Electronic Transport in Molecular Scale Devices

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I. Electronic Transport of Micro & Nano Via-hole Structures for Molecular Electronic Devices

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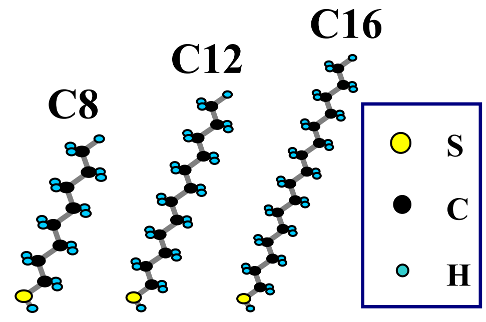
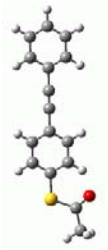
Formation of Alkanethiol Self-Assembled Monolayers

Standard alkanethiol molecule

- **Octanethiol (C8) - $CH_3(CH_2)_7SH$ / length = 13.3Å**
- **Dodecanethiol (C12) - $CH_3(CH_2)_{11}SH$ / length = 18.2Å**
- **Hexadecanethiol (C16) - $CH_3(CH_2)_{15}SH$ / length = 23.2Å**

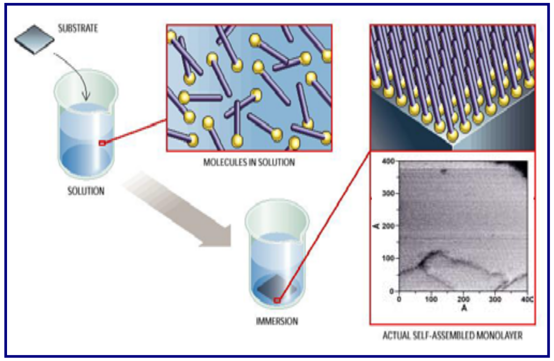


Conjugated molecule: Oligo(phenylene ethynylene) (OPE)



OPE provided by Dr. Changjin Lee (KRICT)

Self-assembled monolayer (SAM)



Reed & Tour, Am. Sci. June 2000

- **A spontaneous chemisorption process**

  $RS\text{-}H + Au \rightarrow RS\text{-}Au + 0.5\ H_2$
- **Chemical bond formation of functional end groups of molecules with the substrate surface**
- **Intermolecular interactions between the backbones**

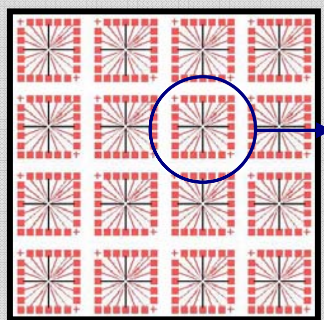
Fabrication of Planar-type Via-Hole Molecular Devices

Design and Fabrication of molecular electronic devices

Optical lithography: ~ 2 μm
Plan: E-beam lithography: ~ 50 nm

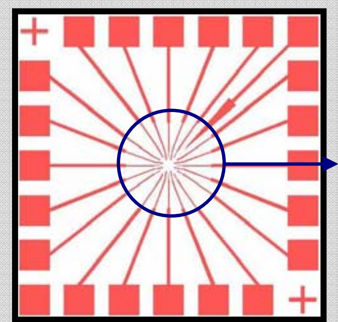
Mask pattern

Unit



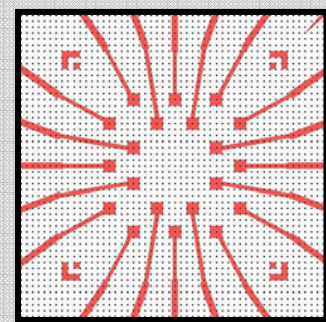
1 cm

Die



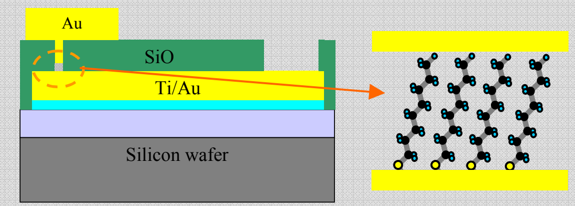
2.5 mm

Devices



190 μm

Schematic of device

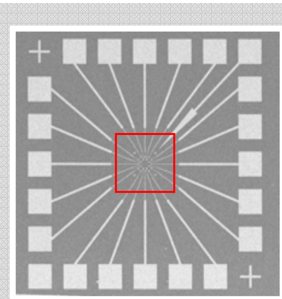


One unit Contain 16 dies
Each die contains 20 devices
Total devices are 320 in a unit

