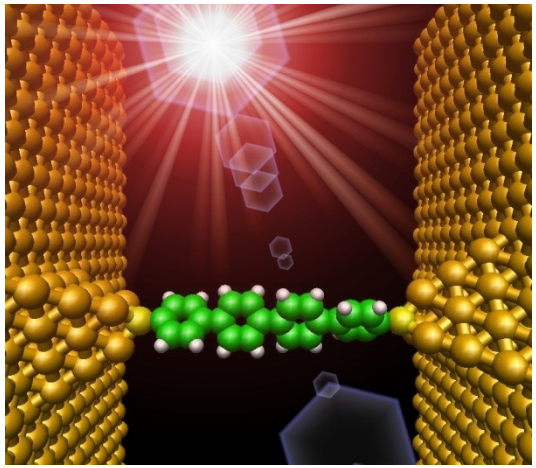
JACOBS UNIVERSITY

Realization of A Unimolecular Rectifier



Seminar - Current Topic Presentation

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Masters of Science in Nanomolecular Science

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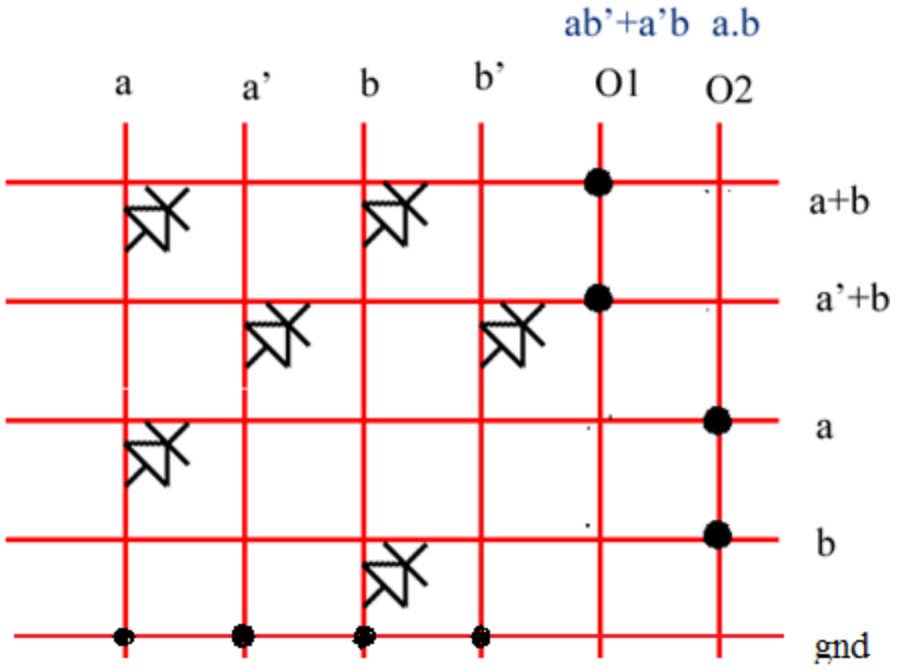
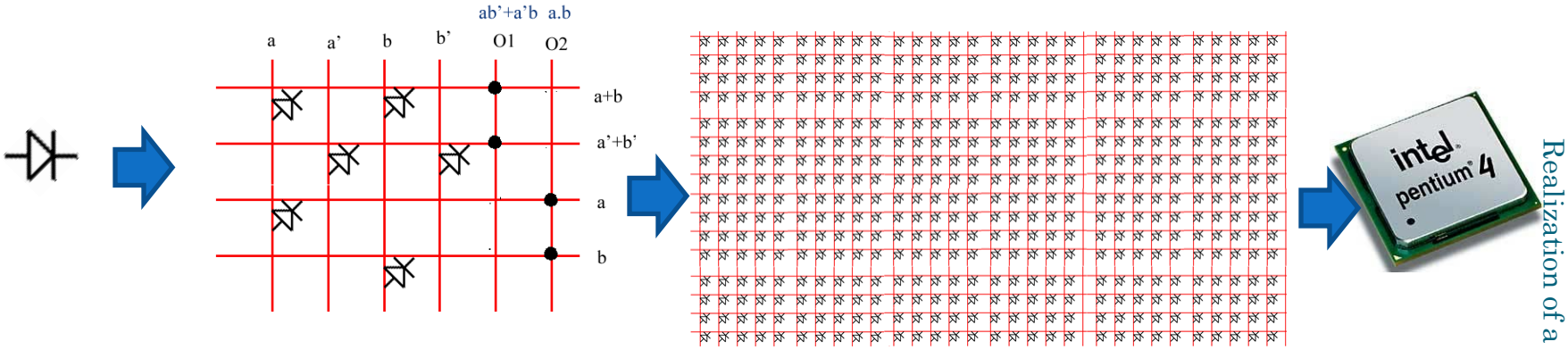
A RECTIFIER-INTRODUCTION

