



Nano-Science Center, University of Copenhagen

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## “Single-molecule electron transfer in solid state three-terminal devices: Status and challenges for molecular electronics with single molecules”

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University of Copenhagen



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SINGLE

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Coupling charge transport to internal degrees of freedom at the single molecule level

**SINGLE**

SINGLE is a project supported by the 7th framework programme for research and technological development (FP7) of the European Union. The research project is a collaborative project - a small / medium scaled focused research project on how to couple charge transport to internal degrees of freedom at the single molecule level. The project will be carried out by a collaboration of these institutions, coordinated by Prof. Thomas Bjørnholm of Copenhagen University:

University of Copenhagen (Nano-Science Center)  
Chalmers Tekniske Hoegskola AB  
Technische Universiteit Delft  
IBM Research GmbH  
Universite de Mons-Hainaut

**SINGLE is supported by FP7**

**SEVENTH FRAMEWORK PROGRAMME COOPERATION ICT**

**Future and Emerging Technologies Programme**

**Collaborators on SINGLE**

NANO-SCIENCE CENTER  
UNIVERSITY OF COPENHAGEN

**CHALMERS**

**TU Delft**  
Technische Universiteit Delft

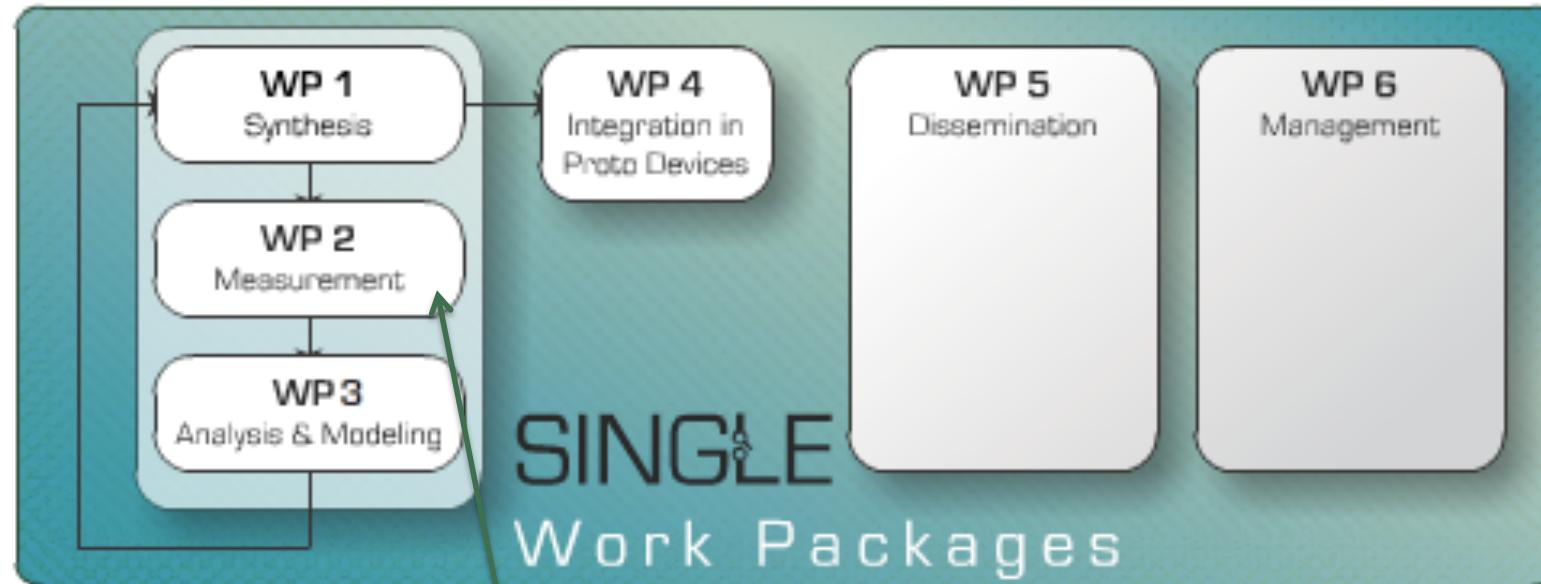
**UMH**

**IBM**

www.single.ku.dk

Bjørnholm  
Kubatkin  
Van der Zant  
Cornil  
Riel





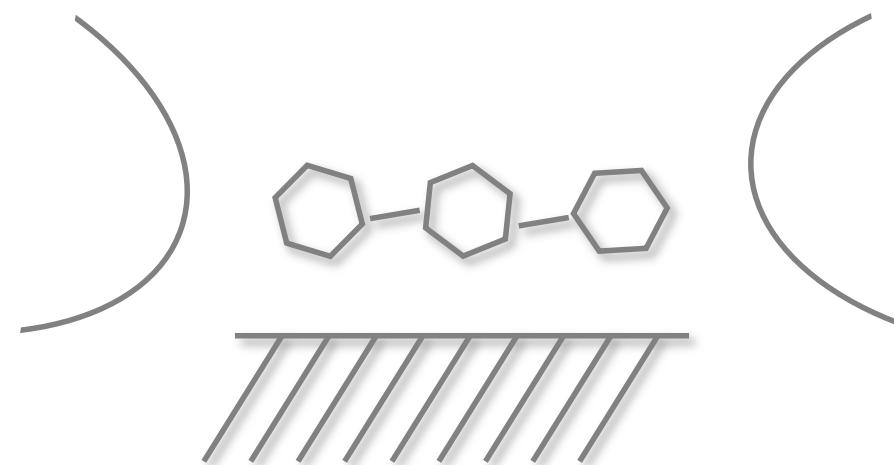
*The work is proceeding in iterative cycles of synthesis, measurements, modeling, and eventually integrating the most promising systems in more advanced prototype systems.*

Measurements by 3 different  
experimental research groups

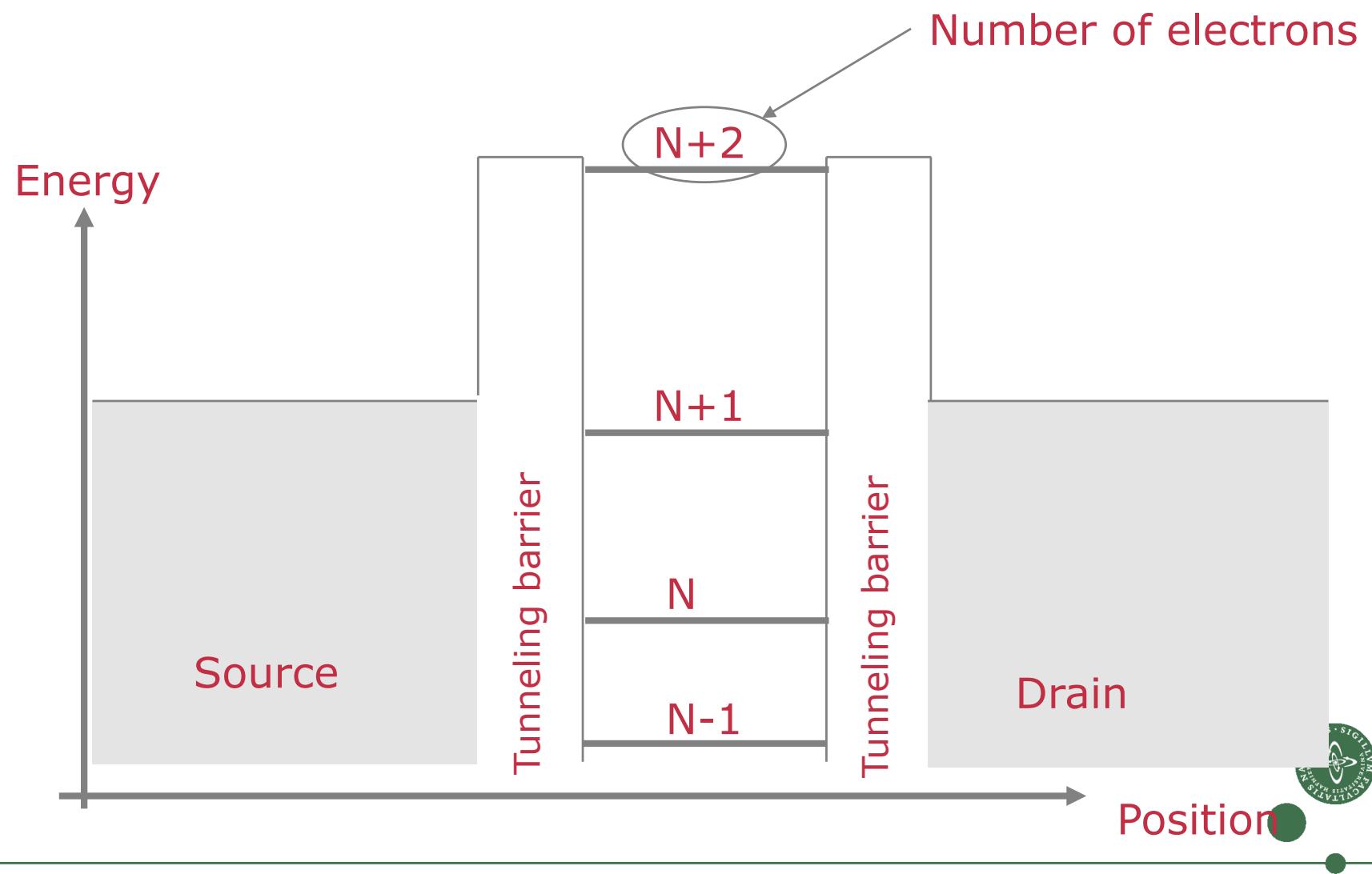


## Question:

What are the key parameters for electron transport through single molecules?