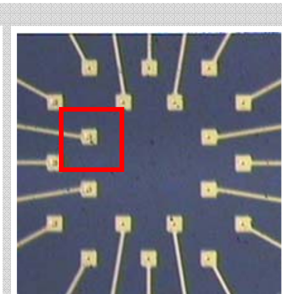
SEM / AFM / Optical images

4” wafer (Collaboration with ETRI, Dr. Hyoyoung Lee)

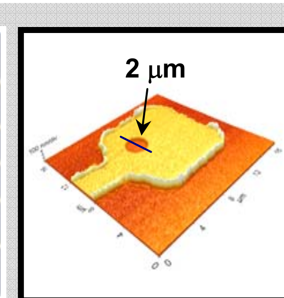
1 cm piece



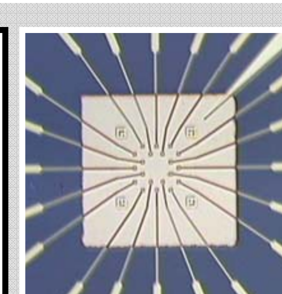
Die



Devices



AFM image of a device



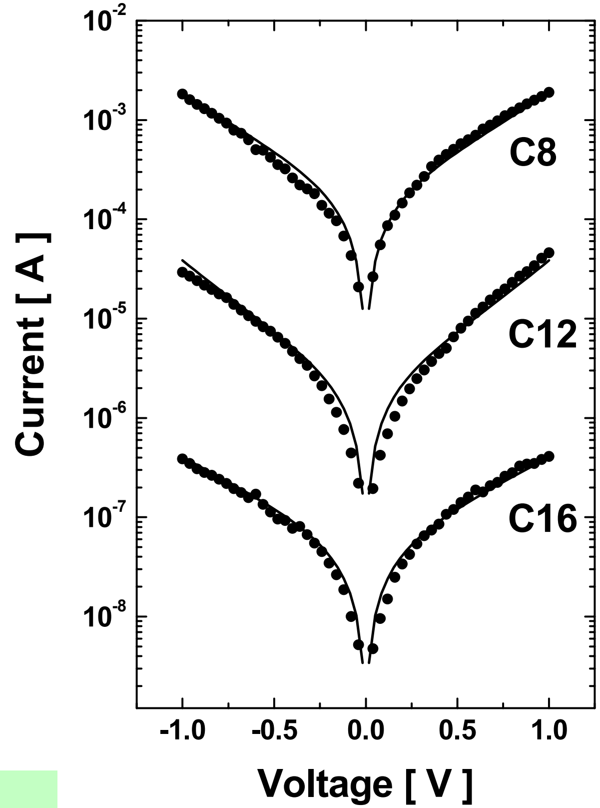
After Top electrode

Yield of Microscale Via-Hole Molecular Devices

1. Yield of molecular devices ?
2. How to define working molecular devices ?

Device yield (micro-via hole molecular devices)

# of fabricated device	Fab. failure	short	Open	Working		
				C8	C12	C16
13440	392	11744	1103	84	57	60
				201		
100%	2.9%	87.4%	8.2%	1.5%		



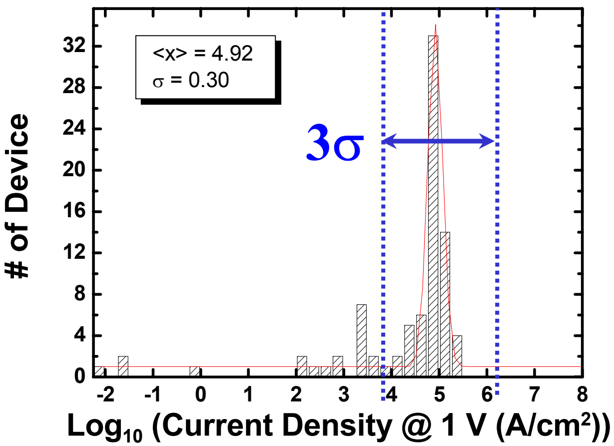
Simmons tunneling fitting results for all working devices

