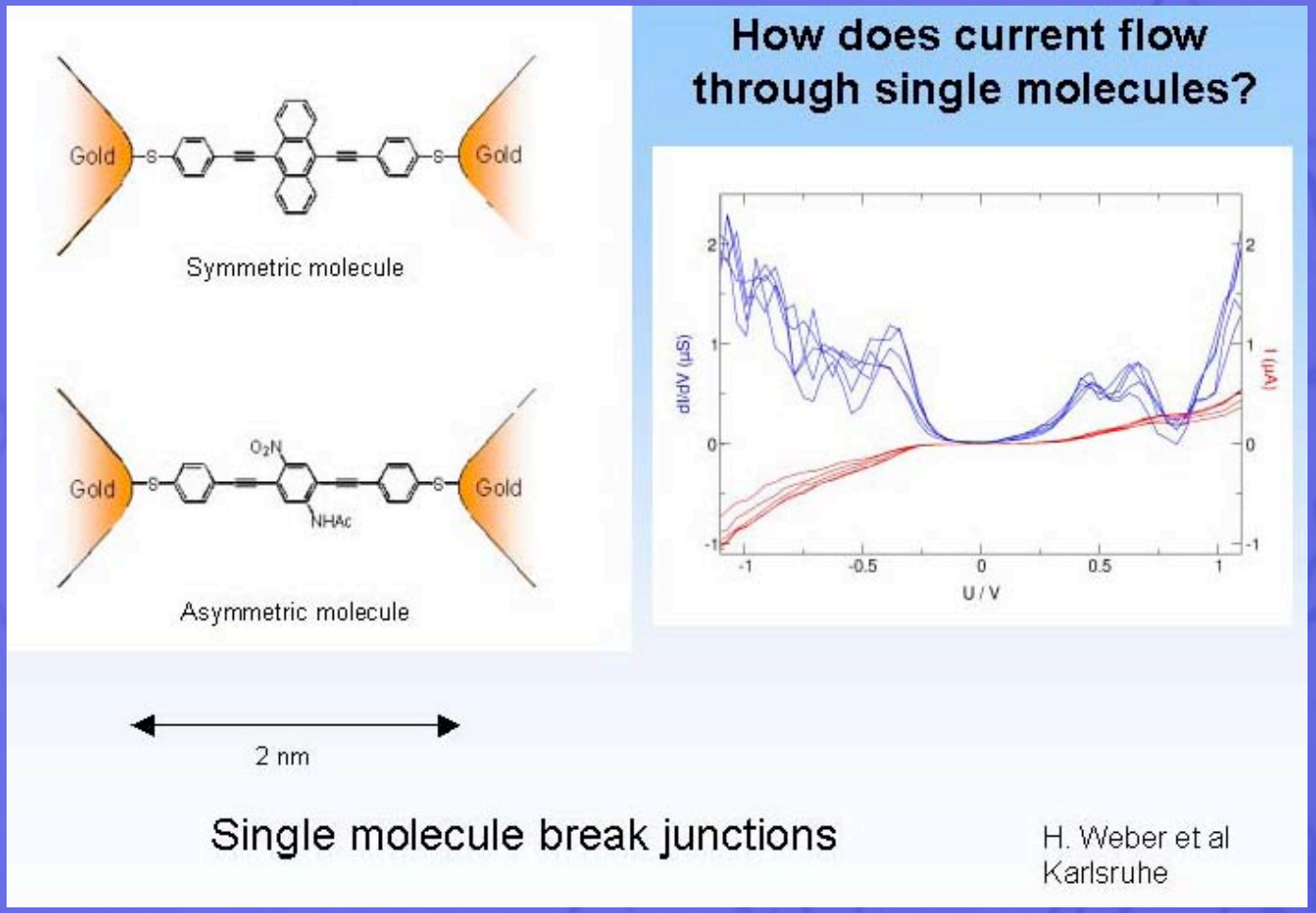
Outline:

- A short review of state-of-the-art;
- DFT atomistic methods;
- The NEGF-DFT implementation;
- Applications of NEGF-DFT;
- Quantum mechanic forces during current flow;
- Summary: outlook to the near future.

Application: molecular transport junctions

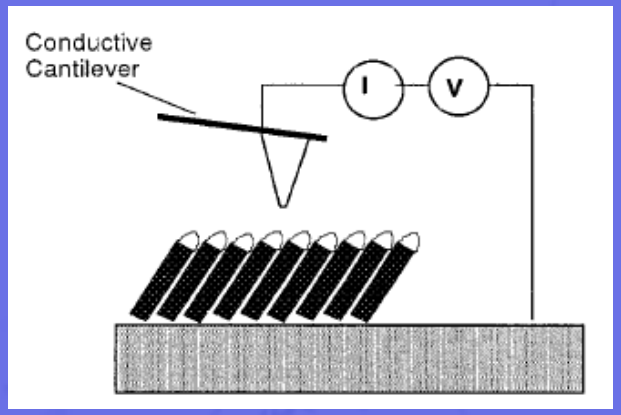


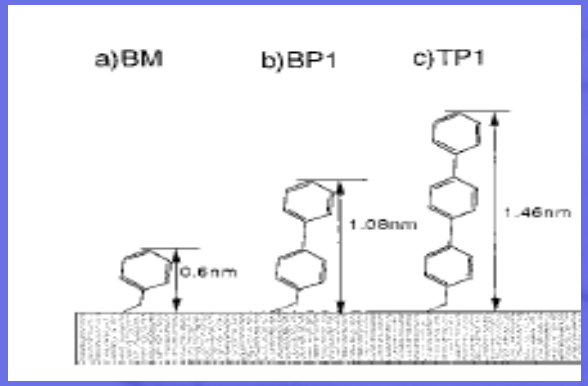
Can we compare with experimental data? There are some difficulties:

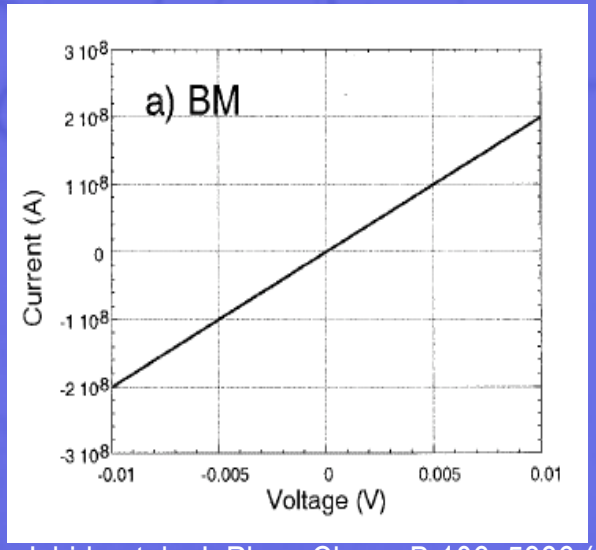
- Do not know experimental device structure;
- Do not know environmental effects;
- Do not know quality of contacts;
- Do not have reliable data on single molecule device;
- Do not have all the physics in our theory;
- …..

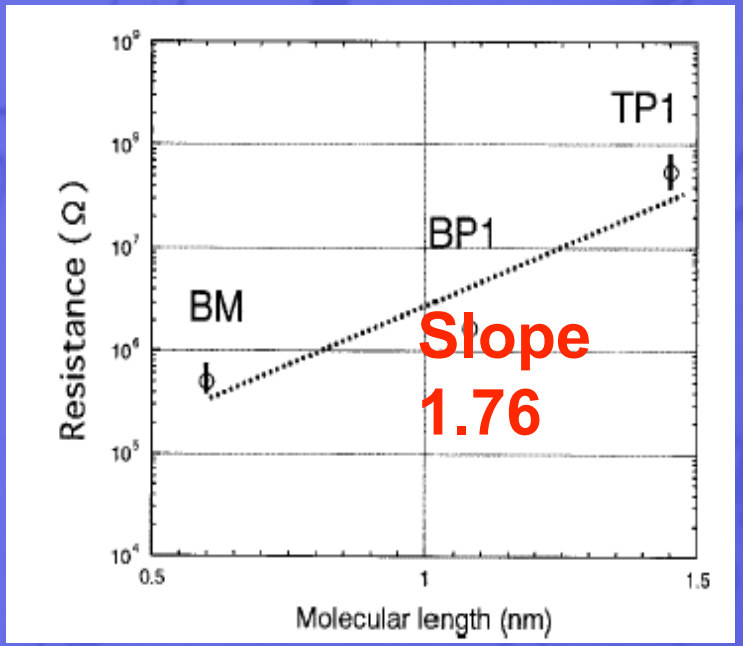
But progress are being made….

Example: resistance of molecular wires



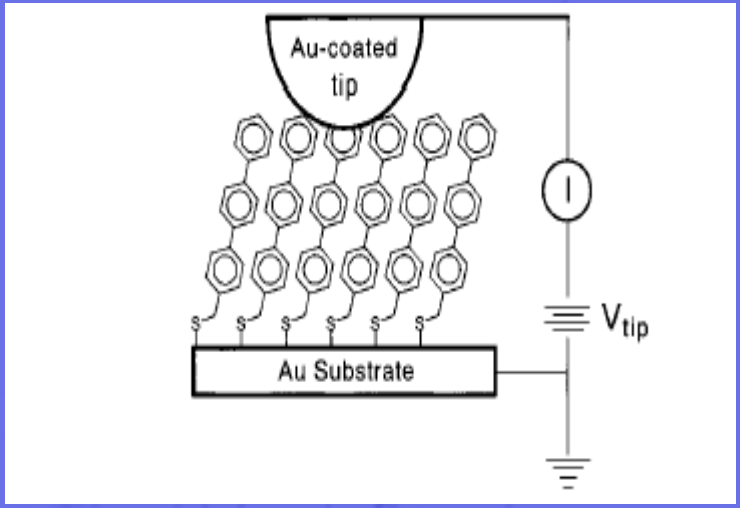


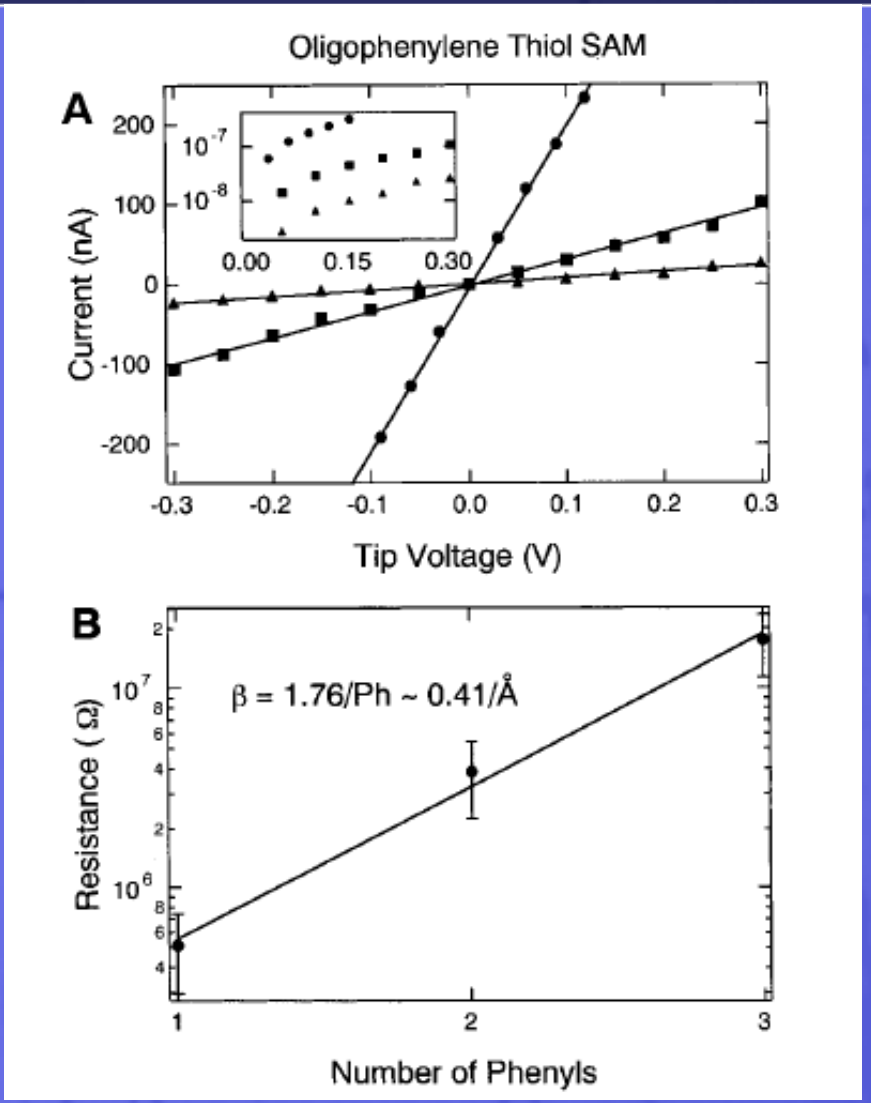




Takao Ishida etal., J. Phys. Chem. B 106, 5886 (2002)