- Allows unidirectional flow of current.
- A semiconductor diode is made by the junction of p-doped and a n-doped semiconductor.



a	b	O1 (Sum)	O2 (Carry)
0	0	0	0
1	0	1	0
0	1	1	0
1	1	0	1

Simple Half adder logic circuit using rectifiers.



Switching device (Rectifier) Logic Circuit N-bit Device Processor

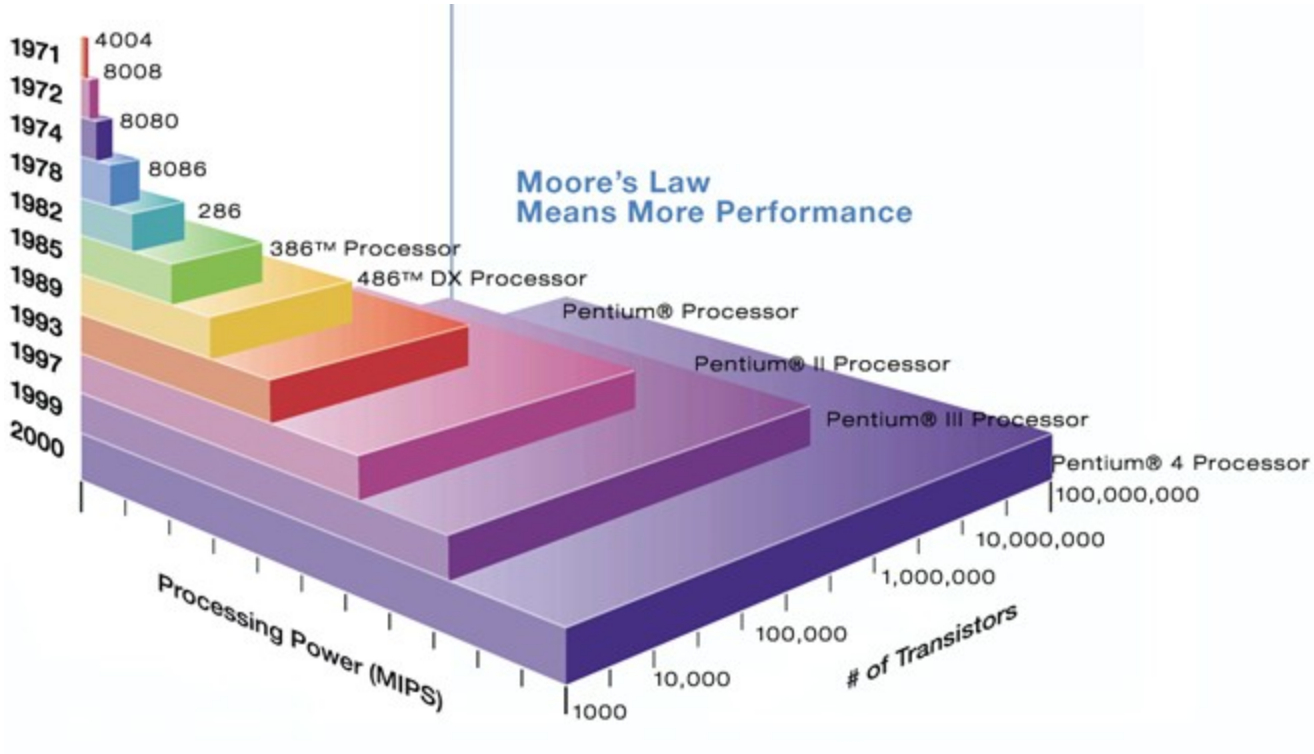
Latest developments in conventional processors:

-Intel® Core™i processors releazed in early 2010, is the first processor with 32nm technology (CMOS channel length).

-Intel Itanium processor (65nm technology) is the first 2 Billion transistor Microprocessor.

Source: Intel.com

Need of a Unimolecular Device



- About every two years number of transistors per chip, cost per bit and the processor speed will double – Intel's co-founder Gordon Moore

Source: Intel.com

Problems with conventional silicon technology

How far we can carry along the Moor's prediction?
Can we prevent the tunneling of carriers and breaking of an oxide layer?
Can we efficiently manage the dissipated heat for shorter channel length?

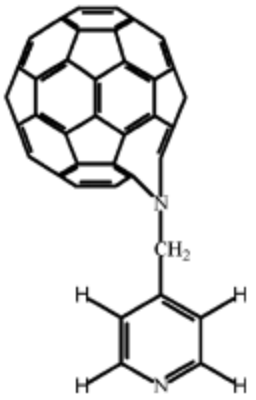
UNIMOLECULAR RECTIFIER

- Device made up of single molecule between the conductors, that allows the flow of electron in a single direction, under proper biasing.
- First conduction mechanism in the unimolecule was proposed by Aviram and Ratner in 1974.
- Unimolecular conduction is favoured by the presence of electron rich moiety (subunit) to the electron poor moiety, but disfavored in the reverse direction.
- Conduction takes place through the HOMO (Heighest Occupied Molecular Orbital) and LUMO (Lowest Unoccupied Molecular Orbital), in a molecule.

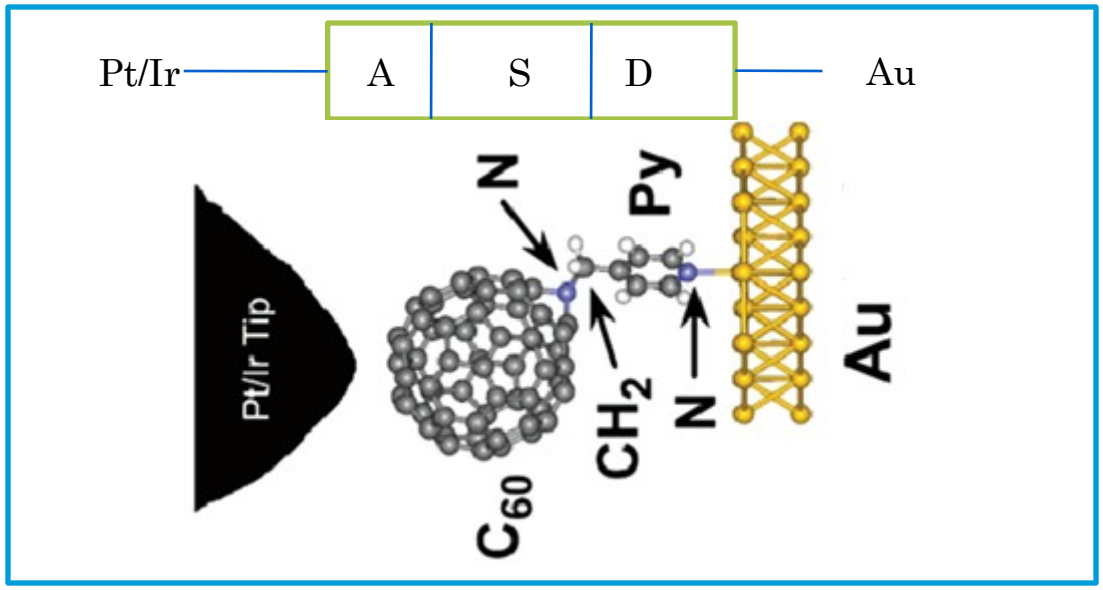
[Areih Aviram, Mark A. Ratner, '*Molecular Rectifiers*', Chem. Phy. Lett. 29, 277-283 (1974).]