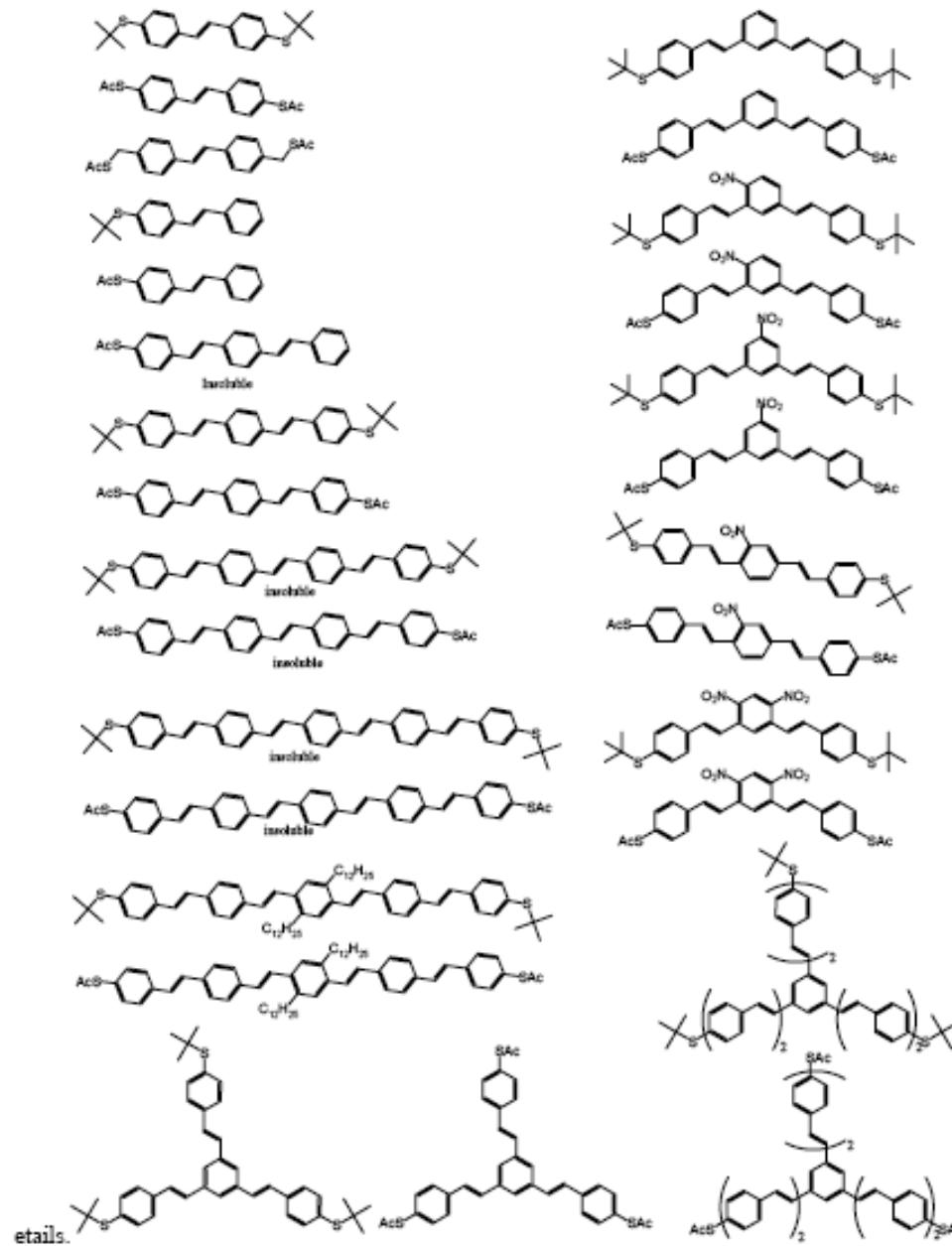
## Energy Levels



## Outline:

- 1) Measurements on thiol end-capped OPV's
- 2) C<sub>60</sub>
- 3) C<sub>60</sub> as the "*alligator clip*": a new generation of molecules

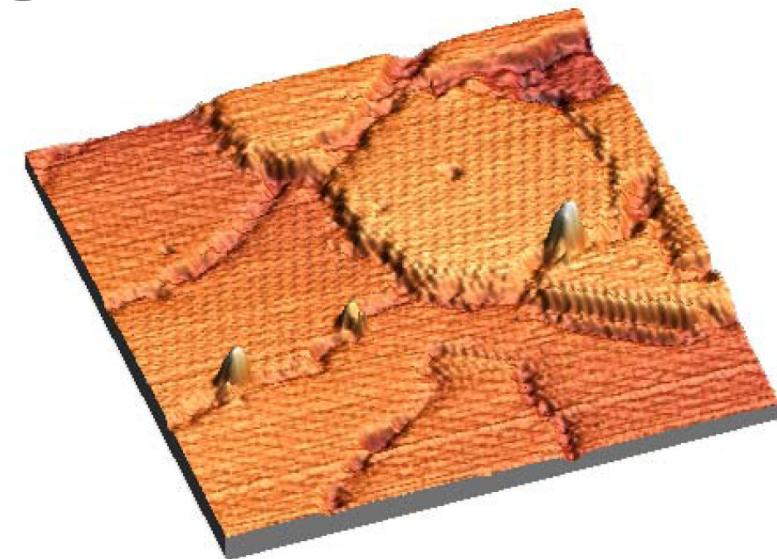
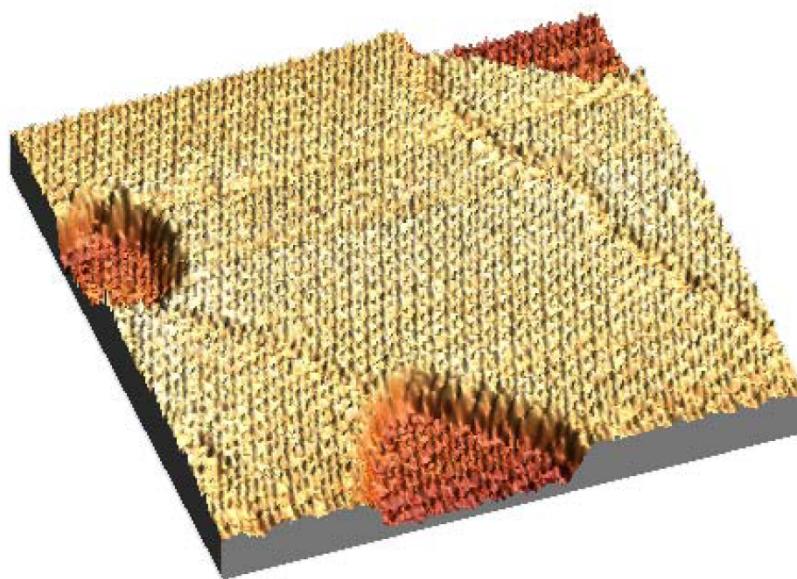
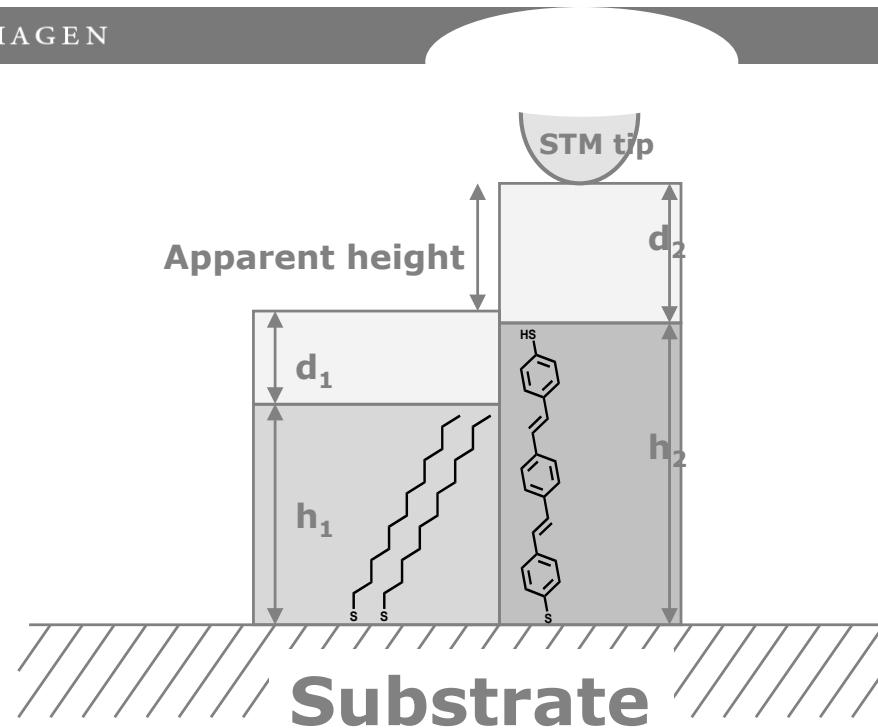