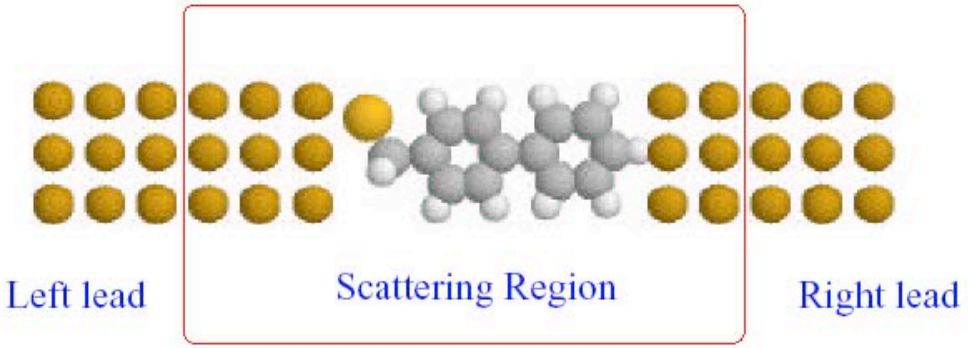
Another independent experiment from a different lab:
David J. Wold etal. J. Phys. Chem. B, 106, 2813, (2002)

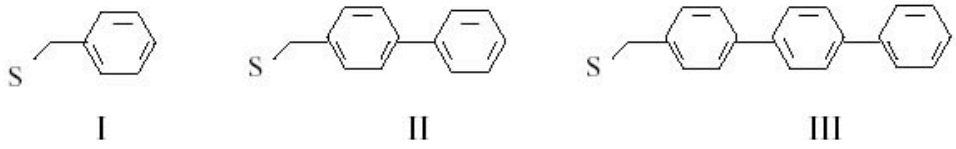




Very similar numbers were obtained as those of Ishida

Our calculations:

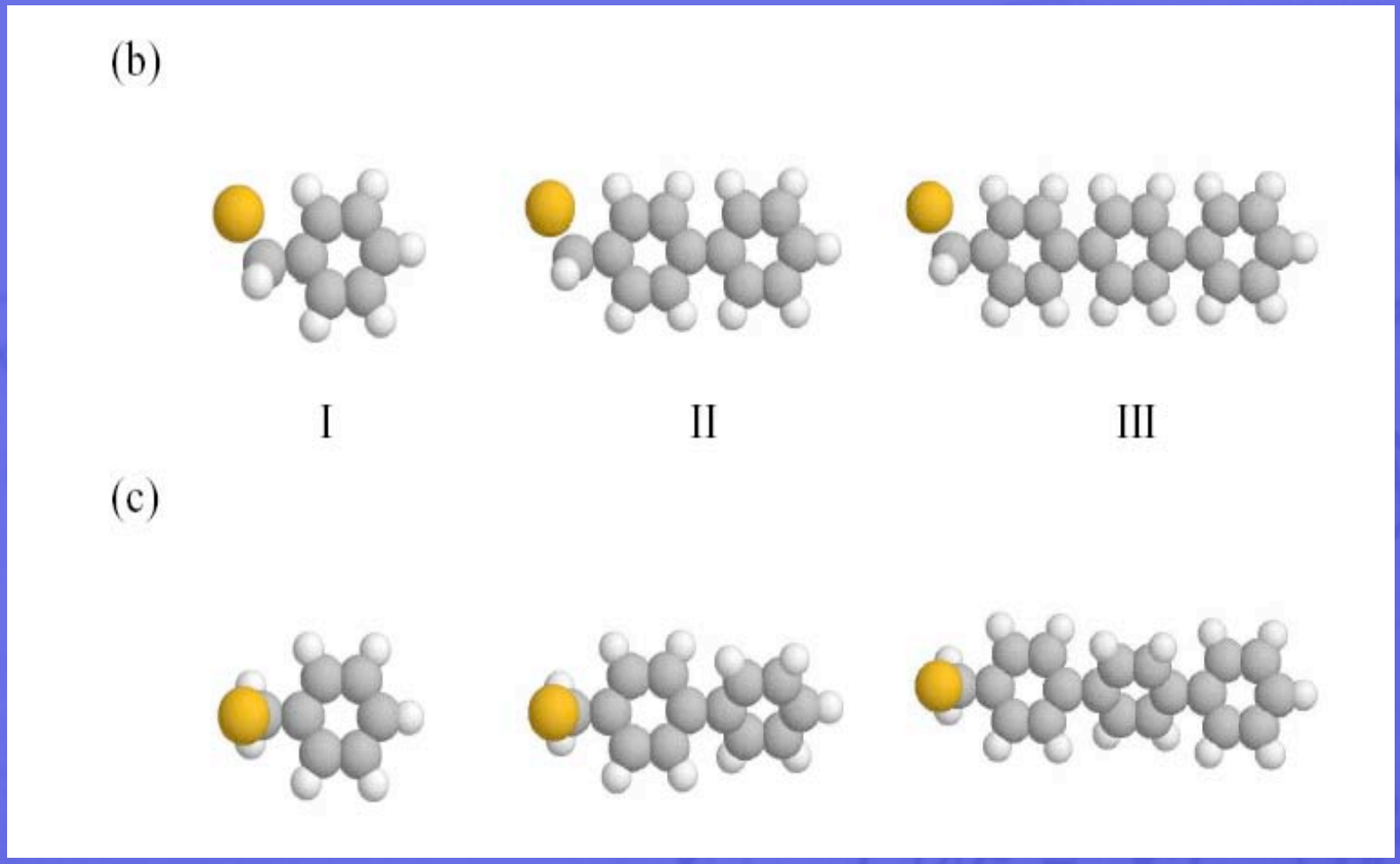




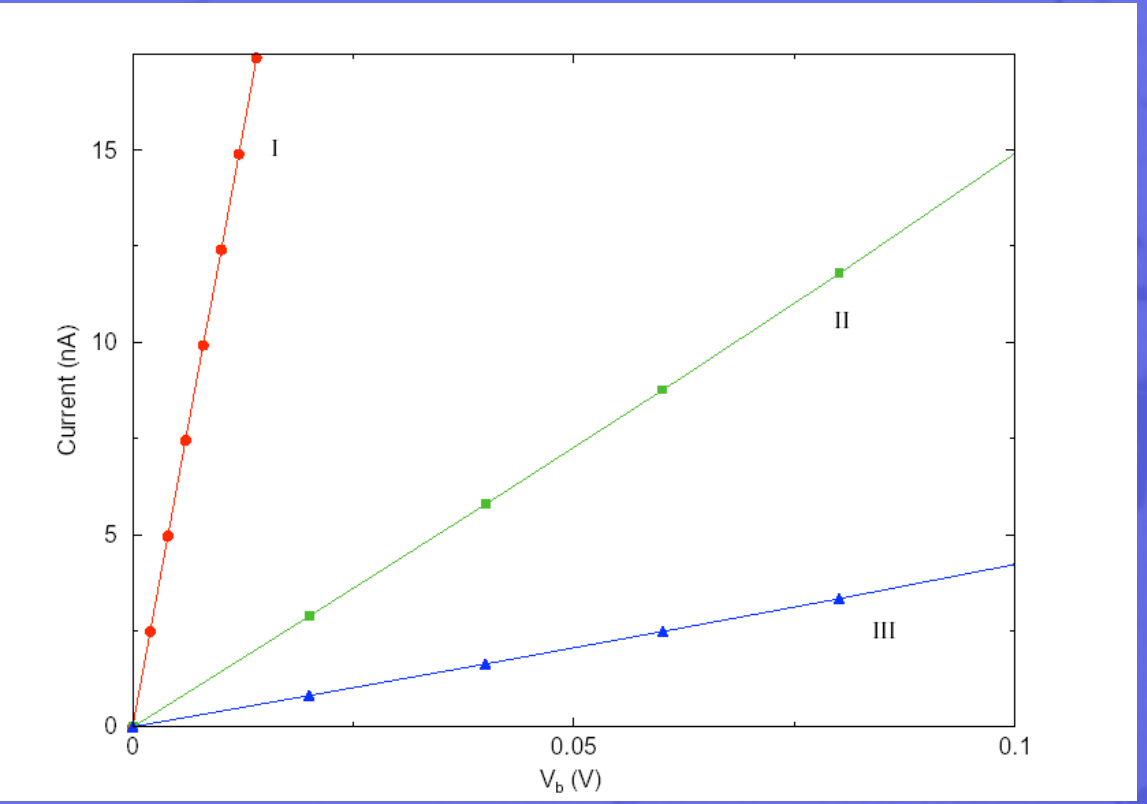
I II III

C.C. Kaun, B. Larade and H.G, PRB (2003)

Planar vs rotated conformations:



I-V curve for planar wire: linear and within a factor of 5 to experimental data

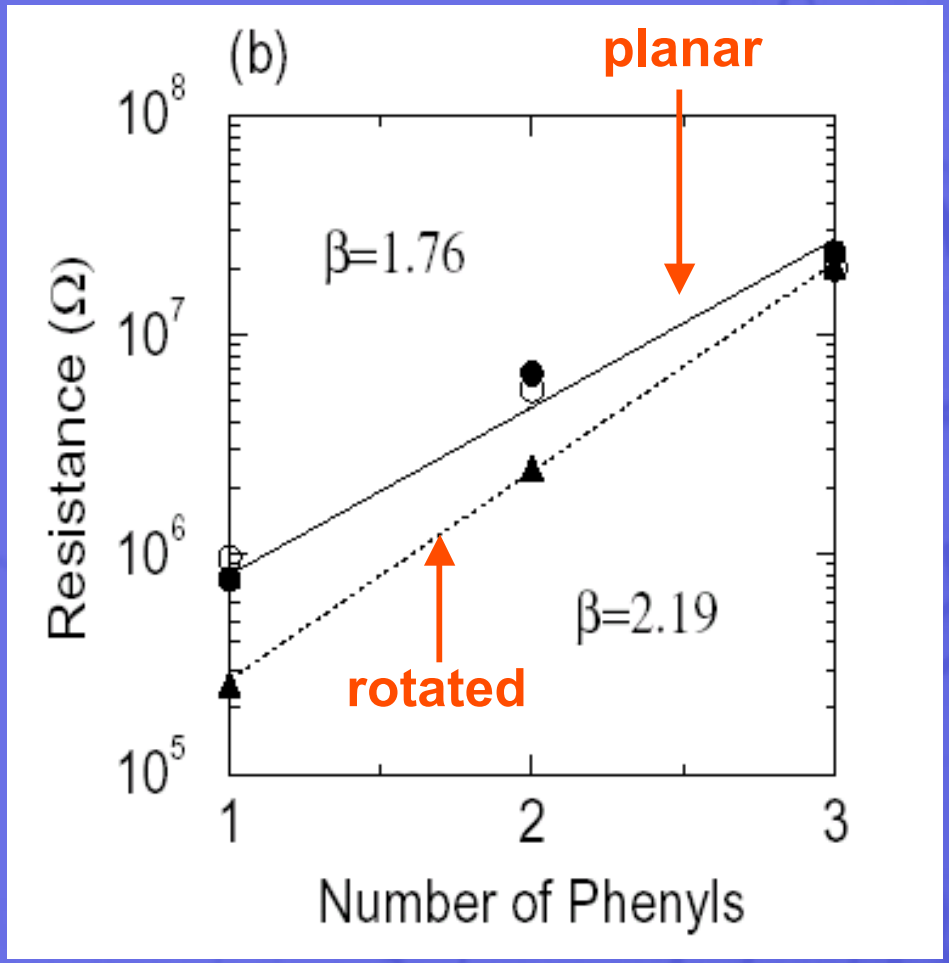


Possibilities: more than 1 molecule in the experimental device; some device details are different.