SINGLE MOLECULAR DEVICE

- Single molecular rectifier C_{60}NPy oligomer present between gold and Platinum/Iridium (Pt/Ir) contact terminals.
- Fullerene molecule act as the electron acceptor (A) group from the Pt/Ir electrode.
- Pyrodyl group act as the electron donor group (D) to the gold electrode.
- CH_2 group forms the sigma (S) bridge, neutral region.
- Can be compared as NP junction diode .

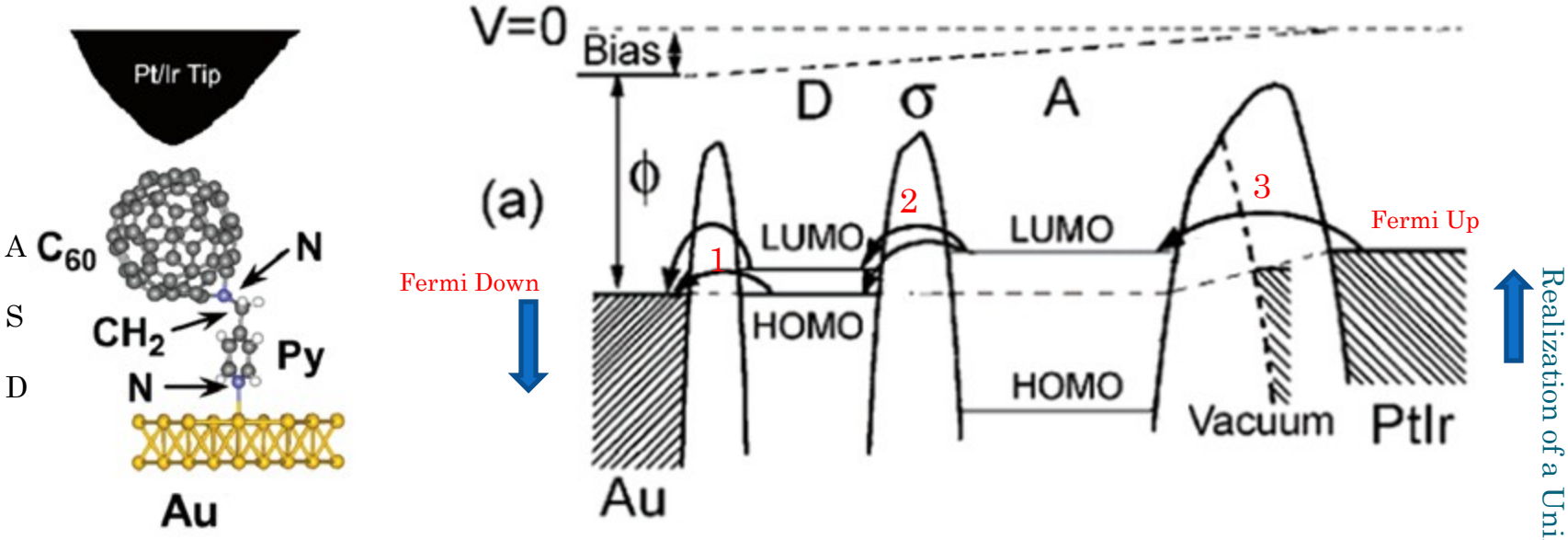


N-3-γ-Pyrodyl aza[60]fulleroid (C_{60}NPy)



[J. Phys. Chem. B 2006, 110, 24505-24512]