Alkanethiol	J at 1 V (A/cm²)	Φ_B (eV)	α	β (Å⁻¹)
C8	78000±46000	1.29±0.49	0.76±0.09	0.87±0.16
C12	2000±400	1.26±0.08	0.72±0.04	0.83±0.04
C16	5.2±4.7	2.67±0.28	0.52±0.04	0.87±0.05

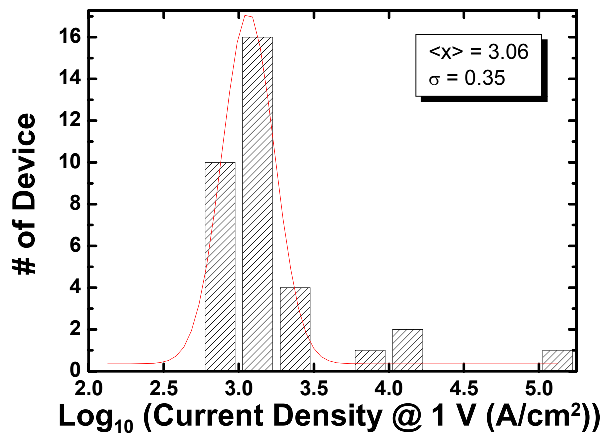
Representative devices determined by Gaussian fitting of J !

Determination of Working Molecular Devices

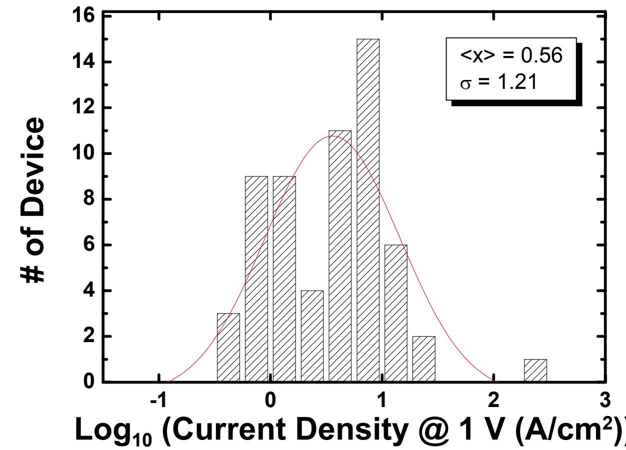
Log (J) for C8



Log (J) for C12

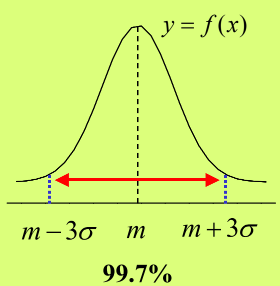


Log (J) for C16

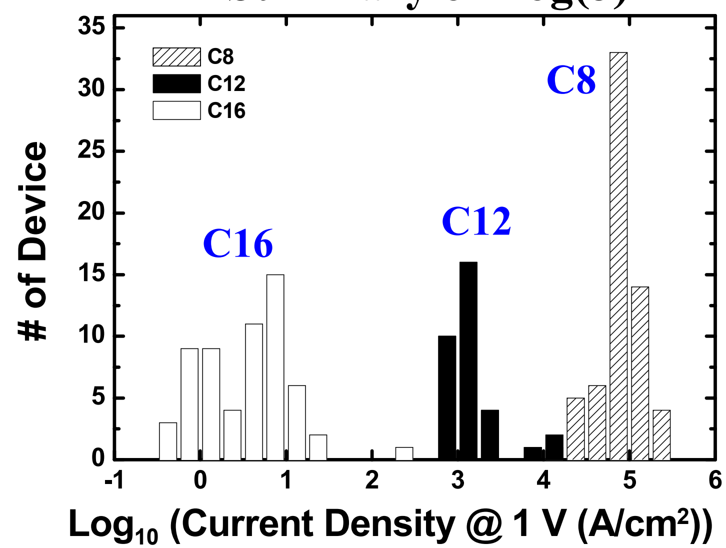


Gaussian fitting (3σ: 99.7 %)