The slope is independent with number of molecues

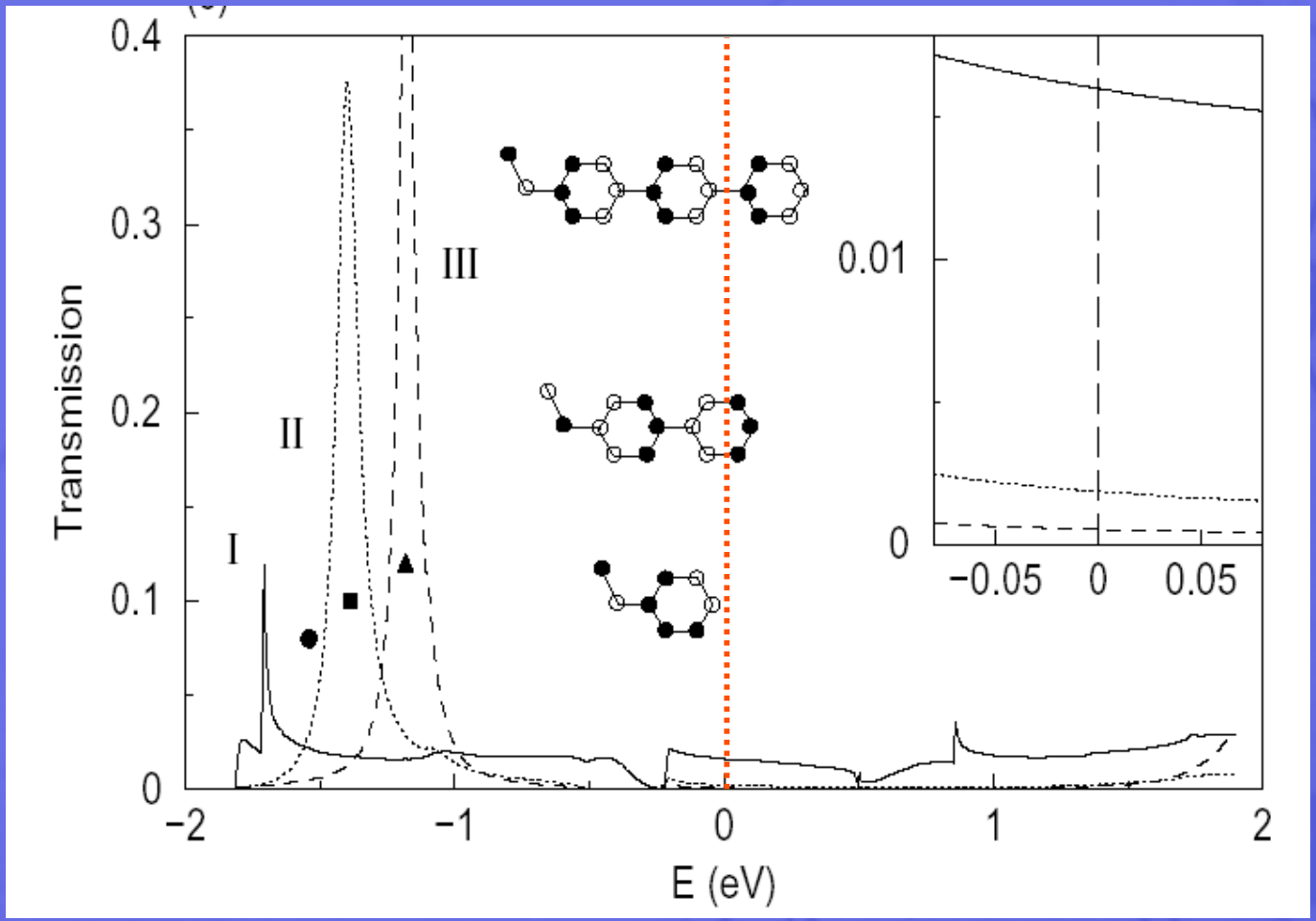
Experimental range:

1.7 and 2.2.

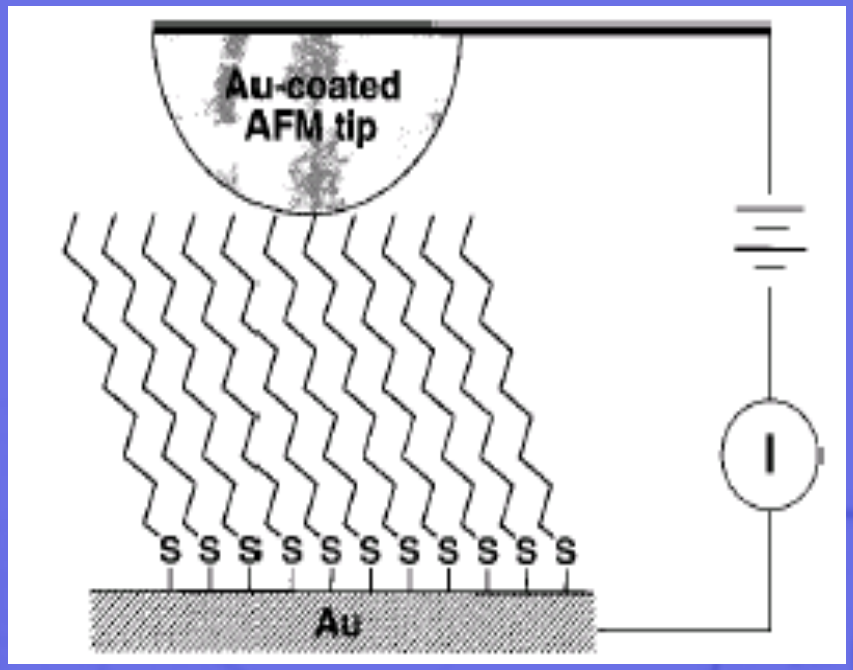


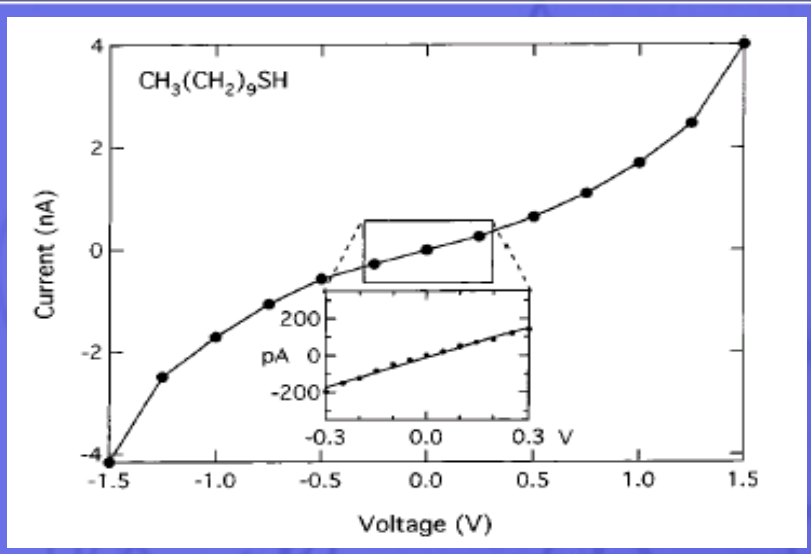
Resistance: order of magnitude comparison can be well made

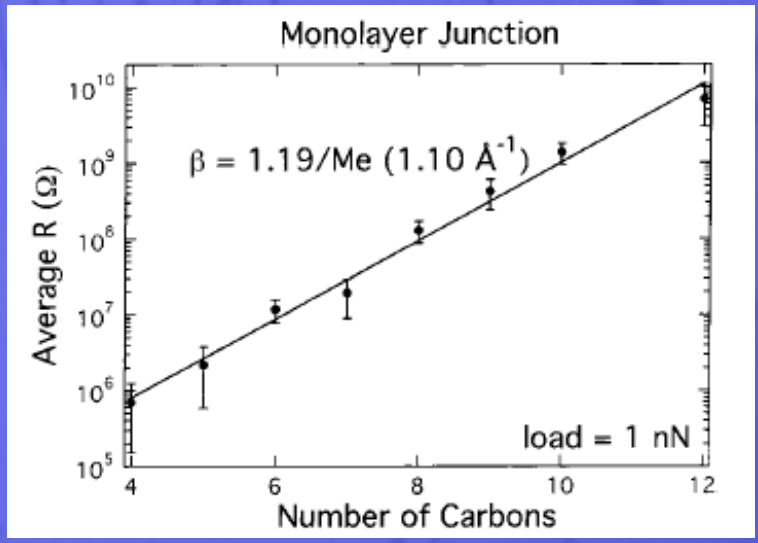
It is a non-resonance conduction: consistent with an exponential increase of resistance.



Another SAM measurement: alkanethiol (Wold and Frisbie, JACS 123, 5549 (2001)





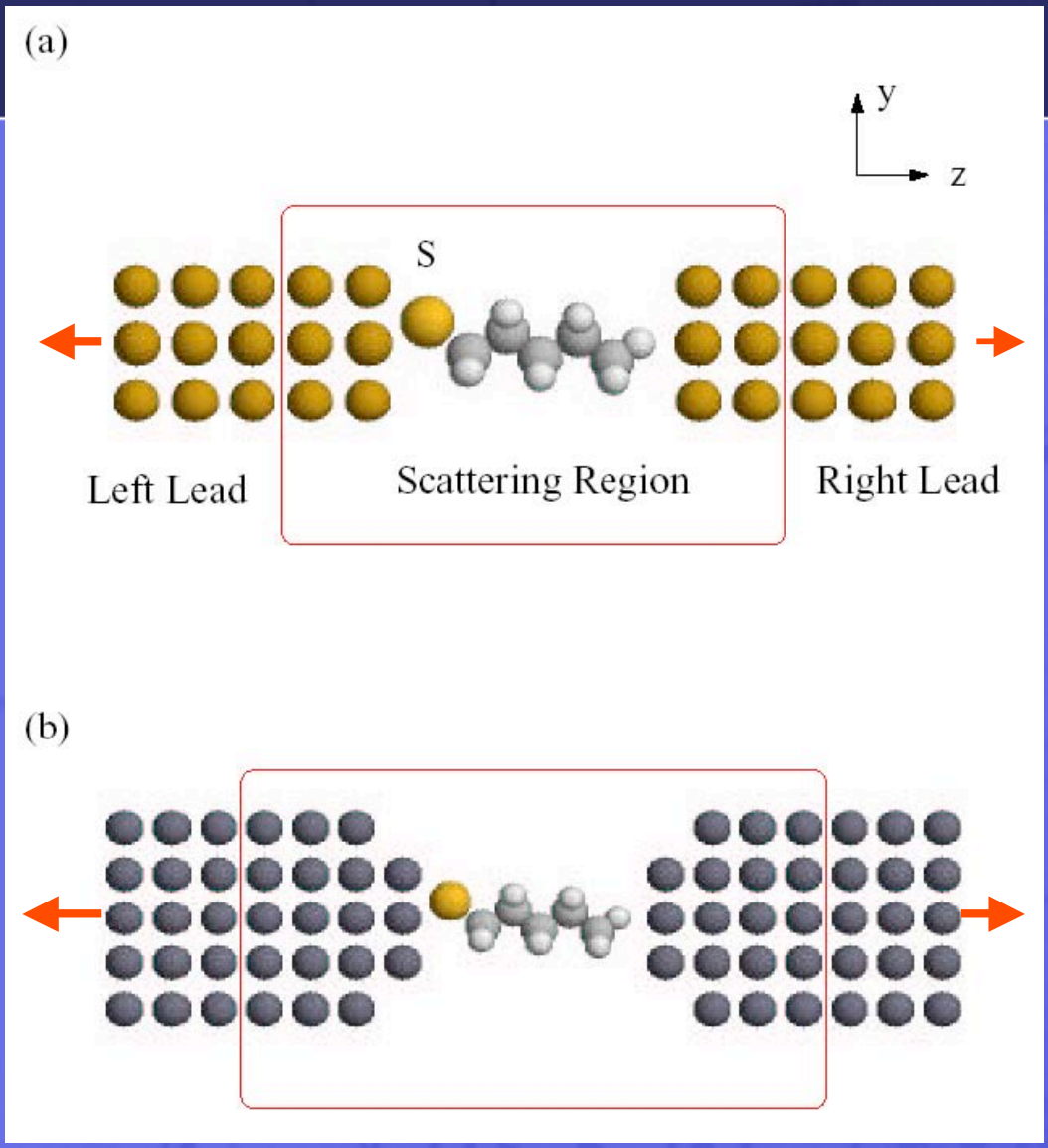


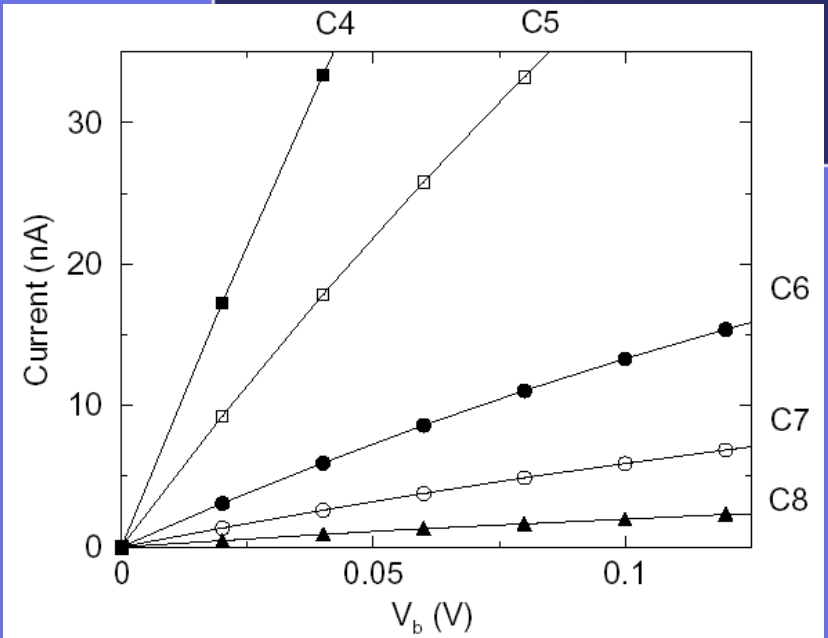
Rather similar results from other groups: M. Reed etal (2003); Lindsay etal Nanotechnology, 13, 5 (2002).