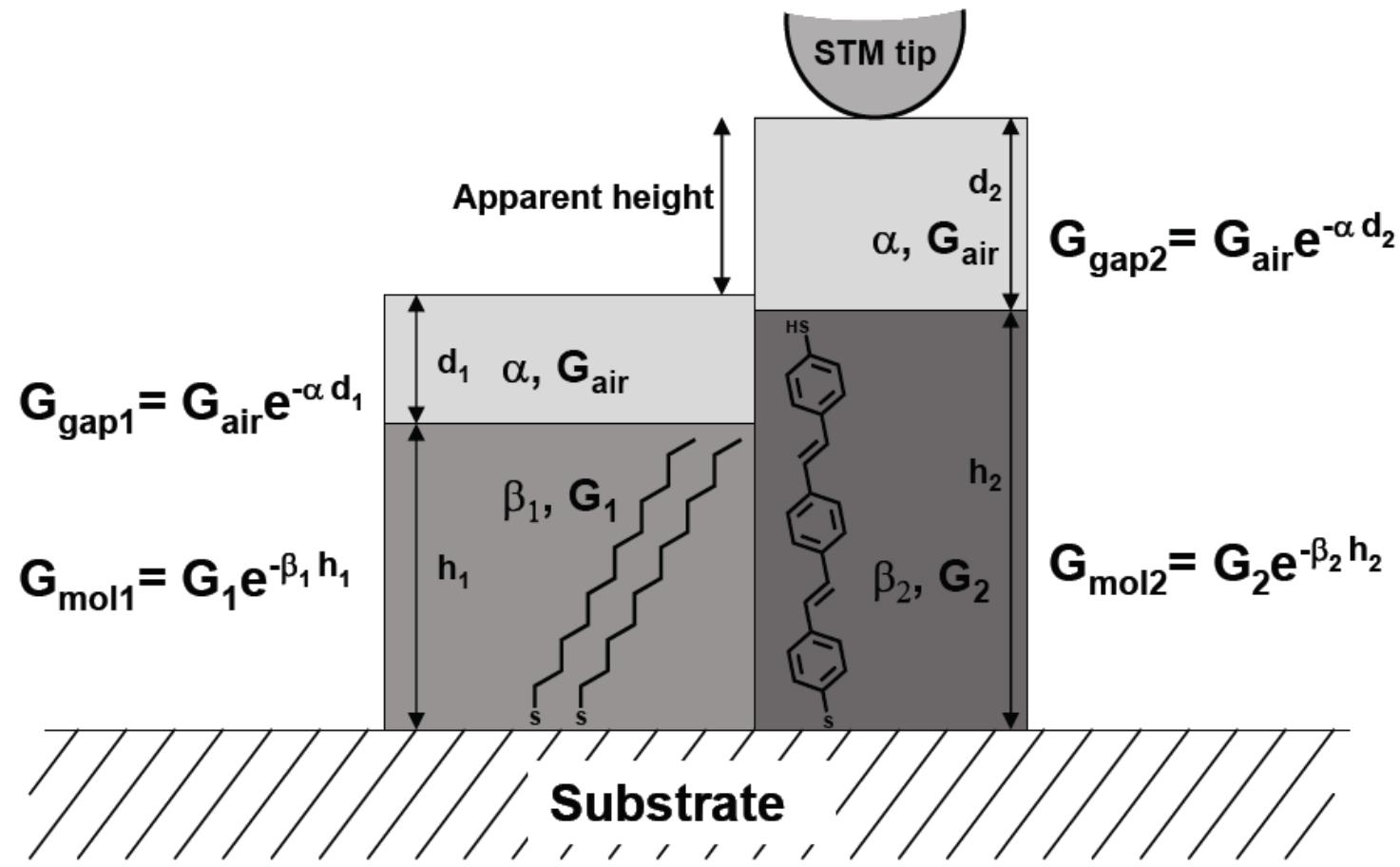


# STM

Goal: to compare the tunnelling properties  
of a series of molecular wires

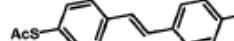
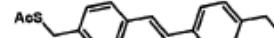
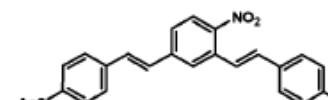
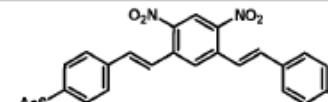
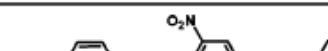
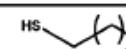


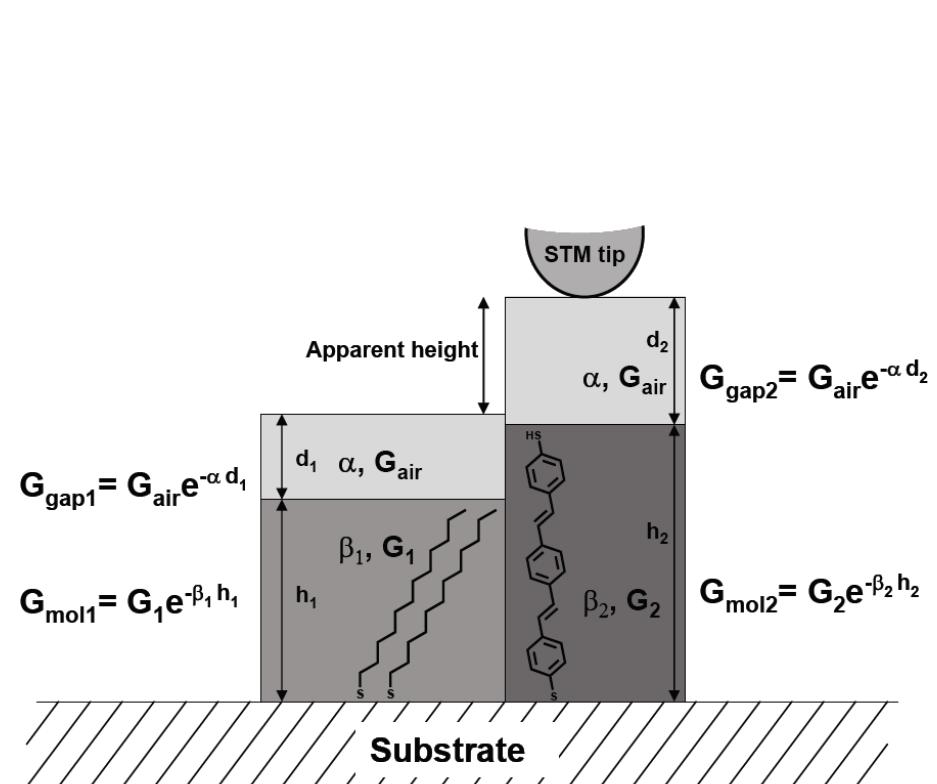




**Assumption:  $G_1 \approx G_2$**



Entry	Molecule	Length (Å)	Apparent height (Å)
1		13.9	4.0 ±0.7
2		14.2	3.5 ±1.0
3		19.5	7.5 ±1.1
4		19.4	6.1 ±2.0
5		16.5	4.1 ±1.6
6		15.9	4.2 ±0.9
7 <sup>6</sup>		13.7	2.0 ±0.9
8 <sup>2</sup>		19.3	4.70 ±1.01
9 <sup>2</sup>		19.3	4.30 ±0.54
10 <sup>12</sup>	 n=10	14	0.0



# STM

- + easy comparison of tunnelling through different molecules
- No control of electronic levels in the molecule

# Solid state 3 terminal device

- + detailed spectroscopic characterisation of the molecule

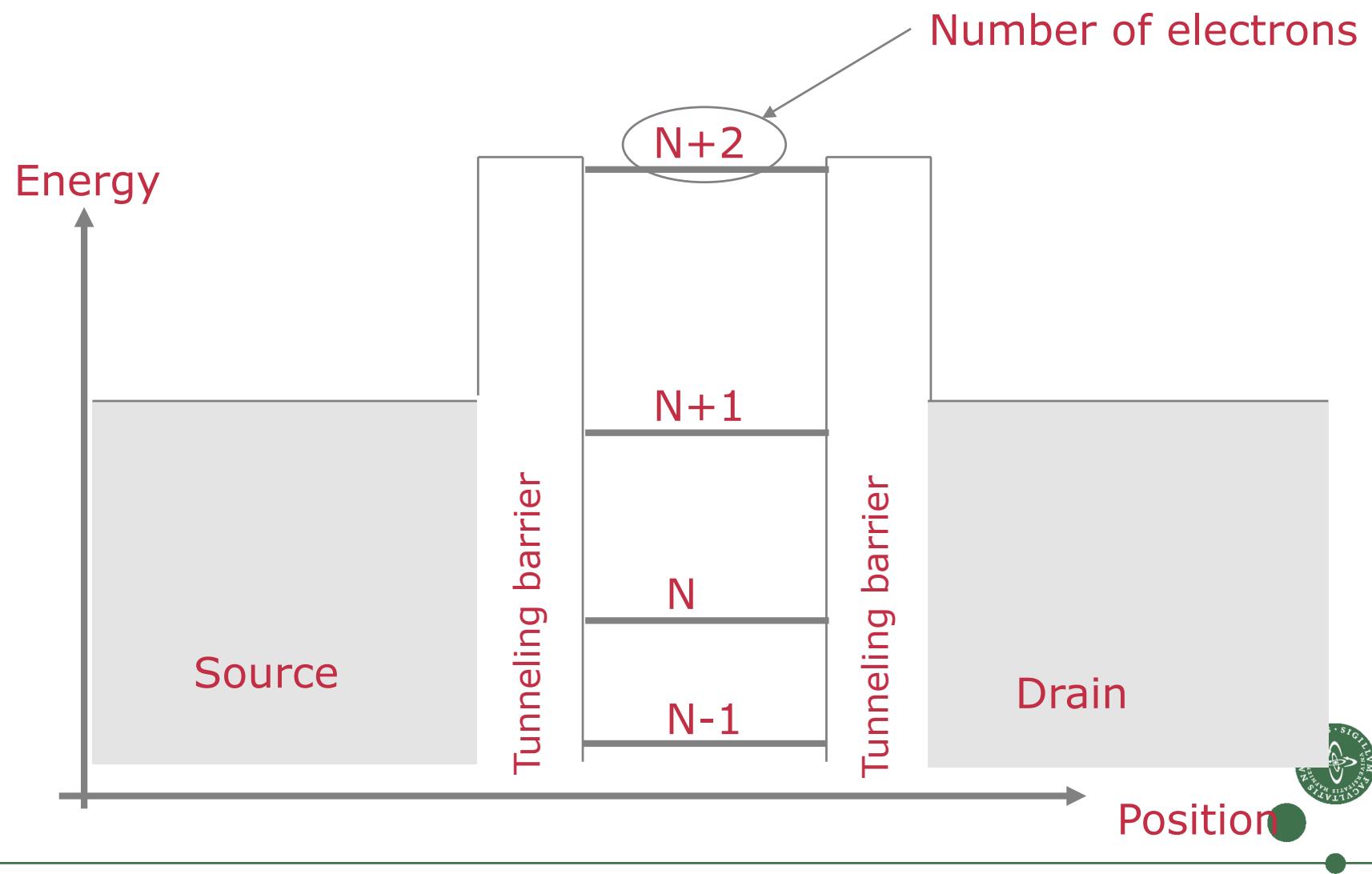
Goal: to study the importance of the contacts between molecule and leads