Conduction mechanism in Unimolecule



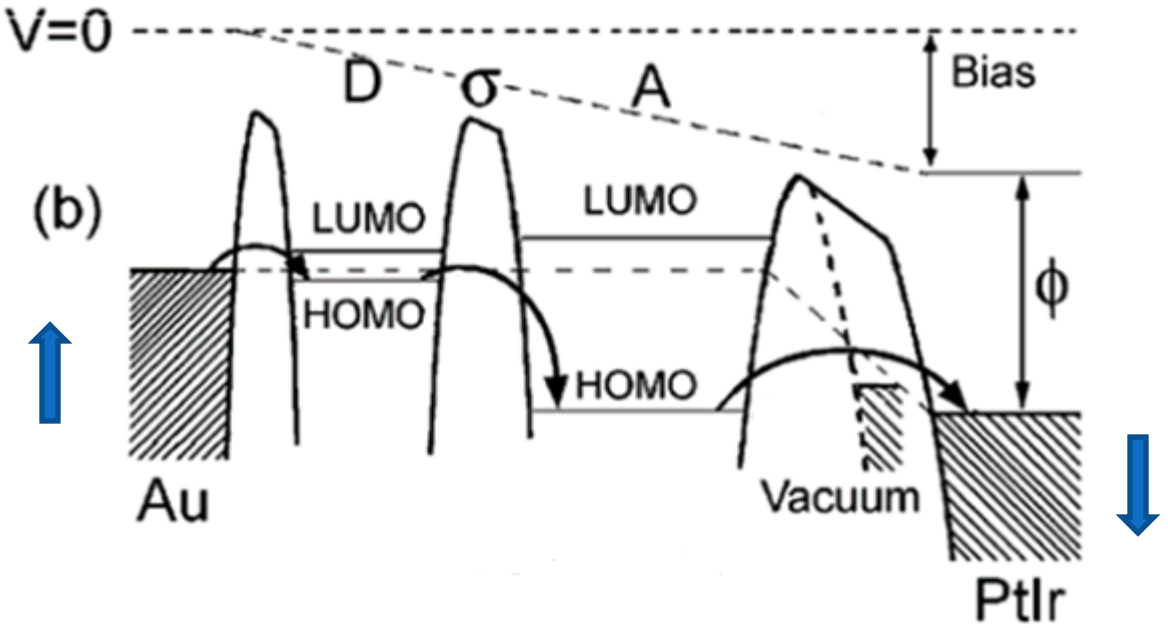
[J. Phys. Chem. B 2006, 110, 24505-24512]

Case 1:Forward biased

Step1: Electron tunnels from HOMO of Donor to Positive Au-Electrode.

Step2: Electrons of Anode (PtIr) tunnels to LUMO of Acceptor molecule through the vaccuum.

Step 3: Electrons from LUMO of Acceptor tunnels to Donor through thin sigma barrier.



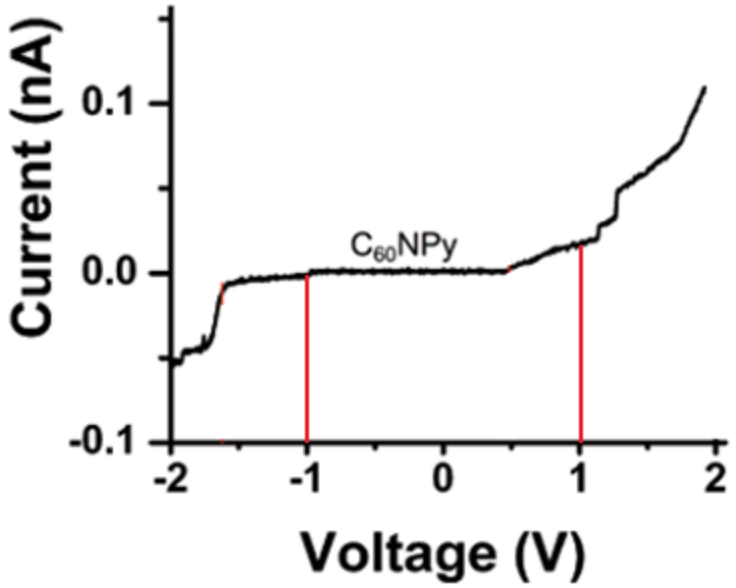
[J. Phys. Chem. B 2006, 110, 24505-24512]

Case 2: Reverse biased

- The reverse conduction is prevented because we need very high reverse bias potential at the Pt/Ir electrode.
- This potential shift the fermi level of electrode much below the HOMO of Acceptor molecule.
- Since, LUMO are empty and HOMO are the filled state, electron can
- only jump along the HOMO level.