Our model:

Au electrodes

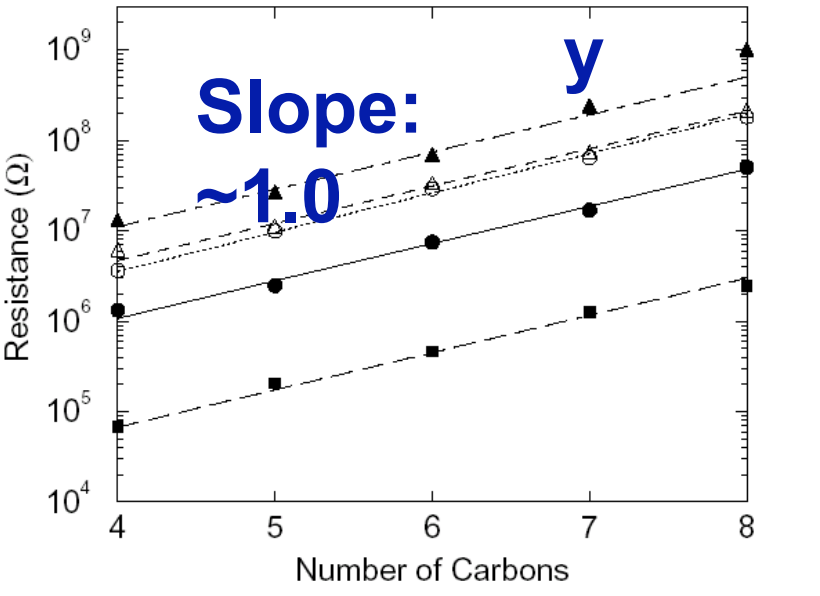
Al electrodes





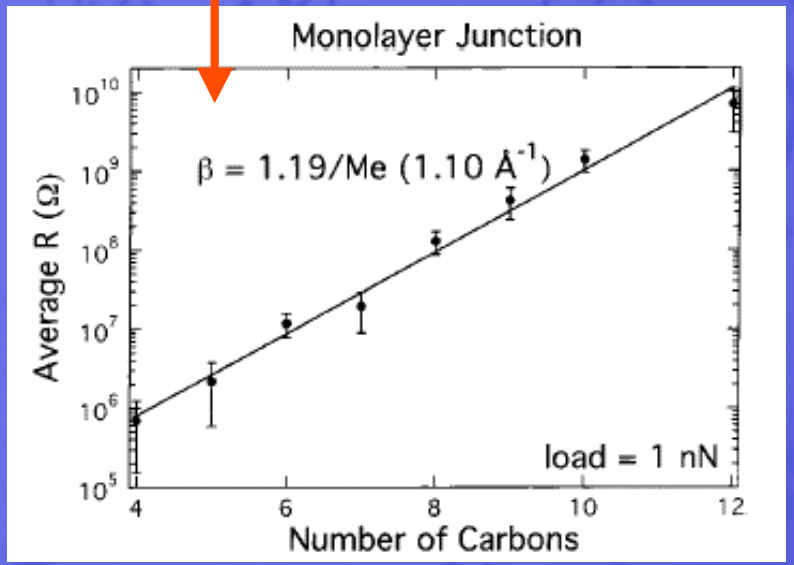
Theory

Slope: ~1.0



Again, not quantitatively too far from real data.

Experimental: average slope is close to 1



Au-alkanedithiol-Au wire: S-atom on both side

- Our calculation: still $R_n = R_o \exp(\beta n)$ ✓
- Our calculated beta is still about 1.0; ✓
- Our R_o is smaller than that of alkanethiol by about a factor of 18. ✓

(Experimental ratio: 16.1 by Lee and Reed, J.Phys. Chem. (2004))

Experiments so far:

1. Cui etal, J. Chem. Phys. 106, 8069(2002): one lead is a quantum dot

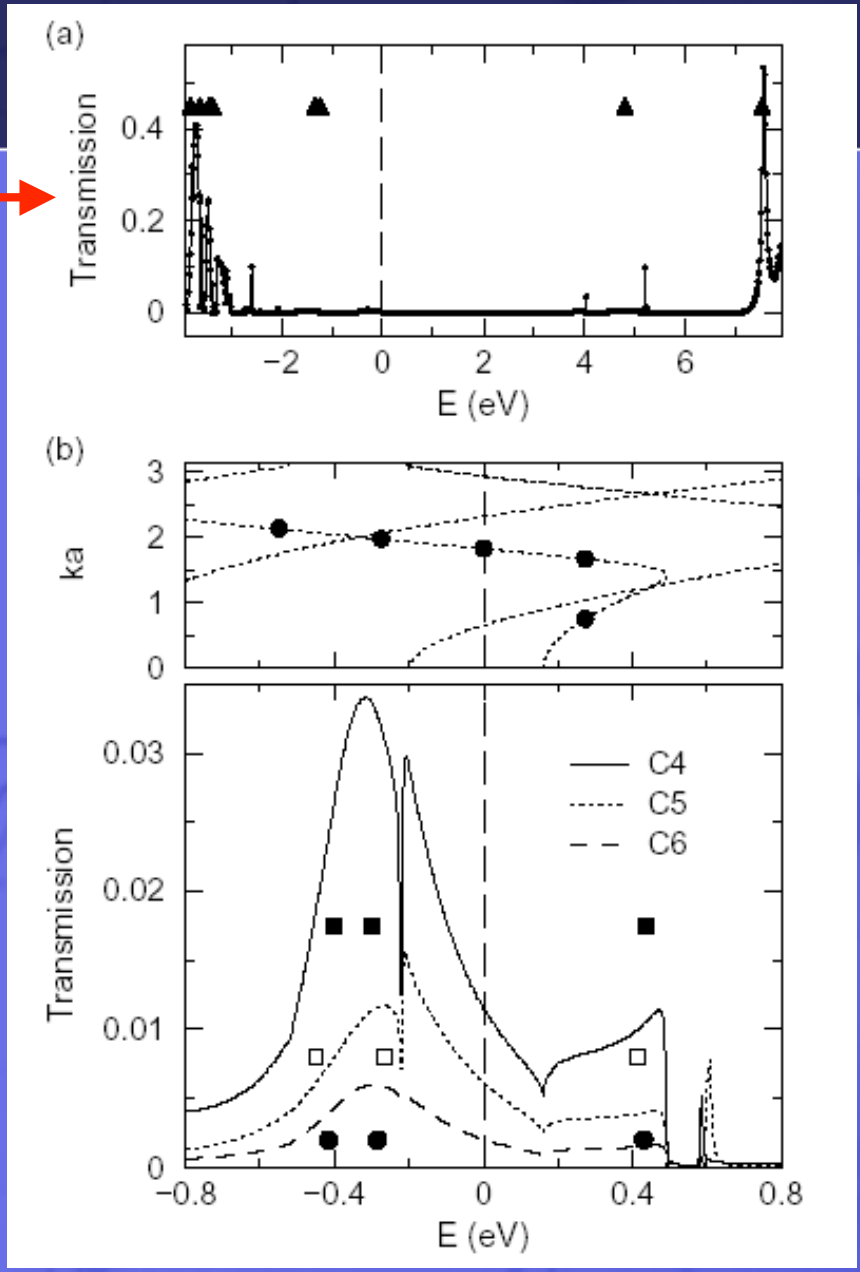
$\beta = 0.57$ → ~ 1 if QD effect is taken out

Lee and Reed, J.Phys.Chem. (2004):
Engellkes etal (Frisbie lab) (2003):

$\beta = 1.05$

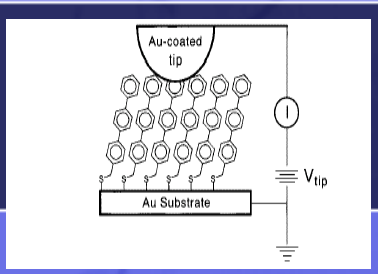
Alkane has a large HOMO-LUMO gap, ~10eV. The Fermi level is inside the gap, but closer to HOMO.

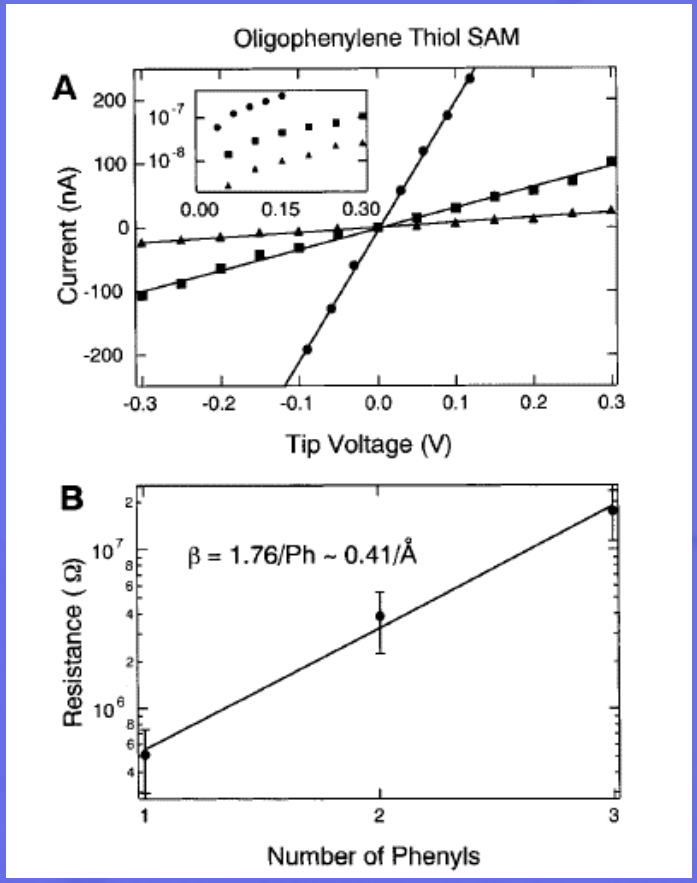
There is a tiny feature near Fermi level which determines the resistance.



C.C.Kaun & HG, NanoLetters 3, 1521 (2003)

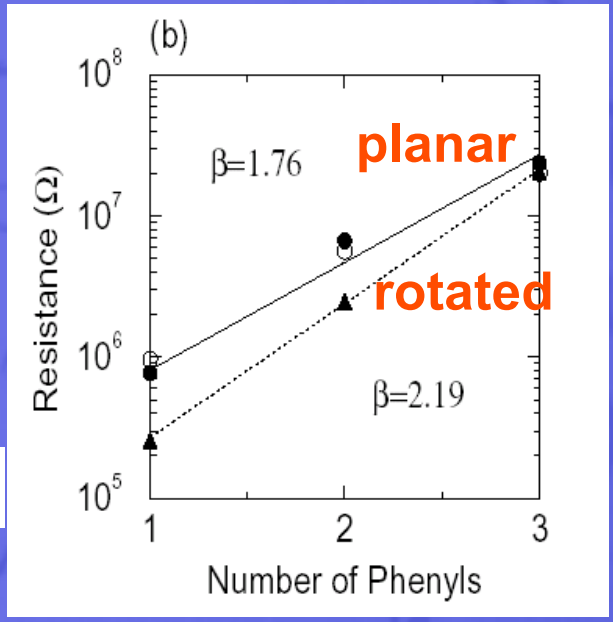
Contact: structural details matter





D. Wold etal. J. Phys. Chem. B, 106, 2813, (2002); T. Ishida etal., J. Phys. Chem. B 106, 5886 (2002)

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

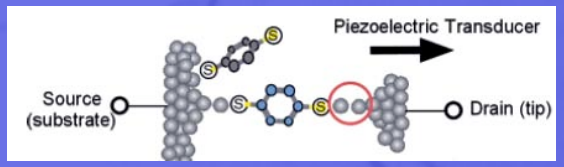


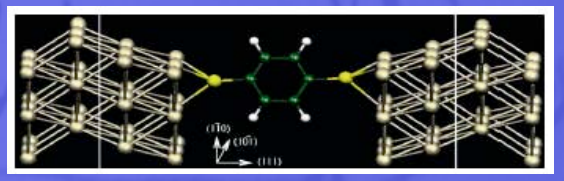
While the scaling factor agrees, the value of absolute value of resistance differs.

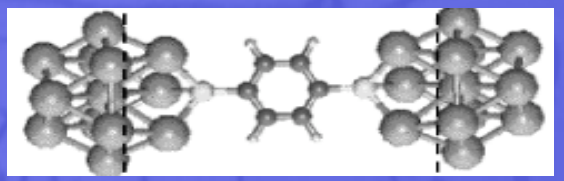
X. D. Cui etal, Science 294, 571 (2001). B. Xu and N. J. Tao, Science 301, 1221 (2003).