$$f(x) = \frac{1}{\sqrt{2\pi\sigma}} \cdot e^{-\frac{(x-<x>)^2}{2\sigma^2}}$$



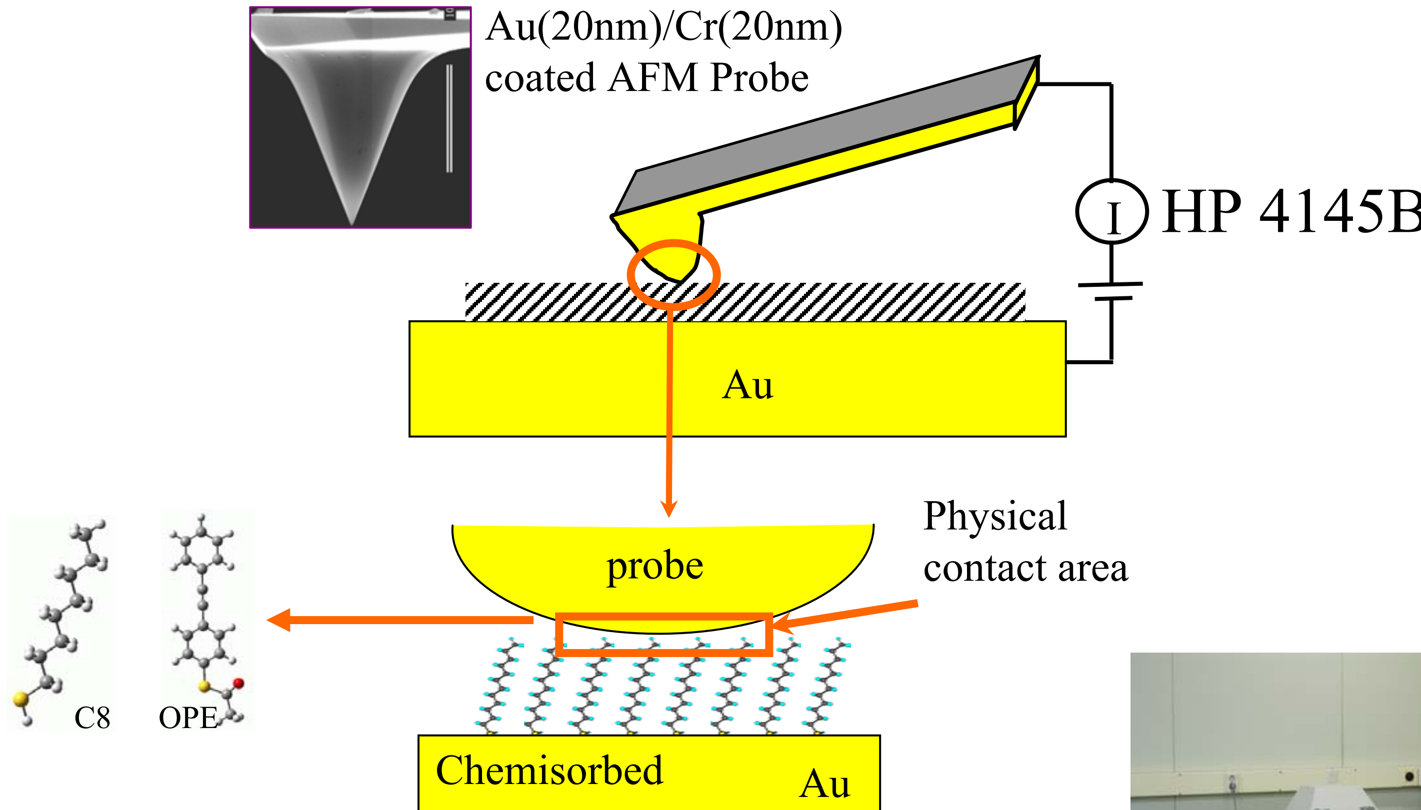
Summary of Log(J)