*Faraday Discussions* 131: 265-279 2006

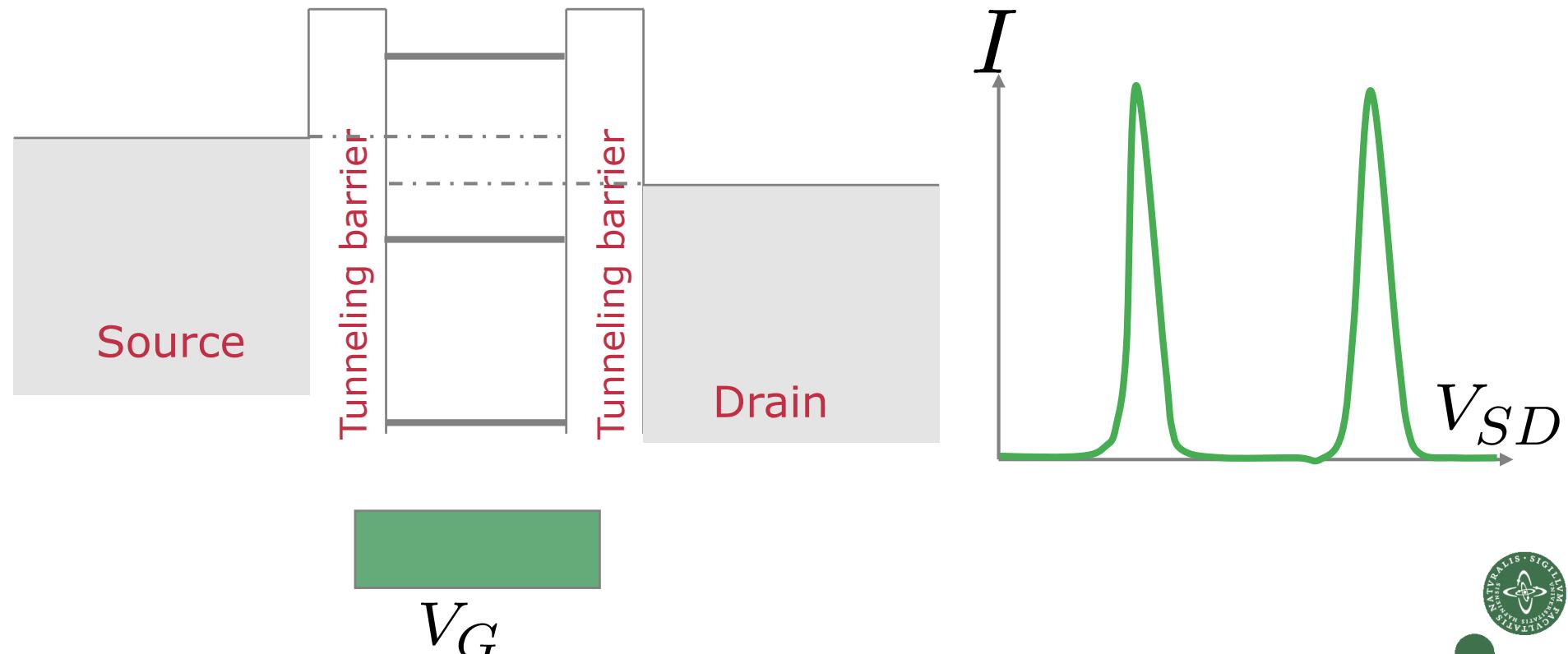
*J. Am. Chem. Soc.* 128 (20): 6574-6575 2006



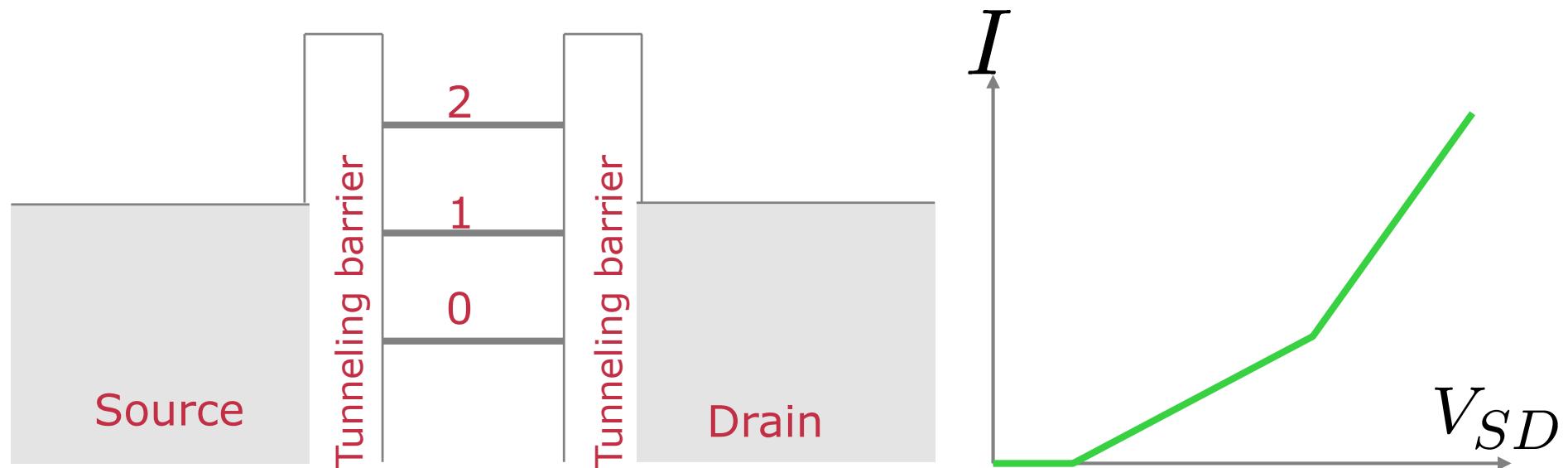
## Energy Levels

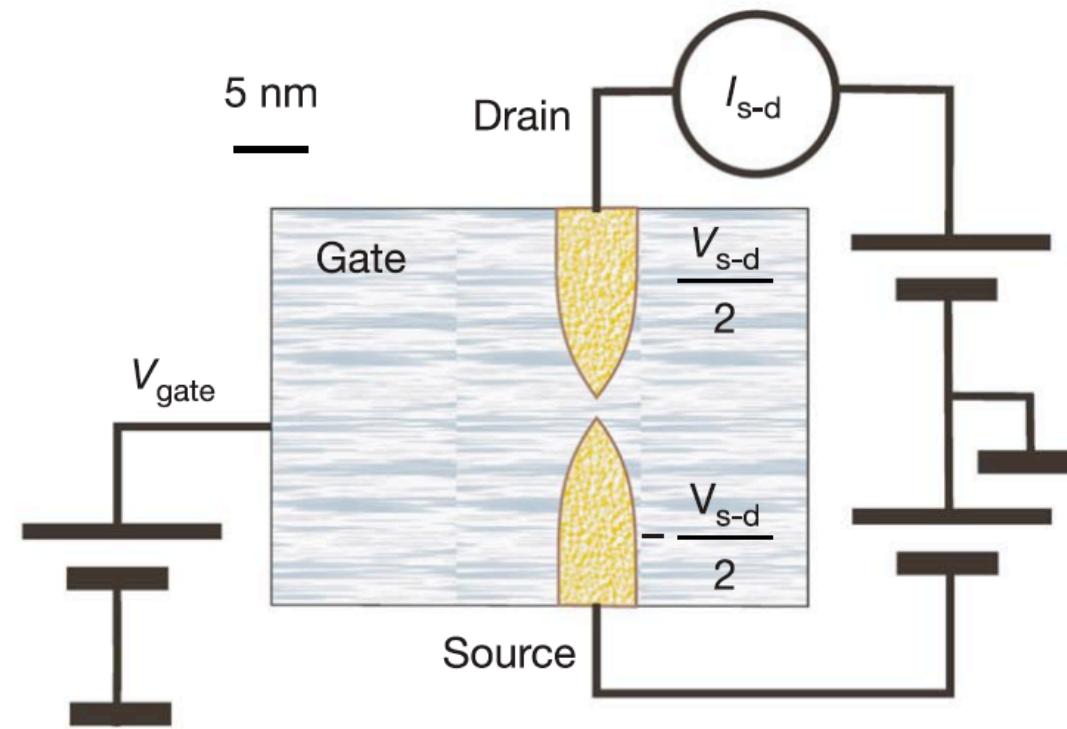
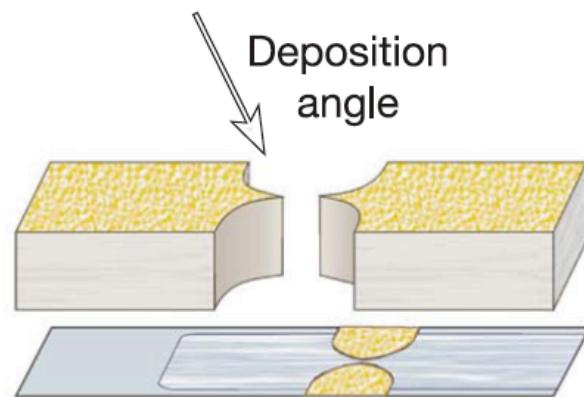