Atomistic transport: conductance of gold-BDT junction

Tao etal. Nano Lett 4, 267(2003). Experiment: measures large number of systems and average.	0.85us
Stokbro etal. Comput. Matter. Sci 27,151(2003) . NEGF + LDA	~20us
Delaney etal, PRL93,36805(2004) Cluster CI + Wigner function on boundary	~0.05us
Bauschlicher Jr. etal. Chem. Phys. Lett 388,427(2004). NEGF+B3PW91 or B3LYP	3-5us
Ning etal., PRB72, 155403(2005) NEGF+B3LYP + correction from UPS reference data	0.6 – 0.9 us
Varga etal. PRL 98,76804(2007). Closed system with complex boundary potential	1.55us

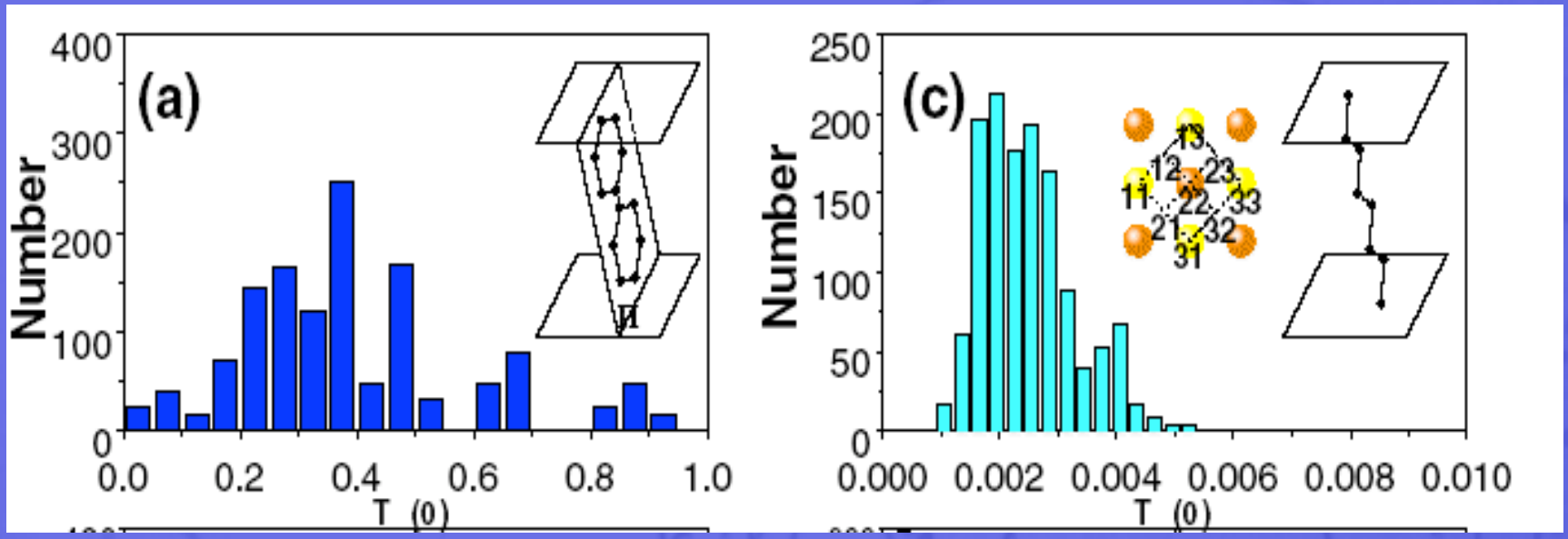






It appears to suggest that Fermi level alignment is critical for this problem.

Statistical analysis of many contacts:



Statistical analysis of about 1000 wires each having slight different contact geometry.

Theory:	Experimental:
G = 0.0023g	G = 0.0012 g

Hu etal PRL 95, 156803 (2005)

Summary of molecular wire:

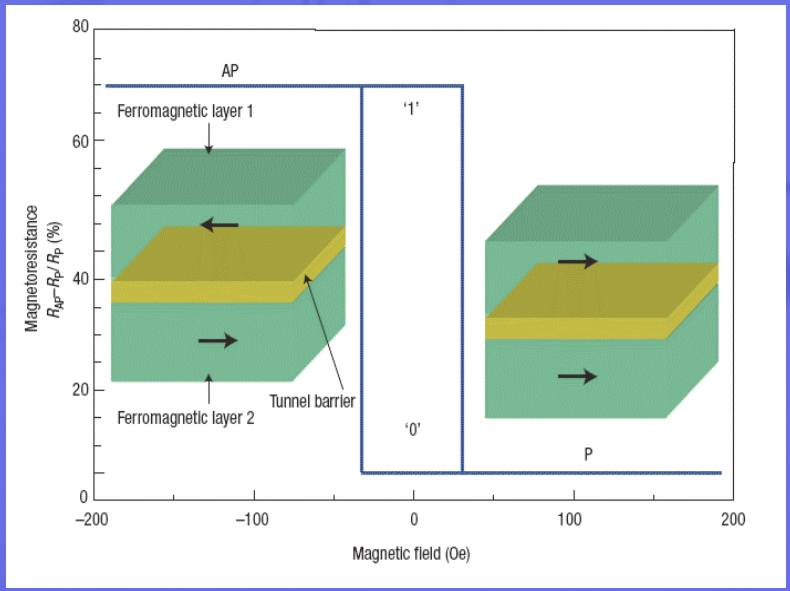
- A non-resonance transport controls these molecular wires. Quantitative consistency to experimental data appears to be obtained on the exponential length scale beta.
- The values of resistance and currents are within a factor of 2~30 to the measured data. The difference is likely due to the presence of multiple molecules in the experimental junction, details of contacts, etc.
- Encouraging but further quantitative work are needed.

Application: magnetic tunnel junctions

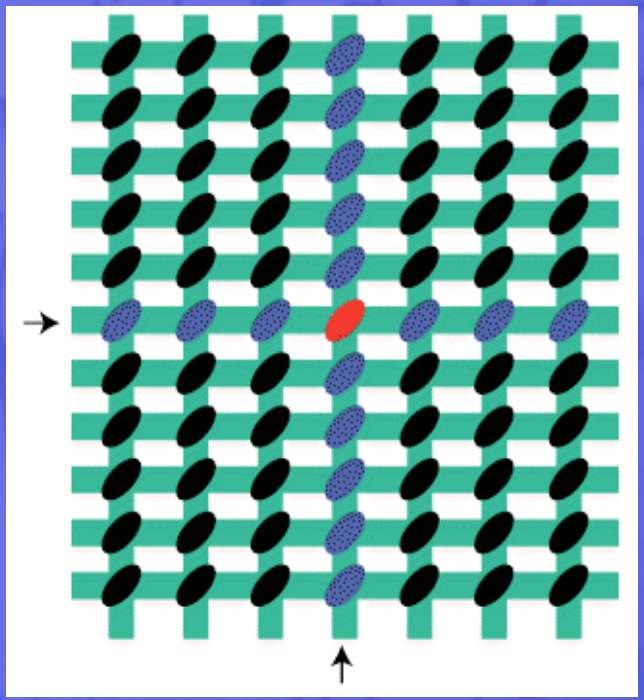
Memory used in digital devices: S-RAM; D-RAM; Flash; …

We desire an "universal memory".

MRAM

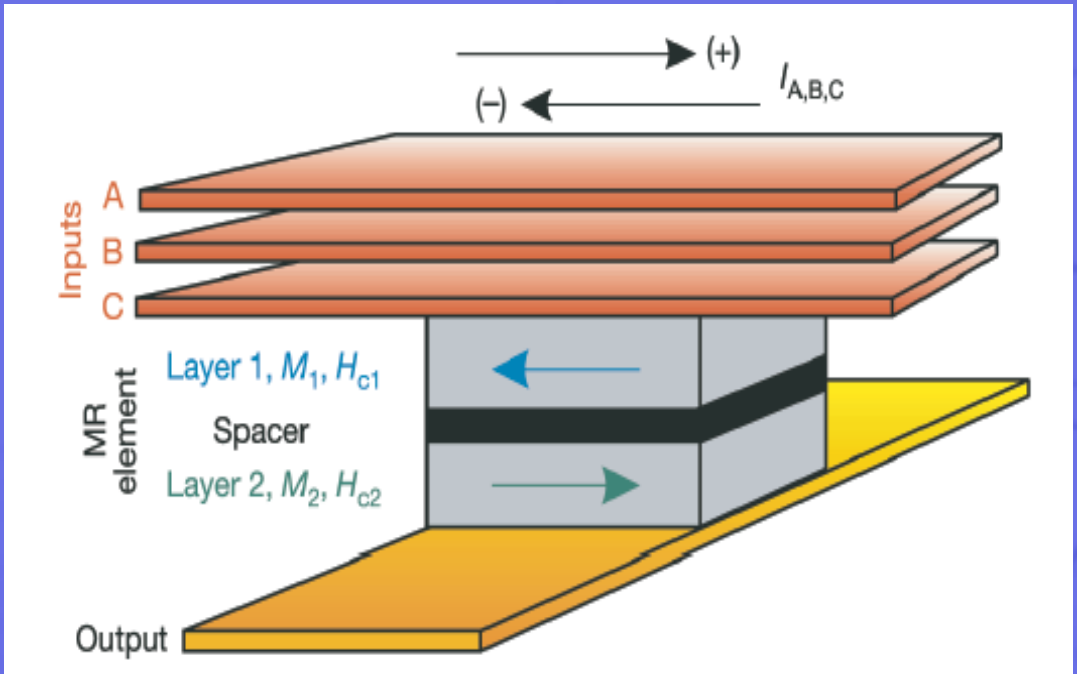


Picture from W. Butler, Nature Mat., 3, 845 (2004).



Picture from J. Akerman, Science, 308, 508 (2005).

The hope for magnetic logic:



Picture from the experimental proposal of programmable magnetic logic cell based on MTJ, A. Ney etal. Natture 425, p485 (2005).

A+B switches M1; A+B+C switches M2. By manipulating with these currents, Ney showed logic operations of AND, OR, etc.

Metal spintronics: magnetic tunnel junctions (MTJ)

up-up:

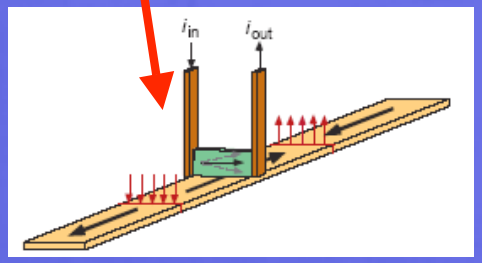
$$I_{tot}^{\uparrow\uparrow} \sim N_{\uparrow}N_{\uparrow} + N_{\downarrow}N_{\downarrow}$$

up-down:

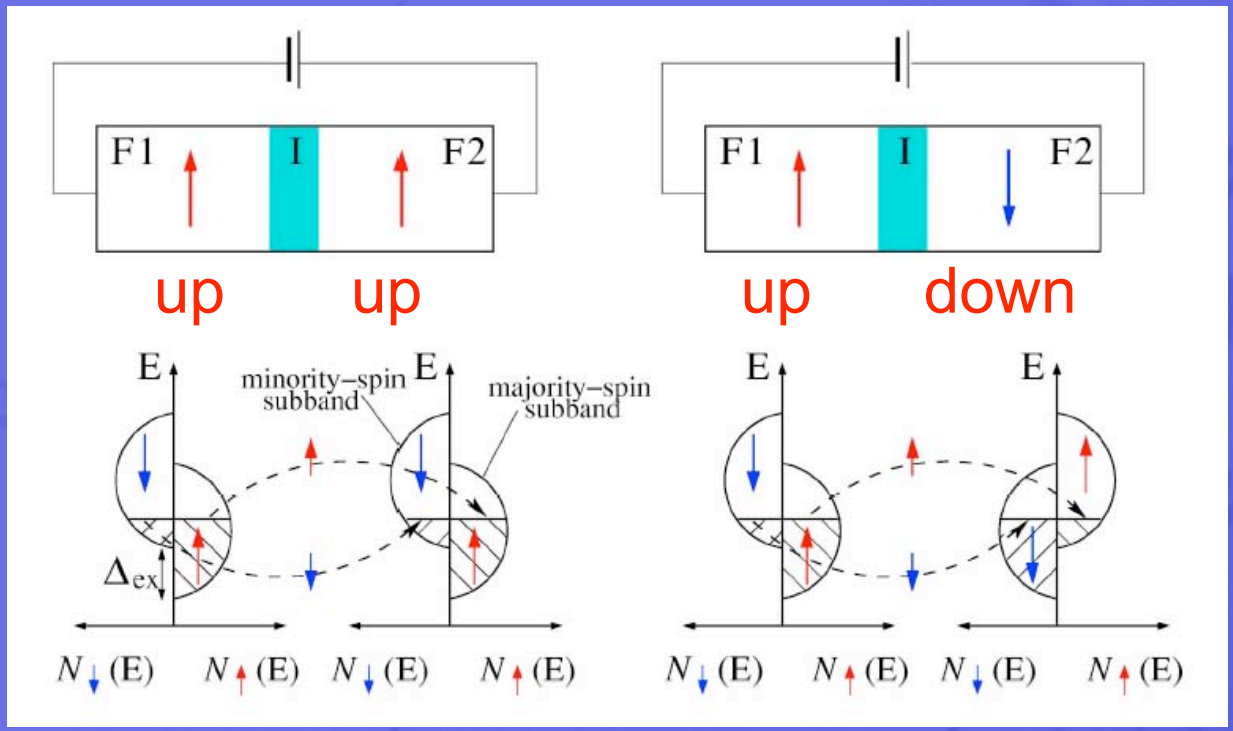
$$I_{tot}^{\uparrow\downarrow} \sim N_{\uparrow}N_{\downarrow} + N_{\downarrow}N_{\uparrow}$$

$$I_{tot}^{\uparrow\uparrow} \neq I_{tot}^{\uparrow\downarrow}$$

Julliere, Phys. Lett. A 54, 225 (1975)