II. Molecular Electronic Junctions Studied by Conducting Atomic Force Microscopy

Hyunwook Song

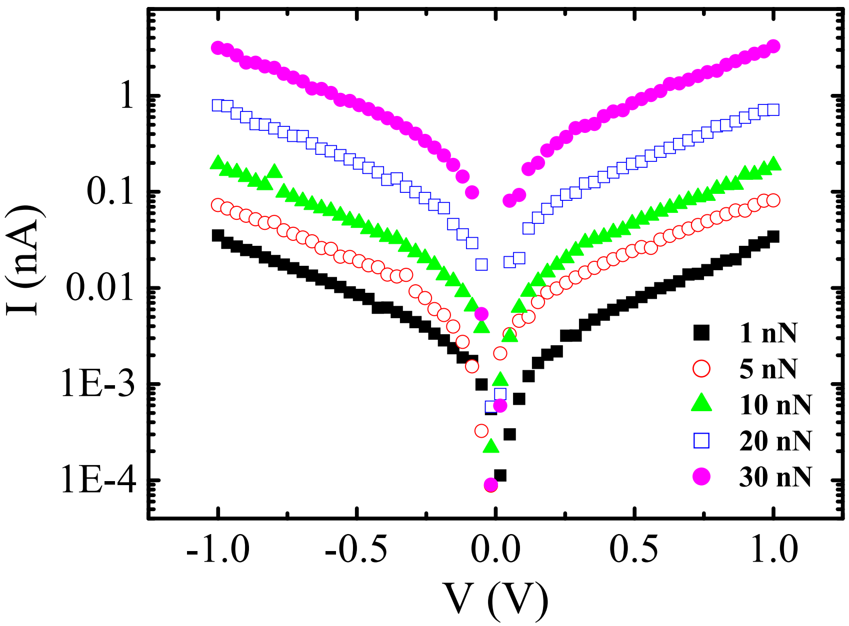
Charge Transport Study by CAFM



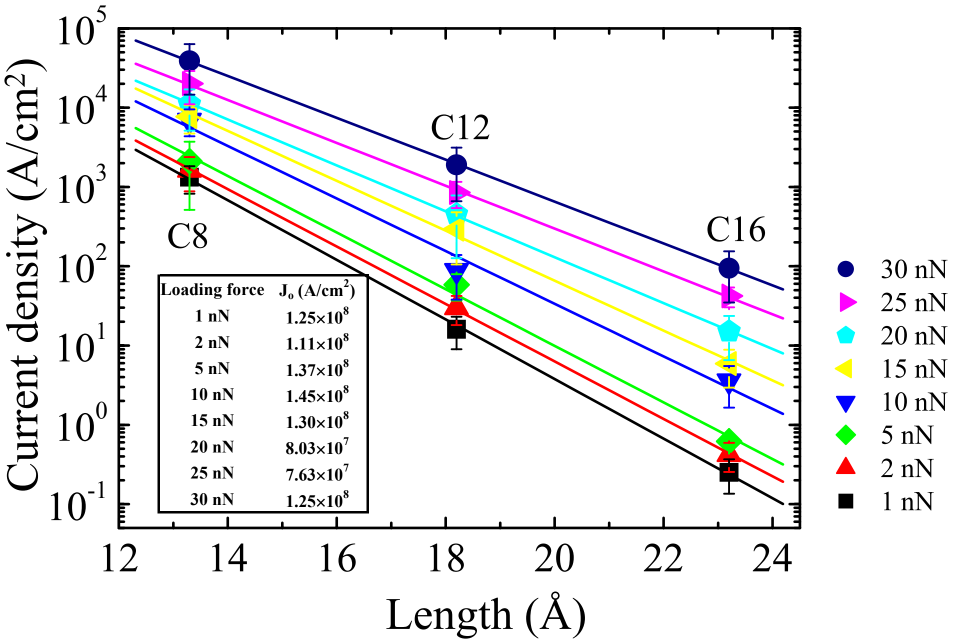
PSIA, XE-100 model
ambient AFM

Force-and Length-Dependent Tunneling

I(V) for C12 (1 to 30 nN)



J @ 1 V (1 to 30 nN)



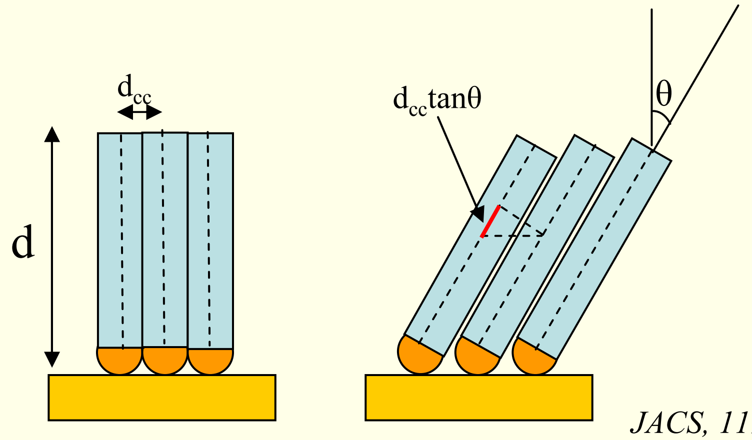
- Larger current with larger loading force
- J: C8 > C12 > C16
- Error bar: sample-to-sample variation