Electrical characteristics

- Rectification ratio (RR)
  - I(V)/I(-V)



[J. Phys. Chem. B 2006, 110, 24505-24512]

RR was found to be 10 (±1V) for C_{60}NPy molecule, when proper biasing was provided.

Application

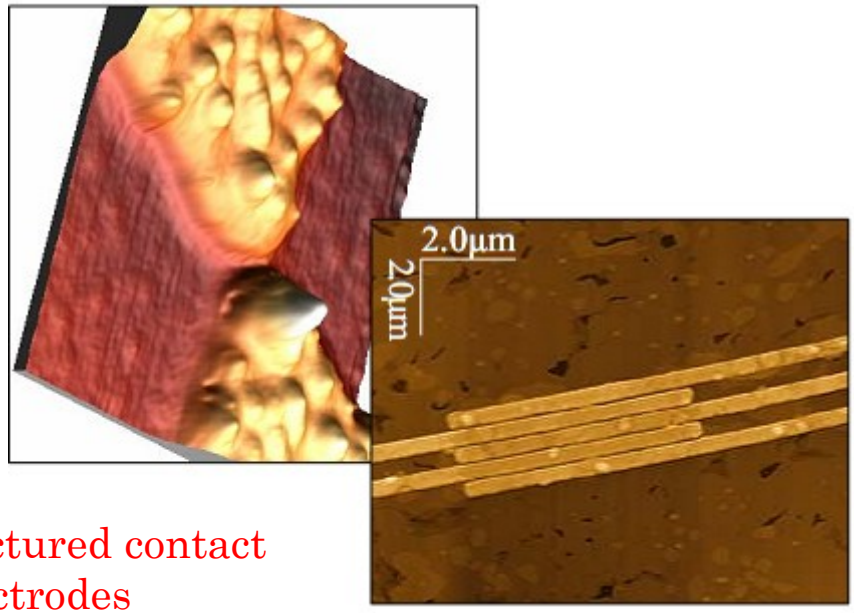
- Size of a rectifier is only few nanometres.
- Considering individual device size as 10nm we can accommodate today available Intel Itanium 9300 series microprocessor (65nm technology) having 2 billion transistors in an area of only $1mm^2$.

Major Problems

- Very low rectification ratio. Ideally, a solid state diode has an infinite rectification ratio.
- Fixation of single molecule across the two metal electrodes.

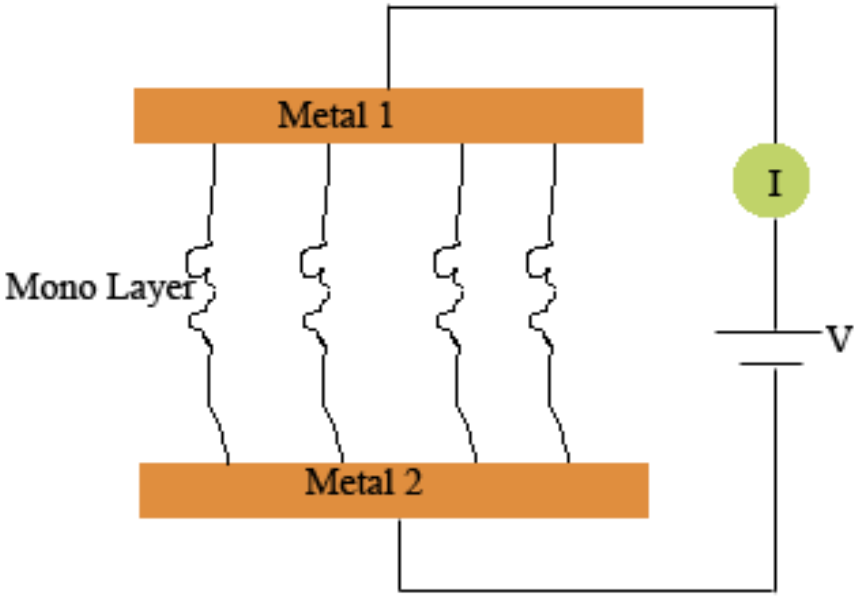
Approach towards Single molecular junction