## Varying Gate voltage

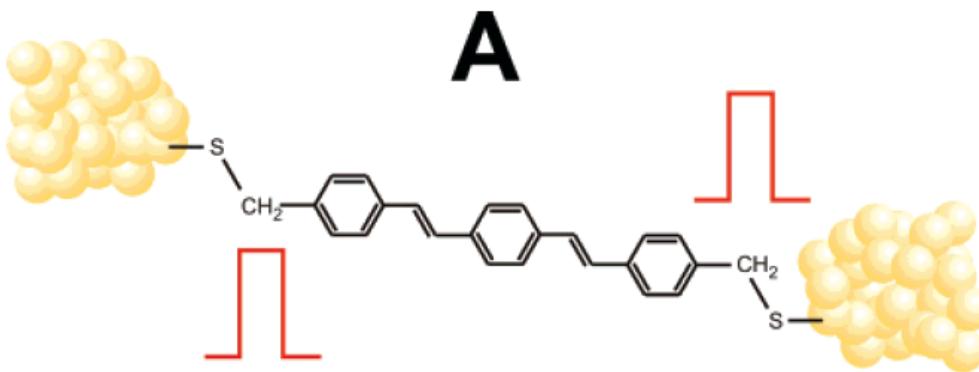


## Varying Source-drain voltage





Kubatkin et al. *Nature* 426 (2003)

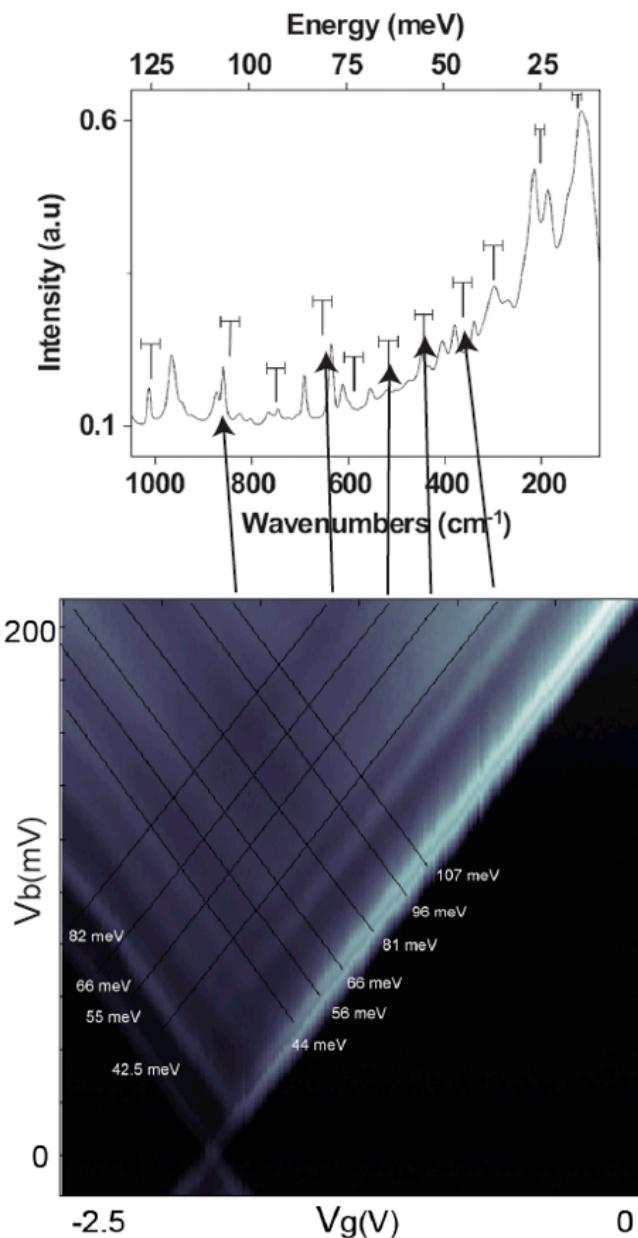
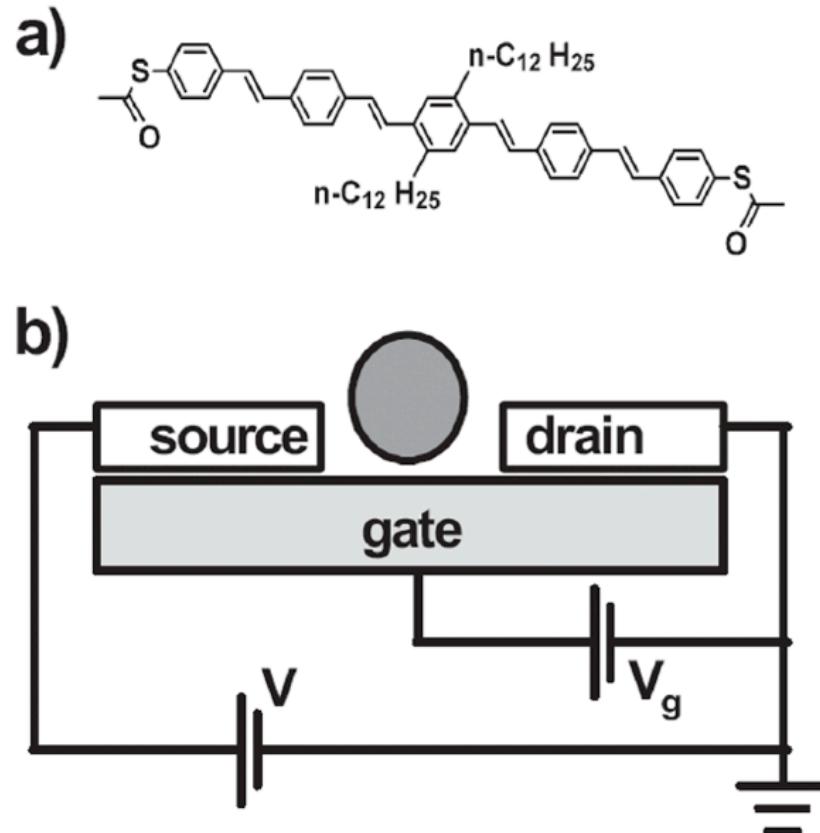


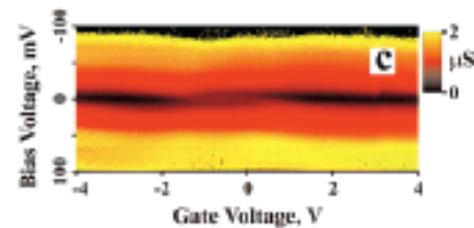
How can we be sure that we are measuring on a single molecule?

What is special about molecules?

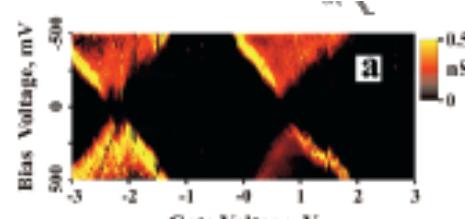
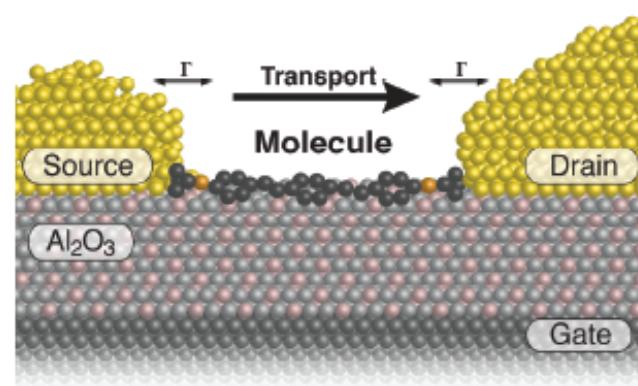
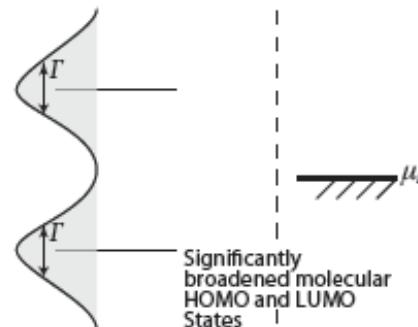
- Molecular vibrations