Exponential dependence

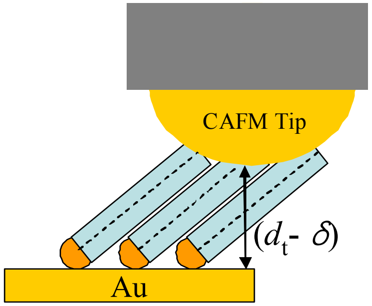
$$R \propto \exp(\beta d)$$

Through-bond vs. Through-space

Tunneling distance in "through space" = $\mathbf{d - d_{cc}\tan\theta + d_{cc}}$



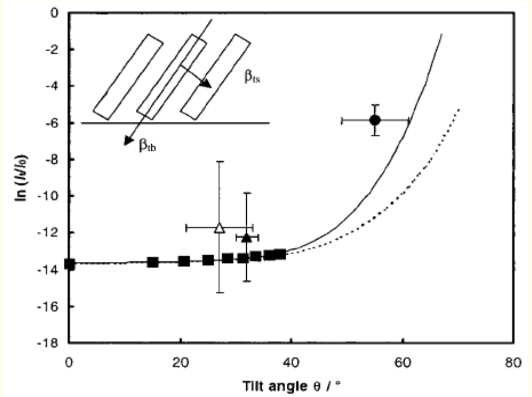
JACS, 119, 11910 (1997)



$$I_t = I_0 \exp(-\beta_{tb} L_M) +$$

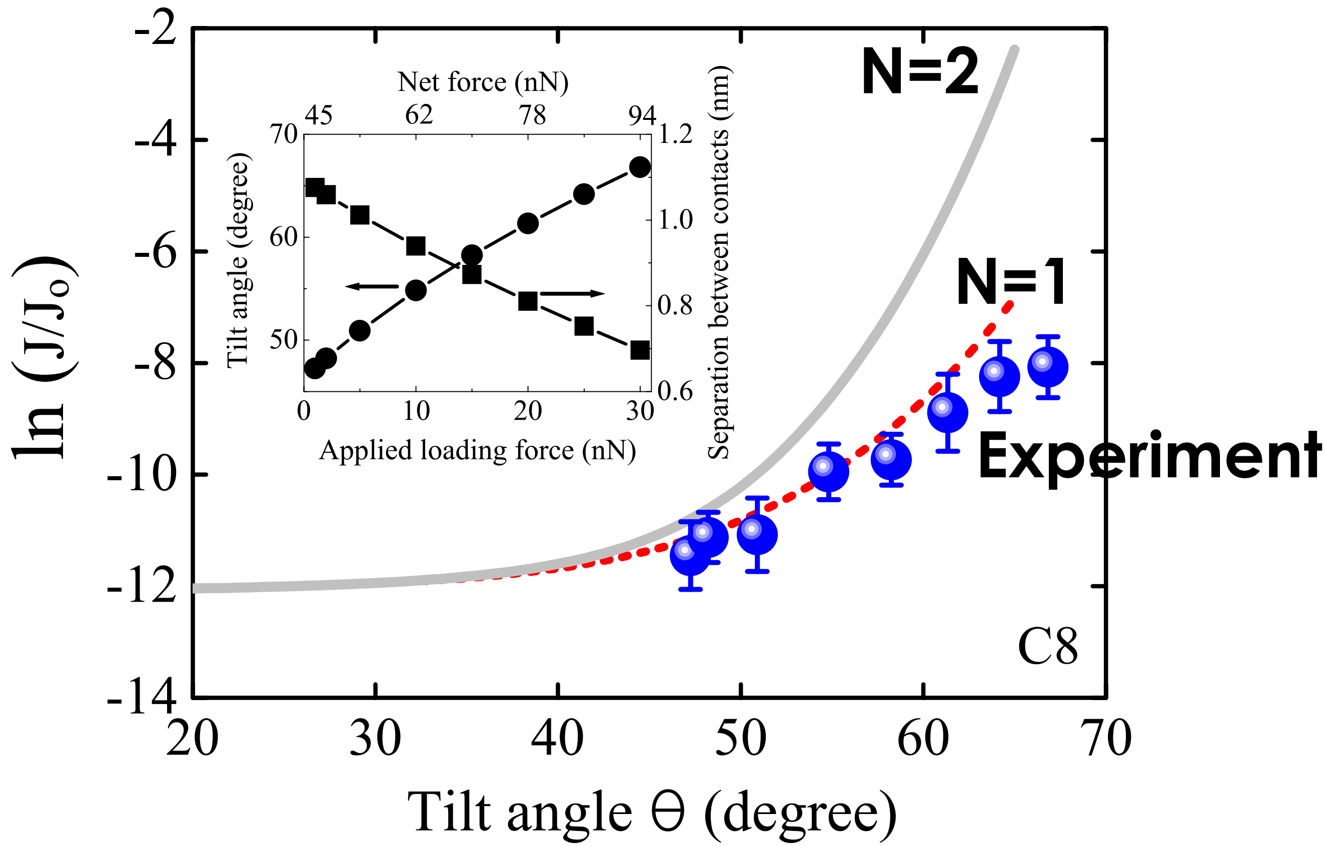
$$I_0 \sum_{N=1}^{\frac{L_M \cos\theta}{d_{cc}}} \frac{n_s!}{(n_s - N)!N!} \exp(-\beta_{tb}(L_M - N d_{cc}\tan\theta)) \times \exp(-\beta_{ts} N d_{cc})$$