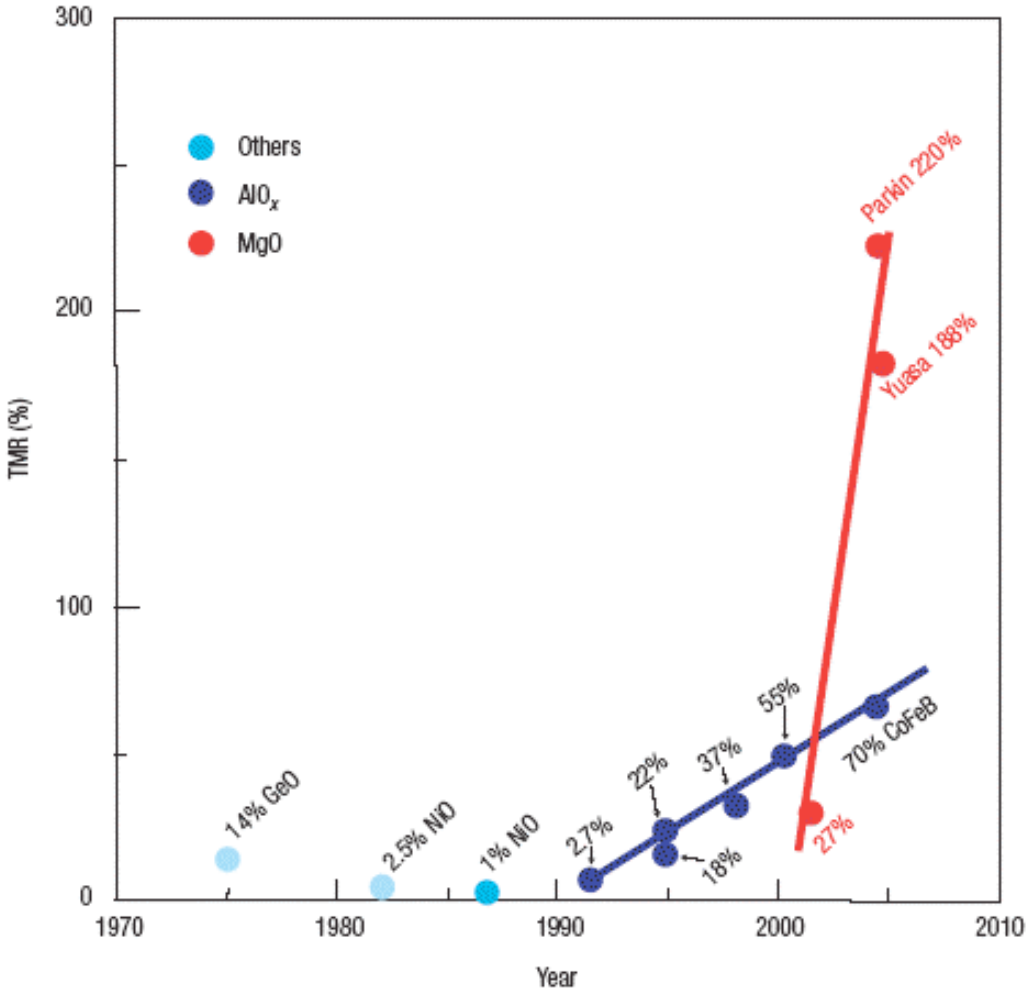
Prinz, Science, 282, 1660 (1998)



Picture from Zutic etal Rev. Mod. Phys. 76, 323 (2004).

Metal spintronics: Fe/MgO/Fe MTJ

- Rapid progress on TMR ratio in recent years due to progress in materials science



Picture from M. Coey, Nature Mat. 4, 9(2005).

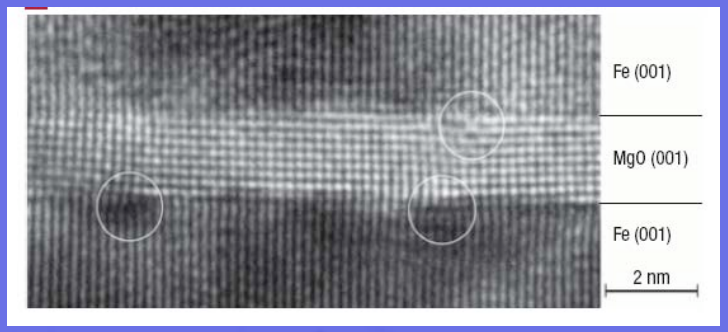
Device merits for applications:

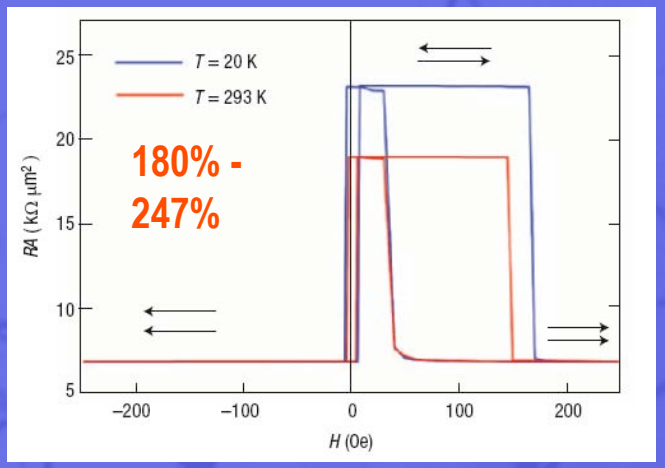
- The greater the TMR, the more sensitive the device. The value of TMR appears to sensitively depend on the tunnelling structure. Theory predicted very large TMR for MgO based junctions. There is a need to understand these materials issues.

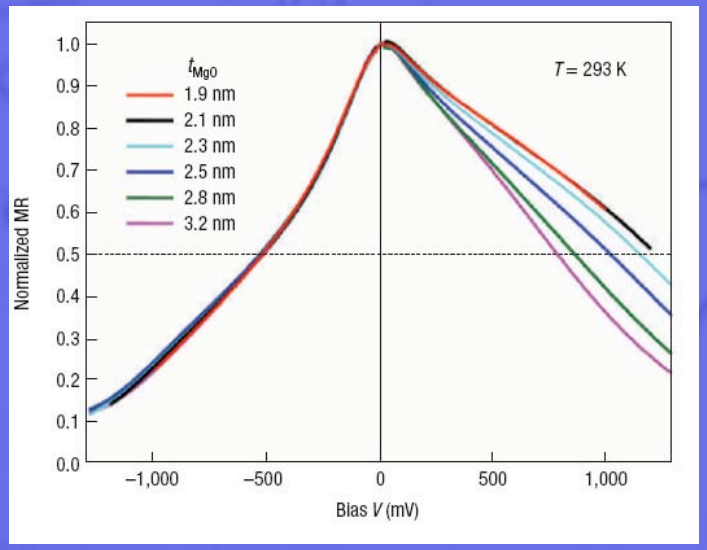
- The smaller the junction, the more devices can be packed per unit area. There is a need to understand tiny junctions made of molecules, clusters, etc.

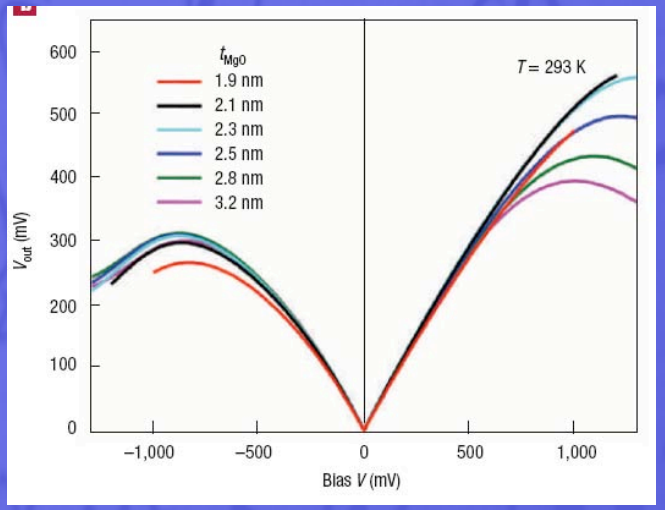
- All of these requires calculation schemes which take into account material and chemical details of the device structure. Most desired is atomic based methods.

Fe-MgO-Fe magnetic tunnel junctions:





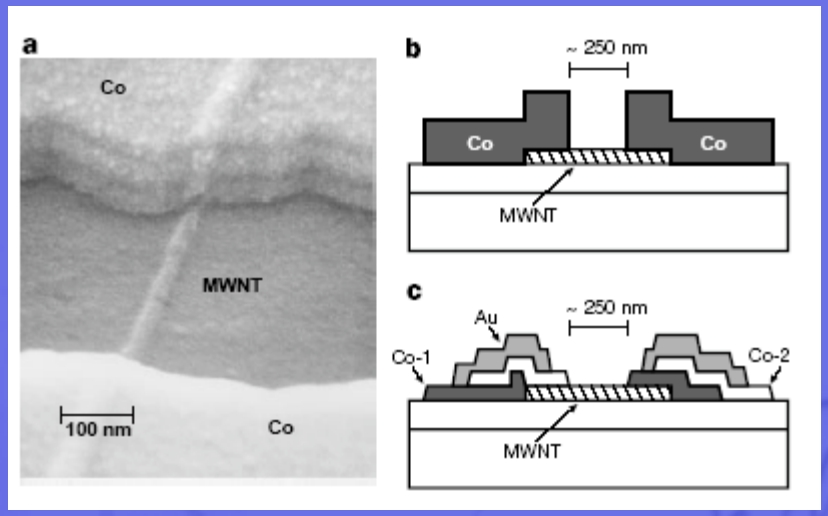




Yuasa et al., Nature Mat. Vol.3, 868 (2004).

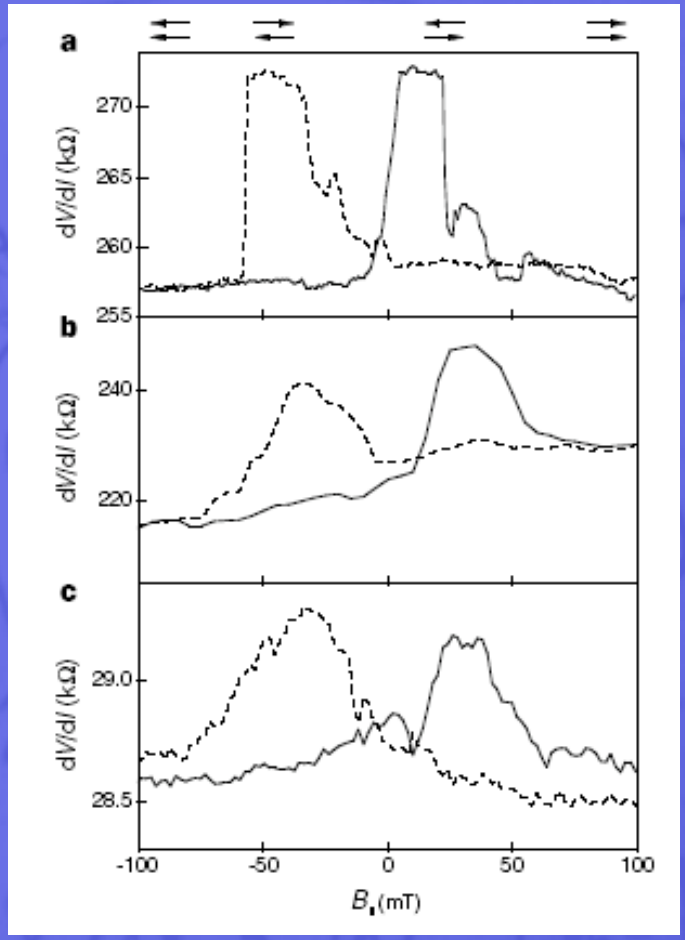
When the tunnel barrier is a molecule: molecular spintronics

Carbon nanotube TMR:



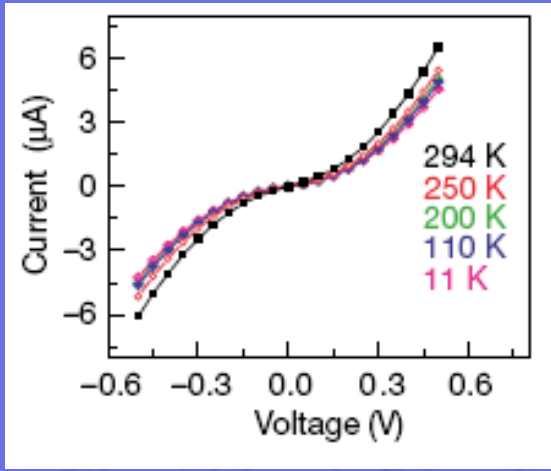
$$\Delta R \equiv \frac{R_{\uparrow\downarrow} - R_{\uparrow\uparrow}}{R_{\uparrow\uparrow}}$$

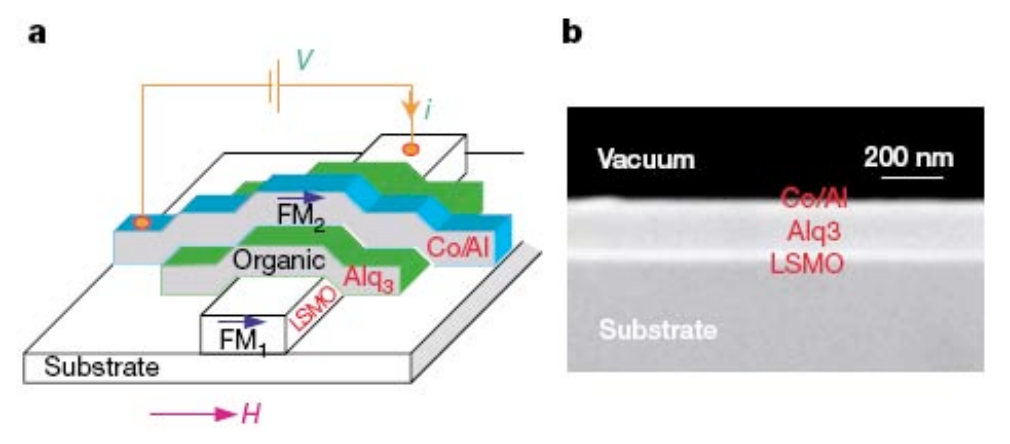
~ 10 %



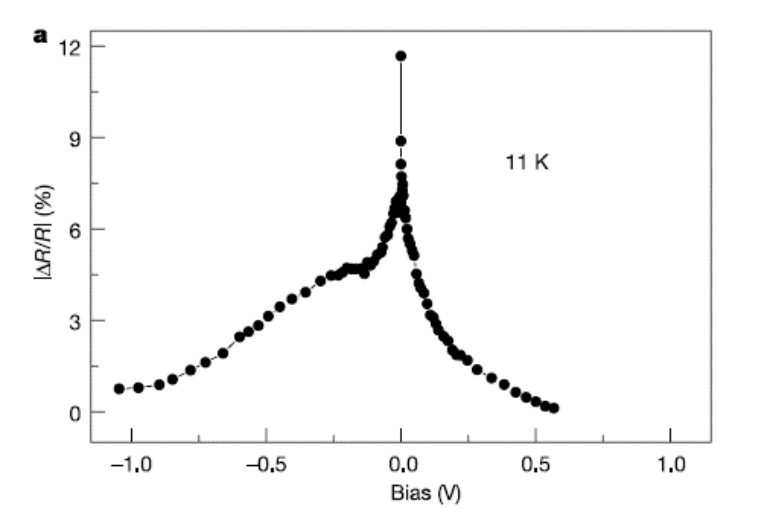
K. Tsukagoshi, B.W. Alphenaar and H. Ago, Nature, 401, 572 (1999).