- E-beam lithography technique-Nanostructure printing
- Scanning Probe Method
- Monomolecular film method
- Mechanically Controlled Break Junction (MCB)



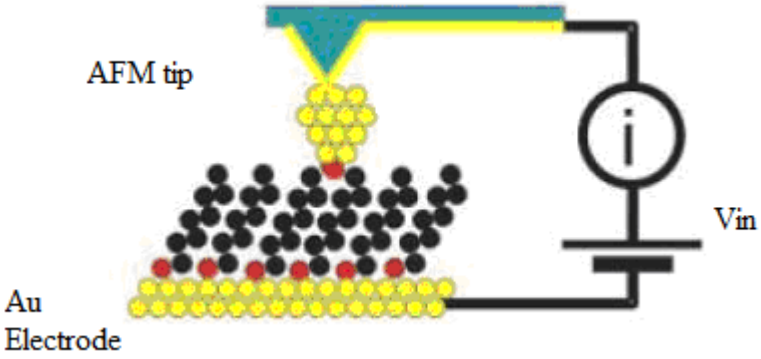
Nanostructured contact electrodes

[Jacobs SEM, Wagner's group]



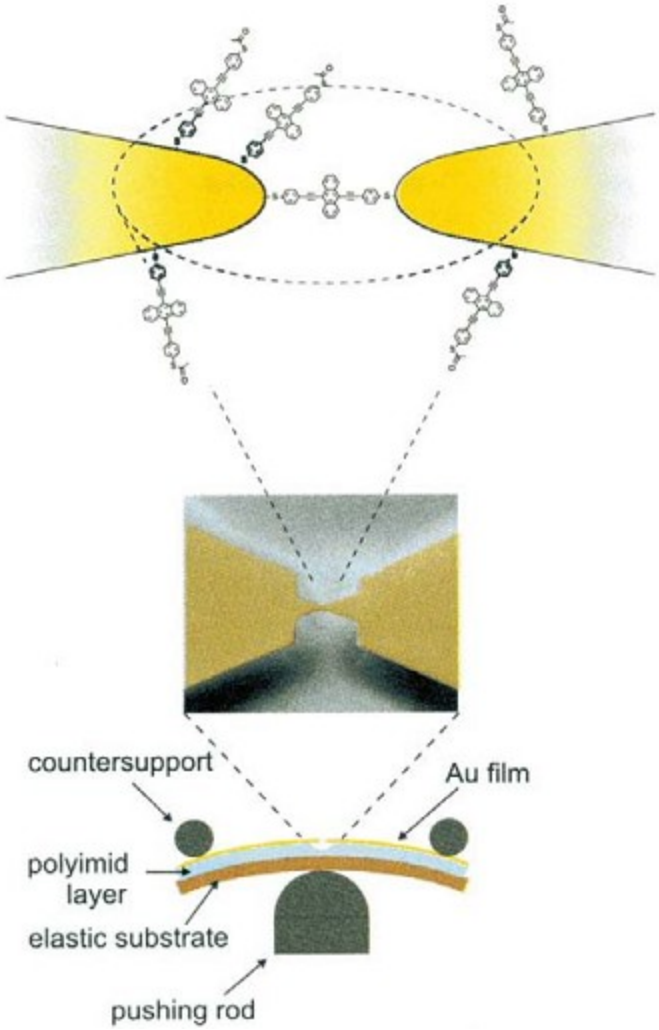
A thin monolayer between two parallel metal surface.