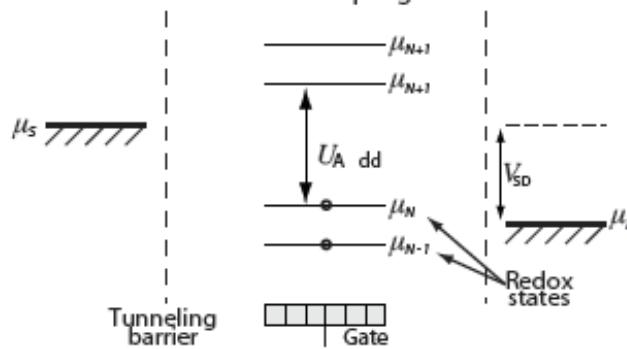




Strong coupling

**Fig. 1**

Weak coupling



## Outline:

1) Measurements on thiol end-capped OPV's

2) *C<sub>60</sub>*

3) C<sub>60</sub> as the "*alligator clip*": a new generation of molecules



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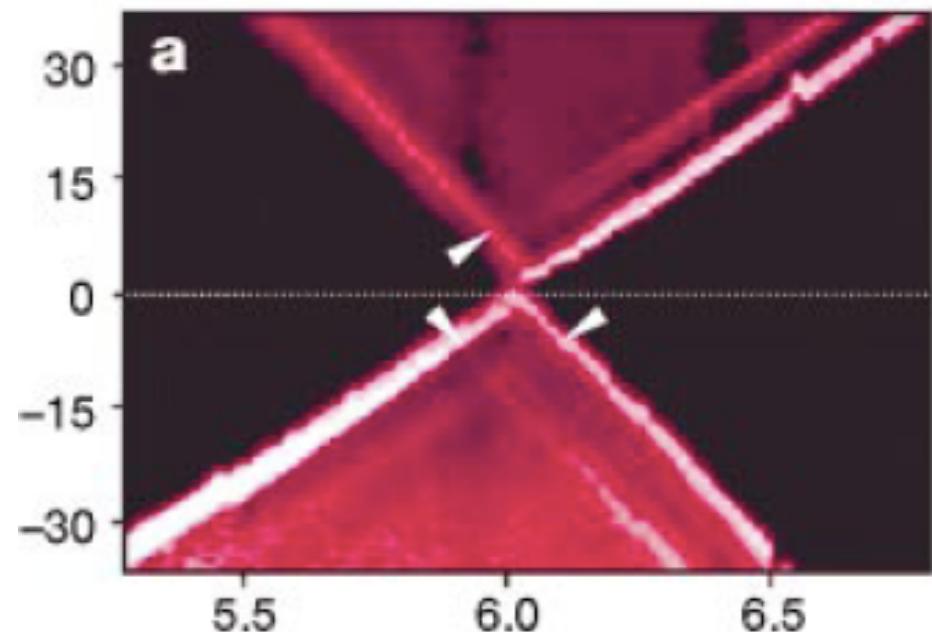
# Nanomechanical oscillations in a single-C<sub>60</sub> transistor

Hongkun Park<sup>\*‡§</sup>, Jiwoong Park<sup>†</sup>, Andrew K. L. Lim<sup>\*</sup>, Erik H. Anderson<sup>‡</sup>,  
A. Paul Alivisatos<sup>\*‡</sup> & Paul L. McEuen<sup>†‡</sup>

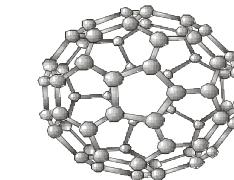
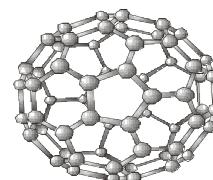
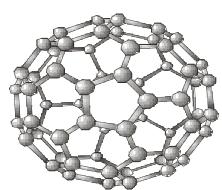
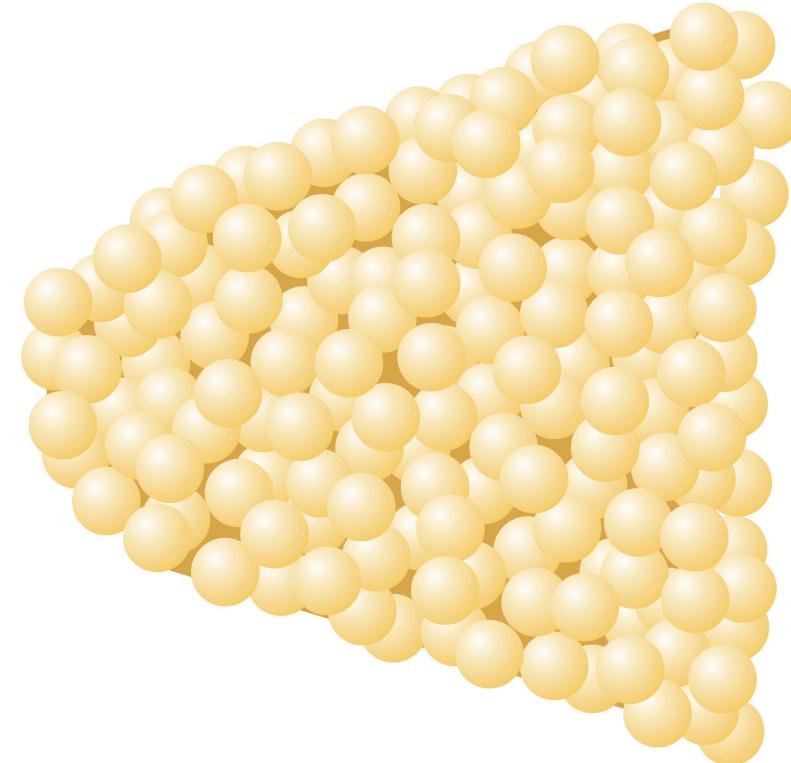
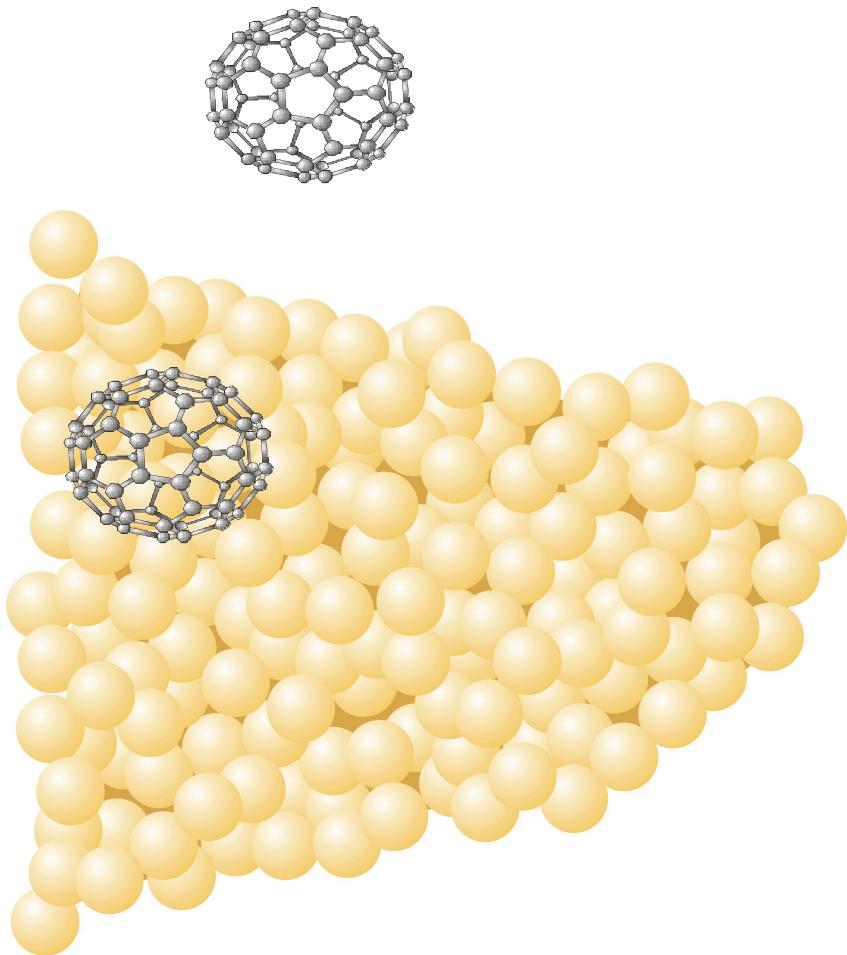
*\* Department of Chemistry and † Department of Physics, University of California  
at Berkeley and ‡ Materials Sciences Division, Lawrence Berkeley National  
Laboratory, Berkeley, California 94720, USA*

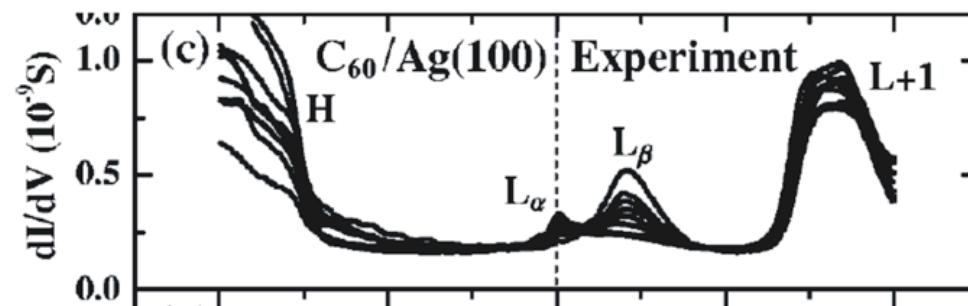
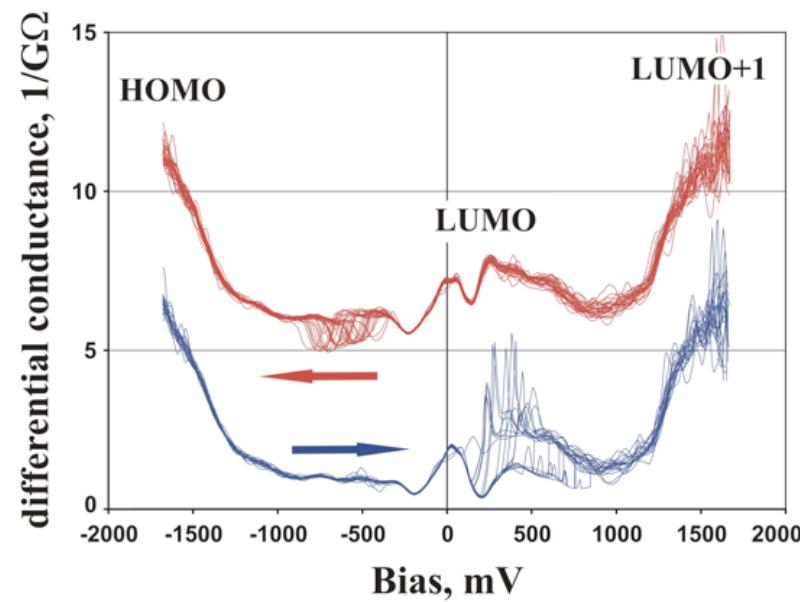
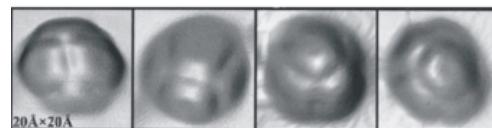
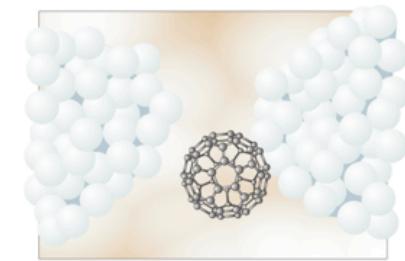
.....

