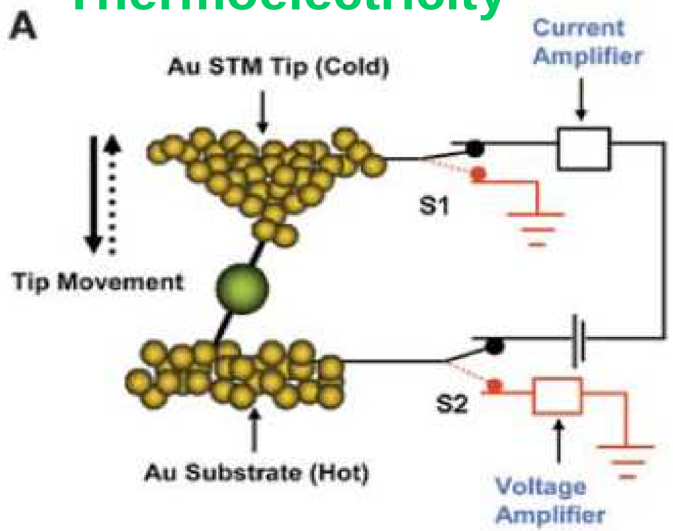
DNA sequencing



Solar cells



Thermoelectricity



Sumary:

- Conductance are quantitative consistent to experimental data
- The structure of electrodes plays an important role.
- Current-driven dynamics can be used to produce oscillating current in molecular junctions
- There are plenty of rooms in the Ballistic regime.

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- Prof. Chi-Shung Tang (National United Univ.)

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