[Appl. Phy. Lett. 66, 3331 (1995)]



A molecule between AFM tip and the electrode.

[Science 292 (2001) 571]

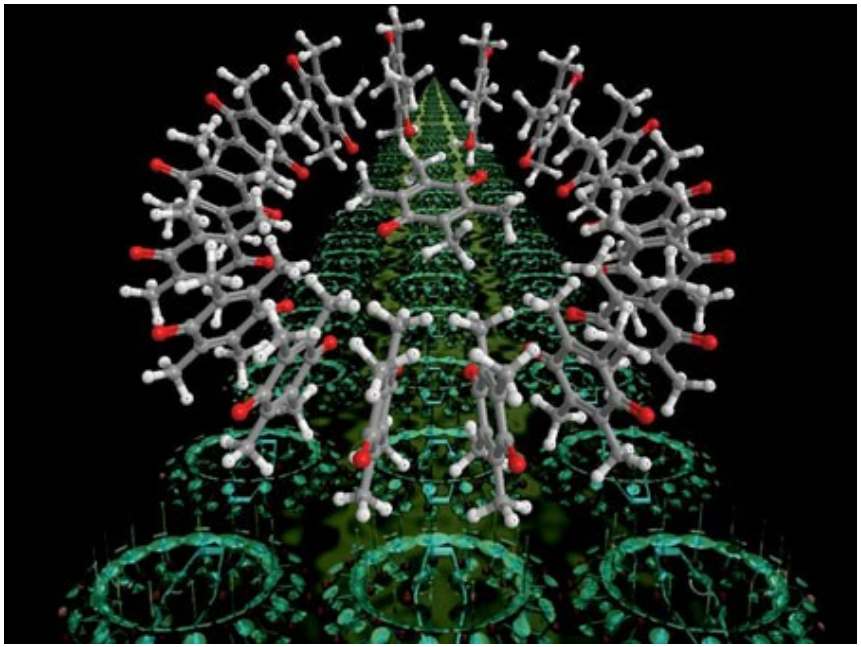


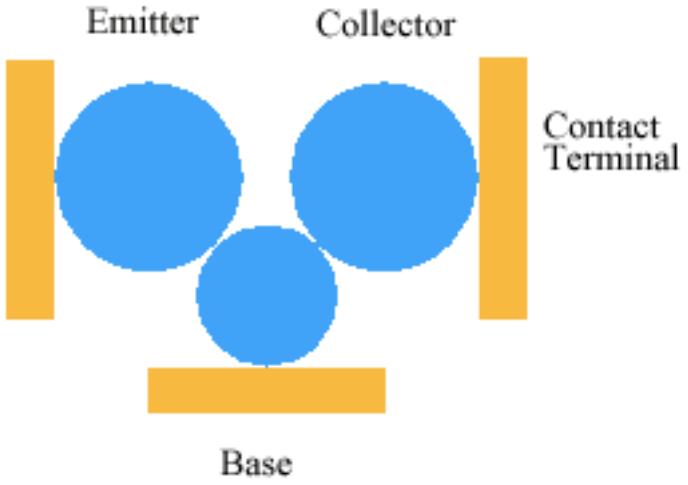
By pushing a rod we can precisely create the nano-scale dimension equal to the size of the molecule using MCB technique.

[Waser , Wiley 2003]

Future Scope- multiterminal input device

- High two high π-electron cloud (E and C-n) region separated from low-electron cloud (B-p) from the σ-region analogous with the solid state bipolar junction transistor (BJT).





Proposed unimolecular transistor.

[Springer, 313-349 (2006)]

- Combination of multiple unimolecular device for parallel processing (first proposed 16-bit molecular processor).

[3668–3672 PNAS March 11, 2008 vol. 105 no. 10]

Conclusion

- Unimolecular rectifiers has huge potential towards low cost device fabrication-nanoprocesso.
- Cost of bit for a device area is decreased rapidly.
- Potential approach for three terminal device understanding and modeling.


Thank you!