C<sub>60</sub> as a model system,  
*Nature* (2000)



# Nanofabrication: catching a single molecule





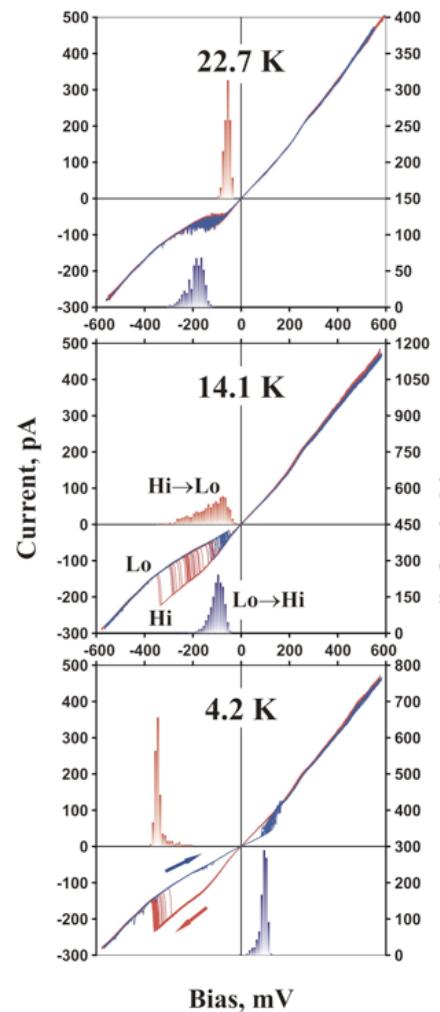
VOLUME 90, NUMBER 9

PHYSICAL REVIEW LETTERS

week ending  
7 MARCH 2003Spatially Mapping the Spectral Density of a Single  $C_{60}$  Molecule

Xinghua Lu, M. Grobis, K. H. Khoo, Steven G. Louie, and M. F. Crommie



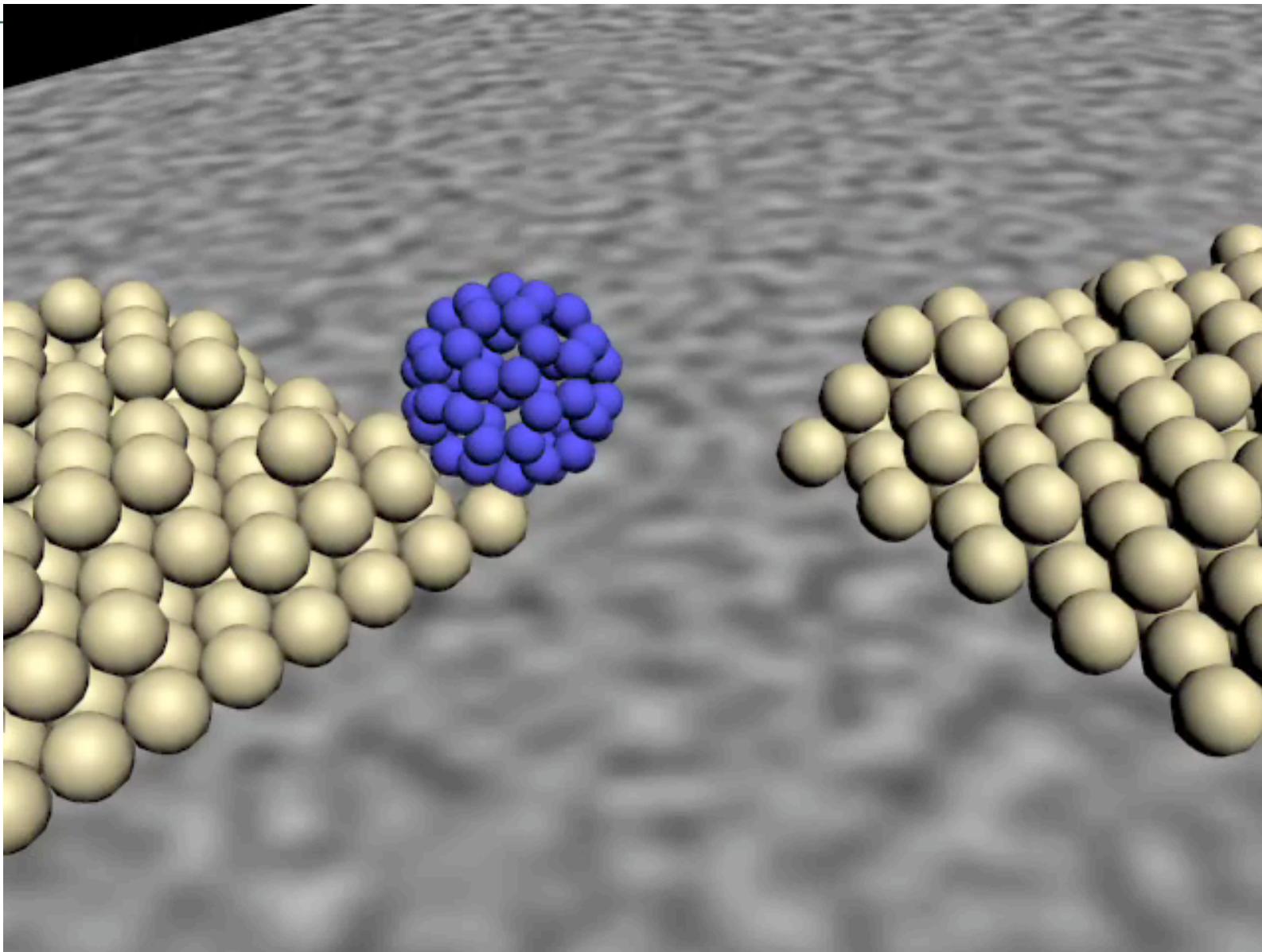
Dripling  $C_{60}$  for six weeks

*Faraday Discuss.*, 131, 337–345 (2006)  
*Nano Lett.* 8, 2393–2398 (2008)  
*Nanotechnology* 18, 165501 (2007)



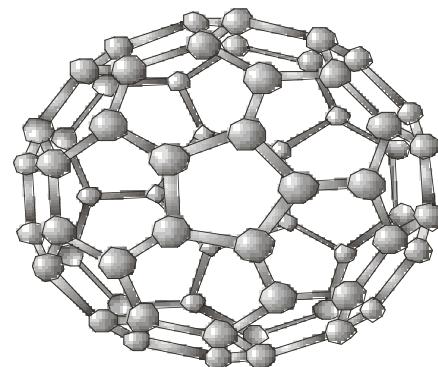


## Faculty of Science



Danilov, Kubatkin *Nano Lett* 2008

## Summary C60:



- In this experimental setup, C60 is strongly coupled to the electrodes\*
- The C60 switches between 2 different states, the system is stable for more than 6 weeks
- The two states might be attachment via 5 or 6 fold symmetry positions

\* In contrast to measurements by Park and McEuen *Nature* 2000

*Faraday Discuss.* 131, 337–345 (2006)  
*Nano Lett.* 8, 2393–2398 (2008)  
*Nanotechnology* 18, 165501 (2007)



## Outline:

- 1) Measurements on thiol end-capped OPV's
- 2) C60
- 3) C60 as the "*alligator clip*": a new generation of molecules