Molecular spintronics: organic semiconductors



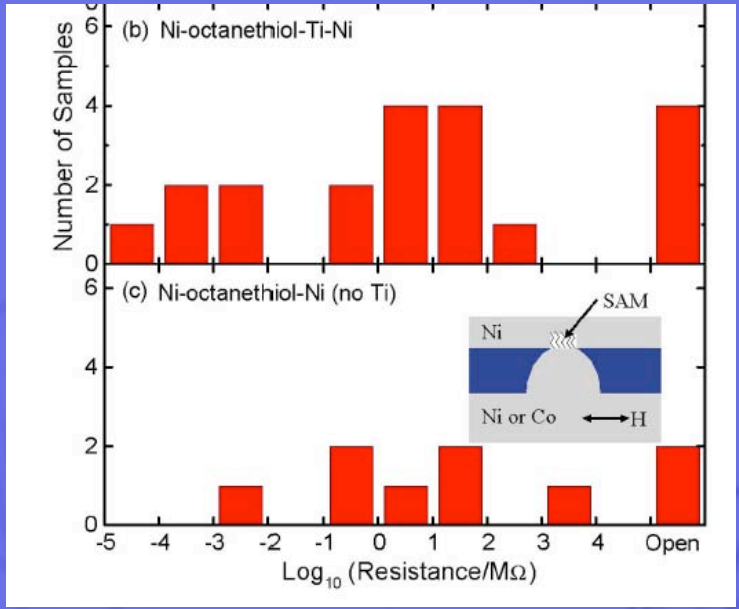


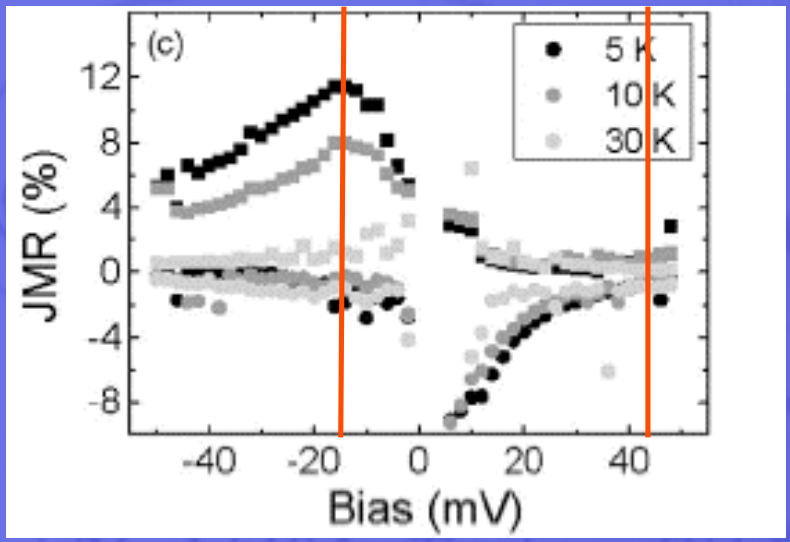
TMR decreases from ~10% due to bias voltage with a scale of roughly 0.2V.



Xiong etal Nature, 427, p821 (2004).

Molecular spintronics: alkane-thiols





TMR decreases from ~12% due to bias voltage with a scale of roughly 0.01V.

Ralph etal, PRL 93, 136601 (2004)

Fe/MgO/Fe MTJ: Two puzzles

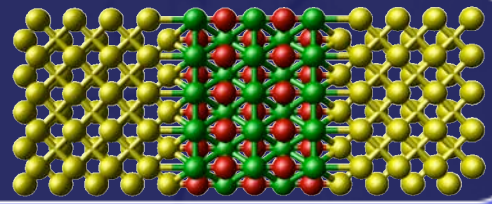
- **Zero bias TMR ratio:**
- **Theory: many thousands percent.**
- **Experiment: several hundred percent.**

- **TMR versus bias voltage:**
- **Theory: either increase with bias, or no dependence.**
- **Experiment: reduce with bias.**

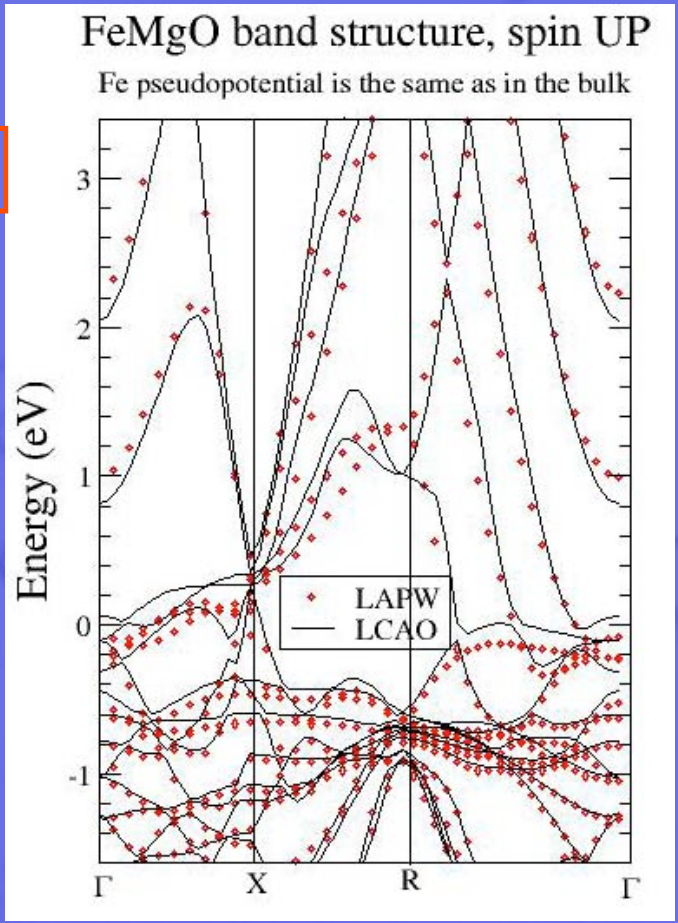
Can we understand these things?

D. Waldron etal, PRL, 97, 226802 (2006).

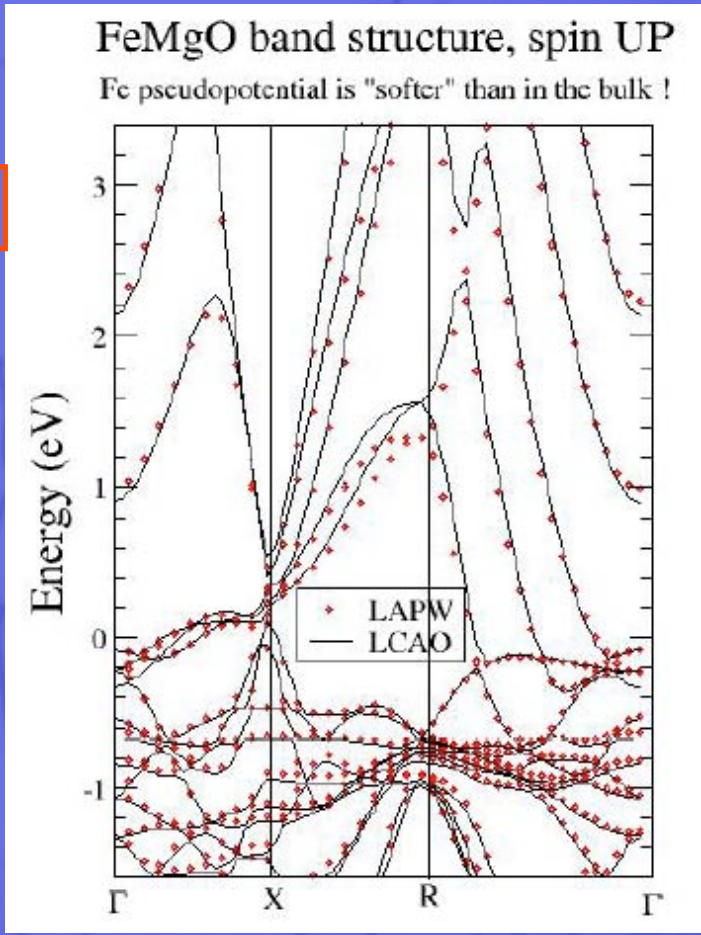
Careful check of basis functions:



bad

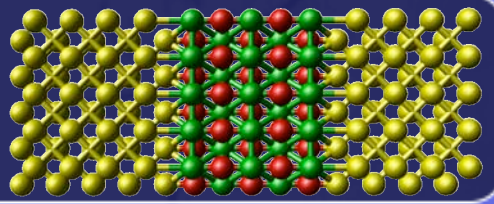


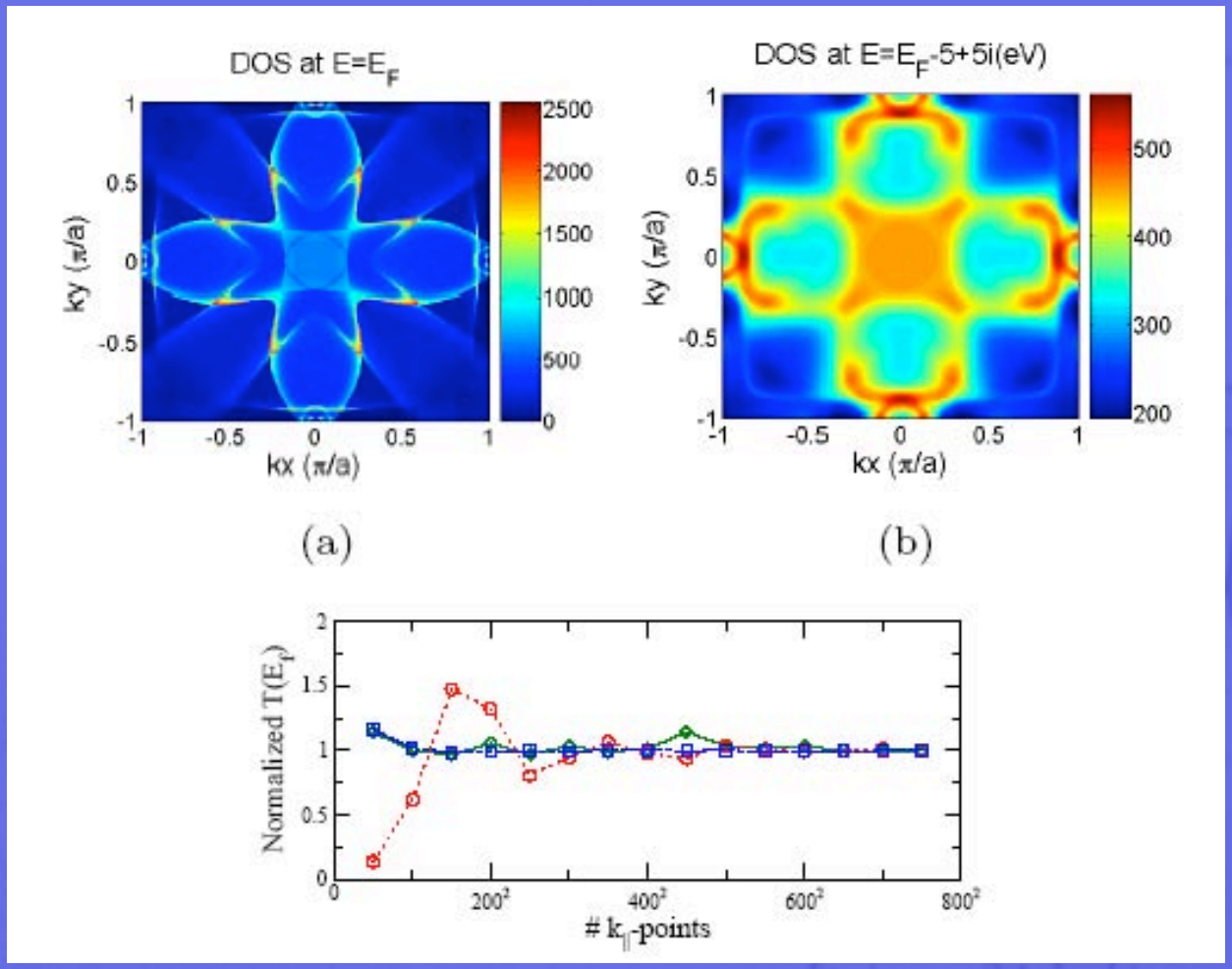
good



It is crucial to have accurate LCAO basis sets.