J. Phys. Chem. B, 106, 7469 (2002)



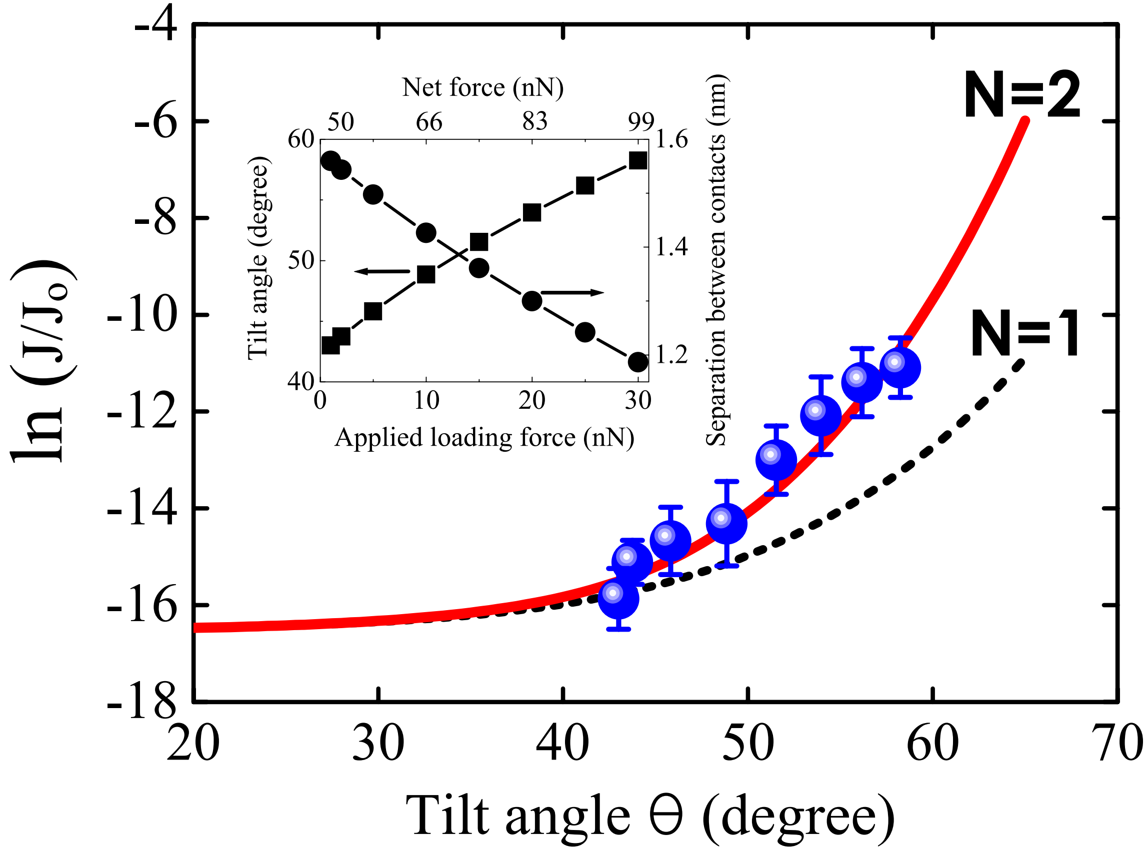
- The dominant transport mechanism of alkanethiol SAM: "through-bond" tunneling
- When tilted considerably, chain-to-chain coupling: "through-space tunneling" appears