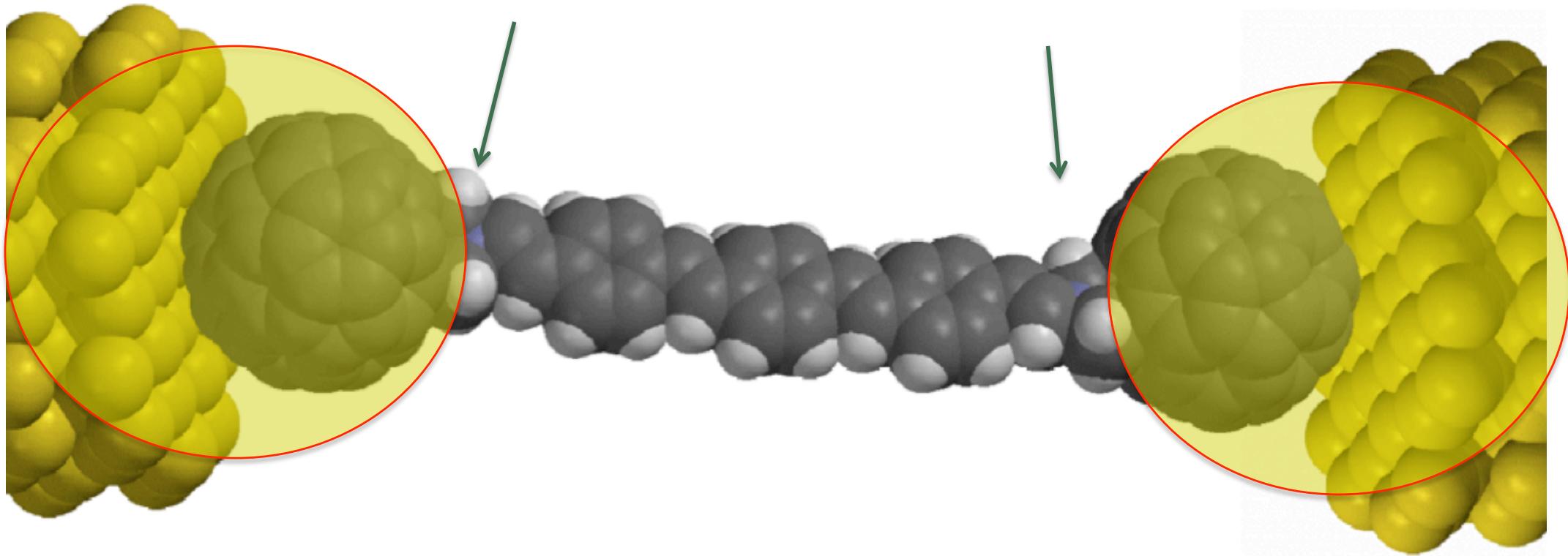


- In molecules, the atoms are placed in a well defined way with respect to eachother
  - The problem is the electrodes, and the interface between molecule and electrode
  - Since C<sub>60</sub> couples strongly to electrodes we might be able to use it to contact a molecule!

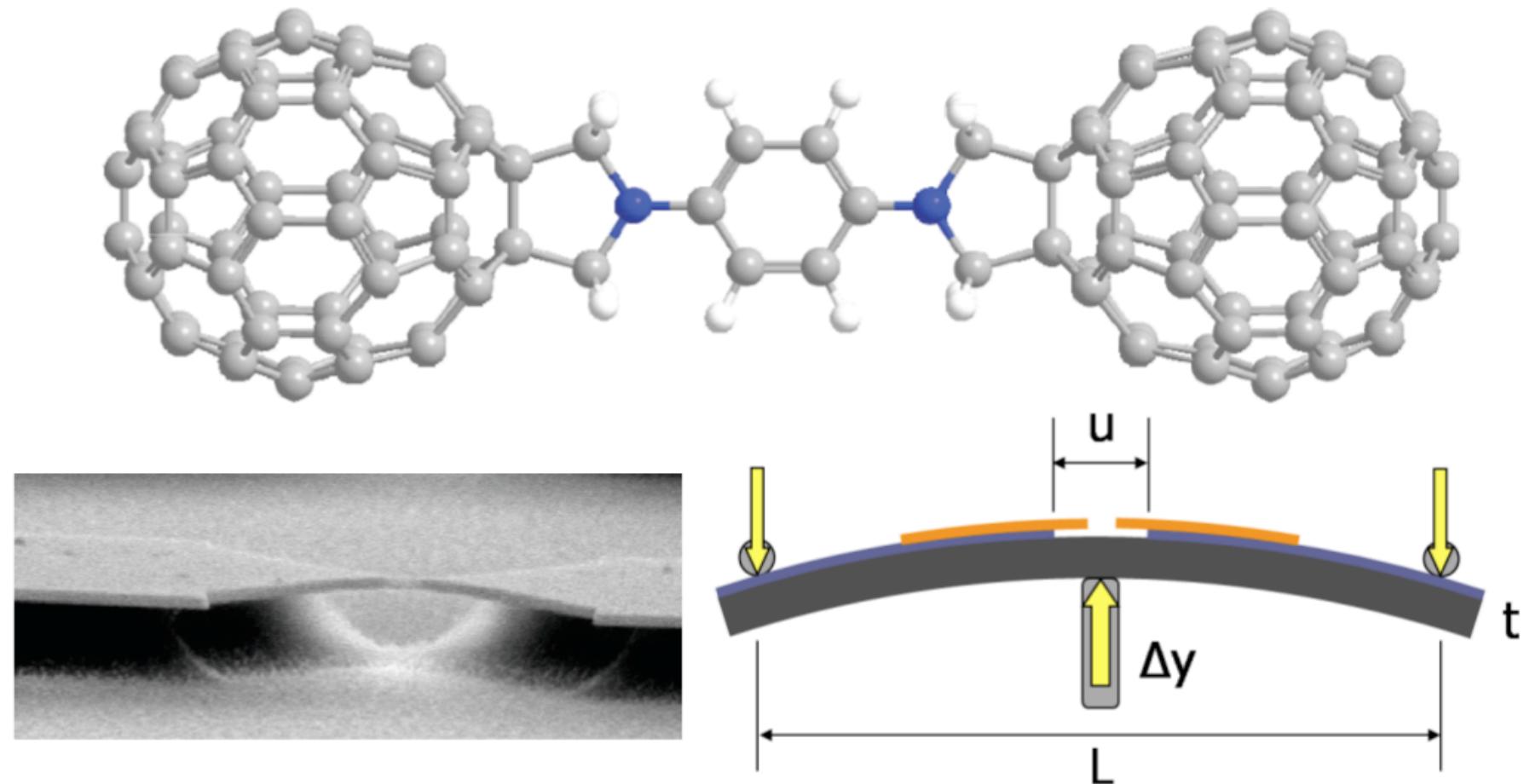




## Covalent defined interface



# (not yet gated) mechanical break junctions



January 25, 2008

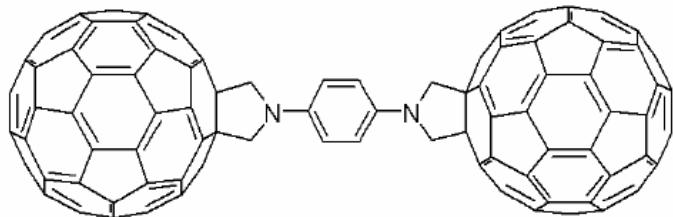
Christian Martin

Work done in collaboration with Jan van Ruitenbeek

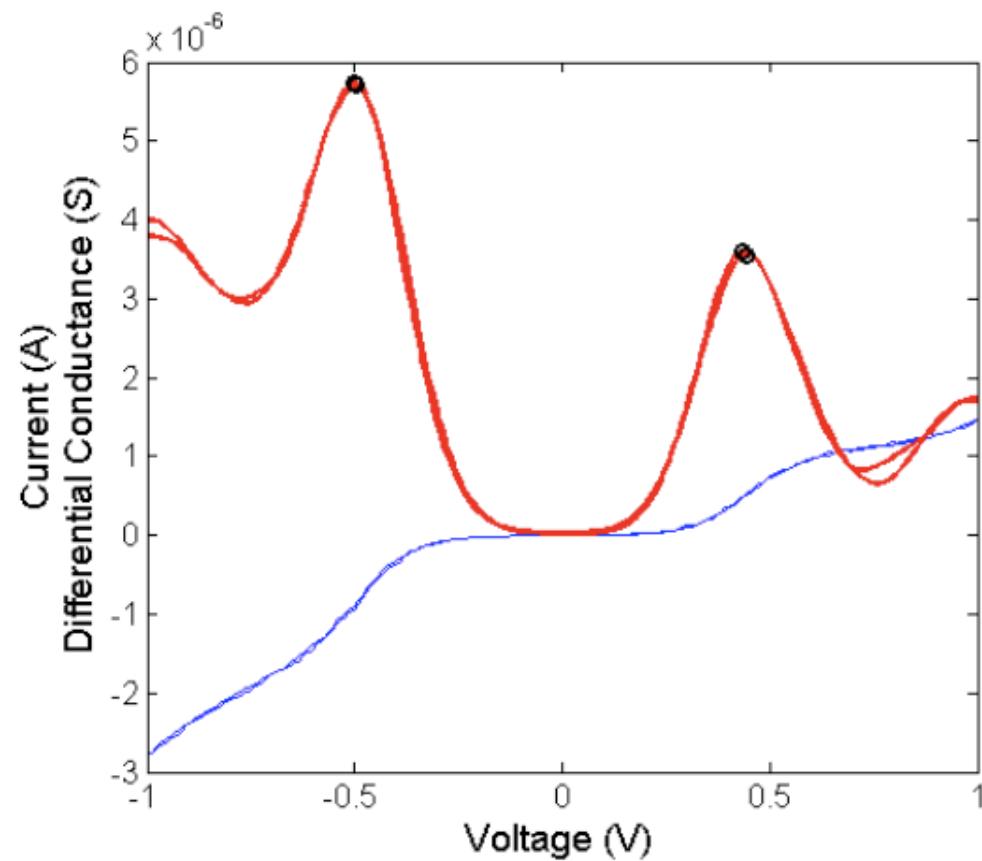
TU Delft



# Very stable current-voltage characteristics



Room temperature measurements.



January 25, 2008

Martin, Ruitenbeek, van der Zant JACS 2008 (accepted)

## Summary:

- We have used STM to compare the tunnelling through different molecules
- We have used *three terminal measurements* to reveal details about the electron transport through single molecules
- We have tested C60 as a new type of alligator clip, and thereby defining the important interface between molecule and electrodes by covalent chemistry



Thank you!