C8: Thru-bond + Thru-space (Single hopping: N = 1)



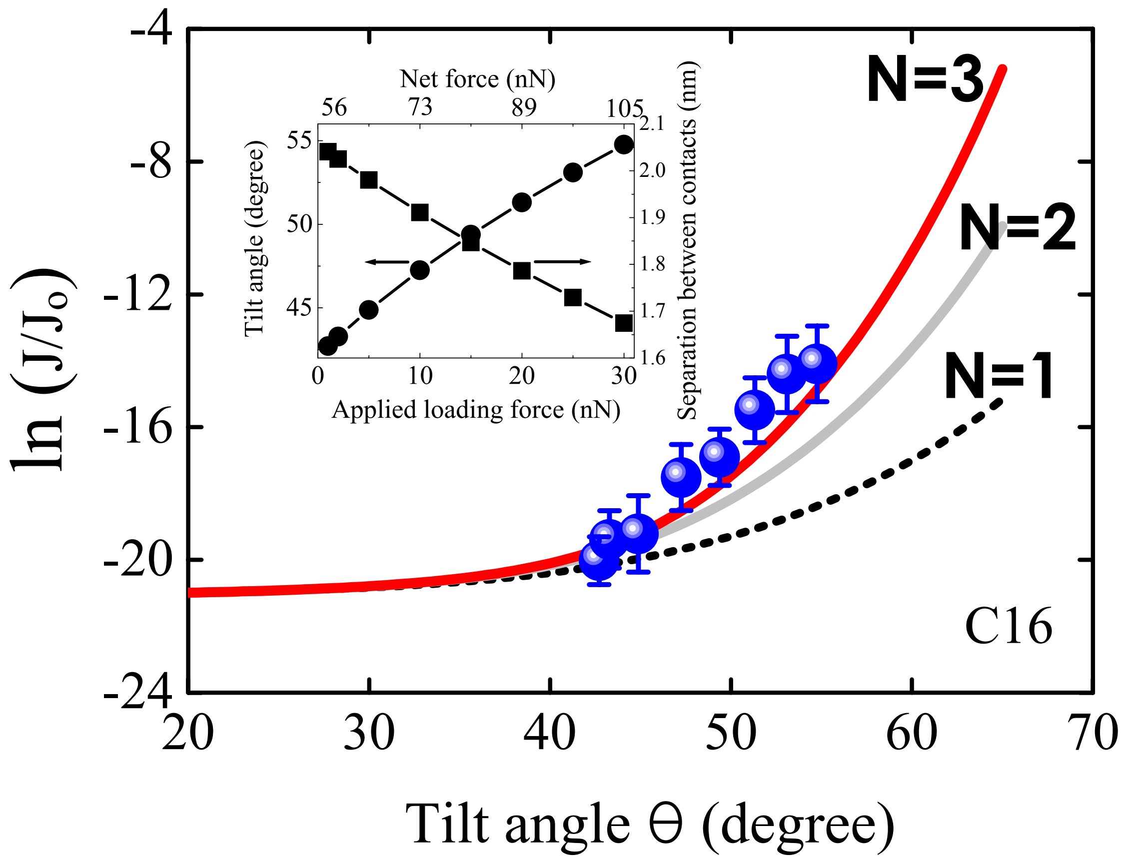
N~1 (N ≤ $L_M \cos \Theta / d_{cc}$)

C12: Thru-bond + Thru-space (Double hopping: N = 2)



N~2 ($N \leq L_M \cos \Theta / d_{cc}$)

C16: Thru-bond + Thru-space (Triple hopping: N = 3)



N~3 (N ≤ $L_M \cos \Theta / d_{cc}$)

Conclusions

- Electronic transport study by CAFM
  - Tip-loading force effects on molecular structural properties
  - Thru-bond vs. thru-space transport

- Fabrication and characterization of micro-via hole molecular devices
  - Detail yield study ~ 1.5 % (out of > 13,000 devices measured)

- Electronic properties of various nanoscale building blocks