Careful check of k-sampling:



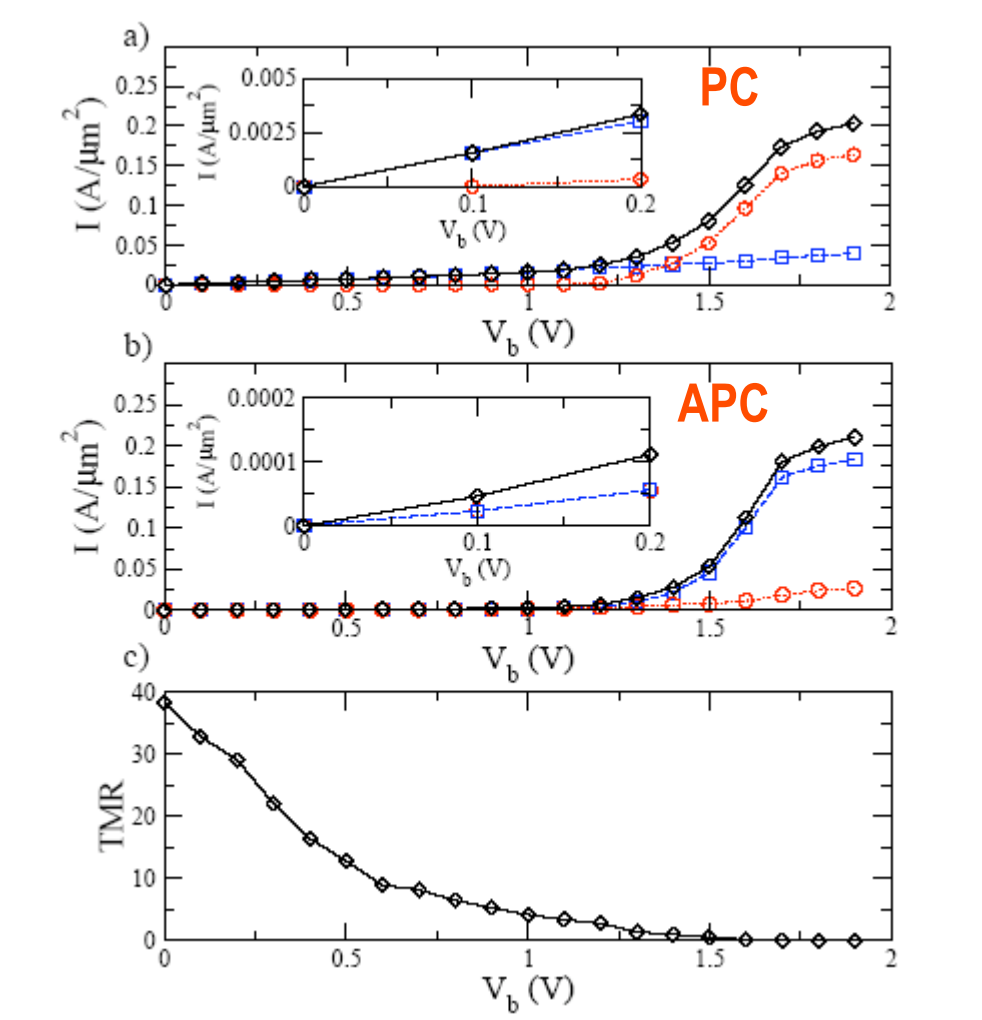


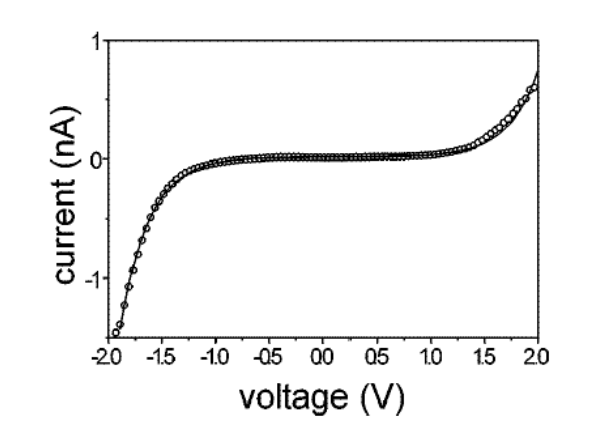
Solid-line (diamonds): APC; dotted-line (circles): $I_\downarrow$ for PC; dashed-line (squares): $I_\uparrow$ for PC.

- Due to resonance states on surfaces of Fe, huge number of k-sample must be done. These resonance states give “hot spots”.

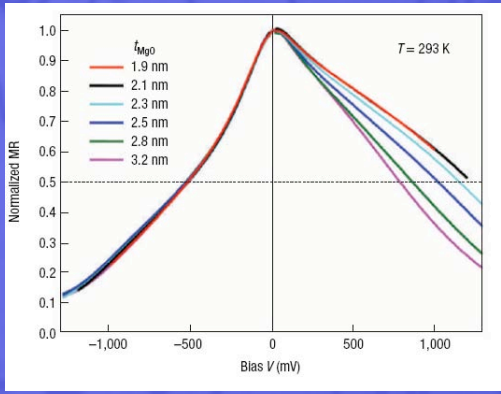
5 layer MgO:

$$TMR = \frac{I_{tot}^{\uparrow\uparrow} - I_{tot}^{\uparrow\downarrow}}{I_{tot}^{\uparrow\downarrow}}$$



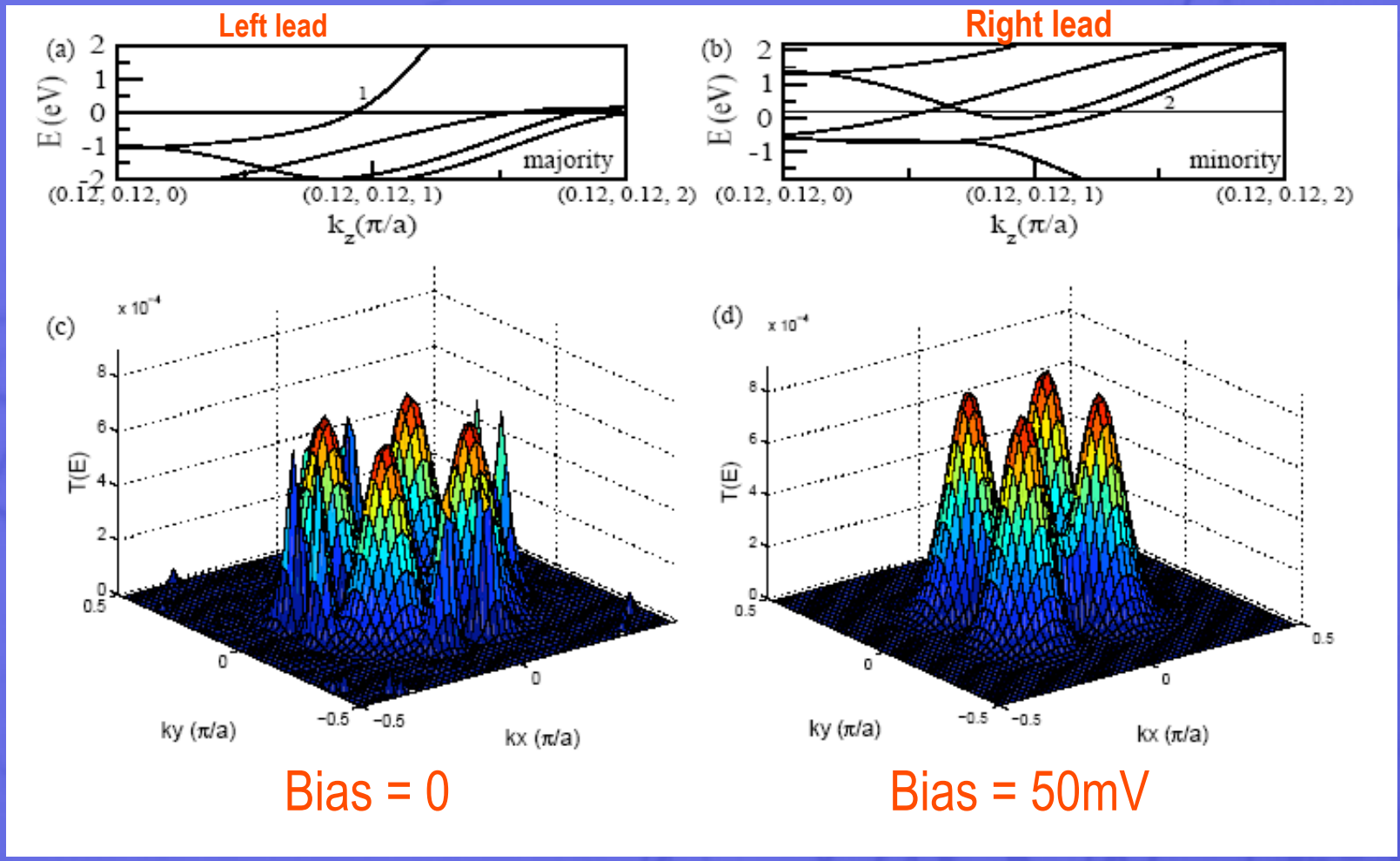


5-layer MgO, measured by Wulfhekel et al APL 78, p509 (2001). STM-MgO-Fe



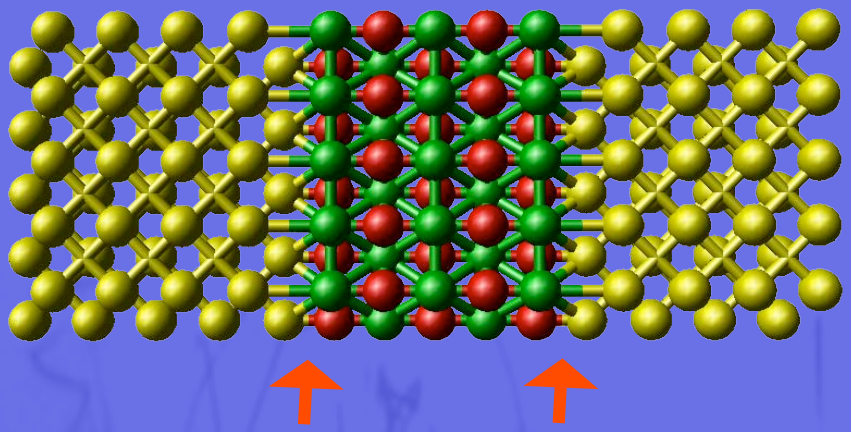
Yuasa et al., Nature Mat. Vol.3, 868 (2004).

Fe-MgO-Fe: transverse momentum resolved T(E) for APC

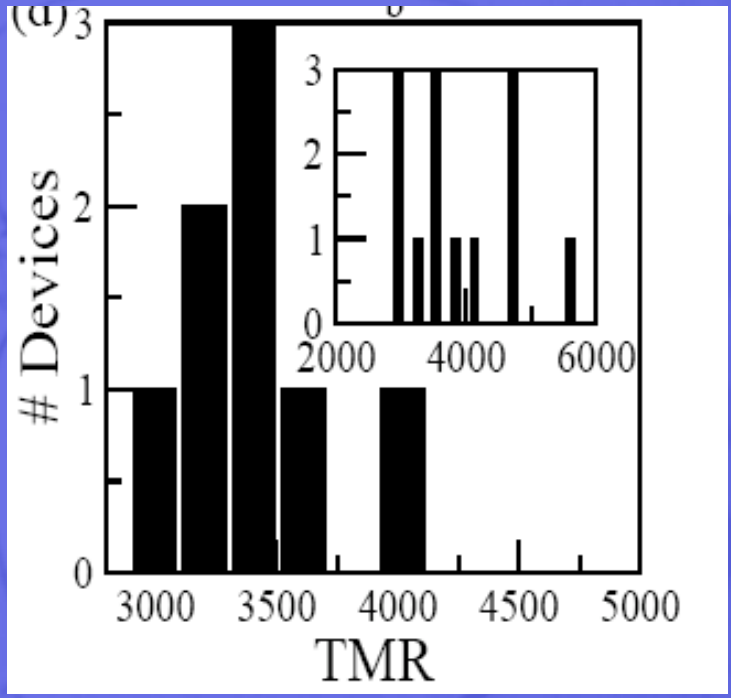


It is the drastic increase of APC current as a function of bias that quenches TMR.

Zero bias TMR: effects of small structure changes



Randomly change
interface bonds by ~1%.



Also, randomly change all bonds by ~1%.

These small structure changes do vary the value of TMR, but not enough to reduce it to the current experimental level (250%).

The remaining puzzle: zero bias TMR too large

Experimental data of Yuasa etal: ~200% (room T); Ohno etal: ~800% (5K);

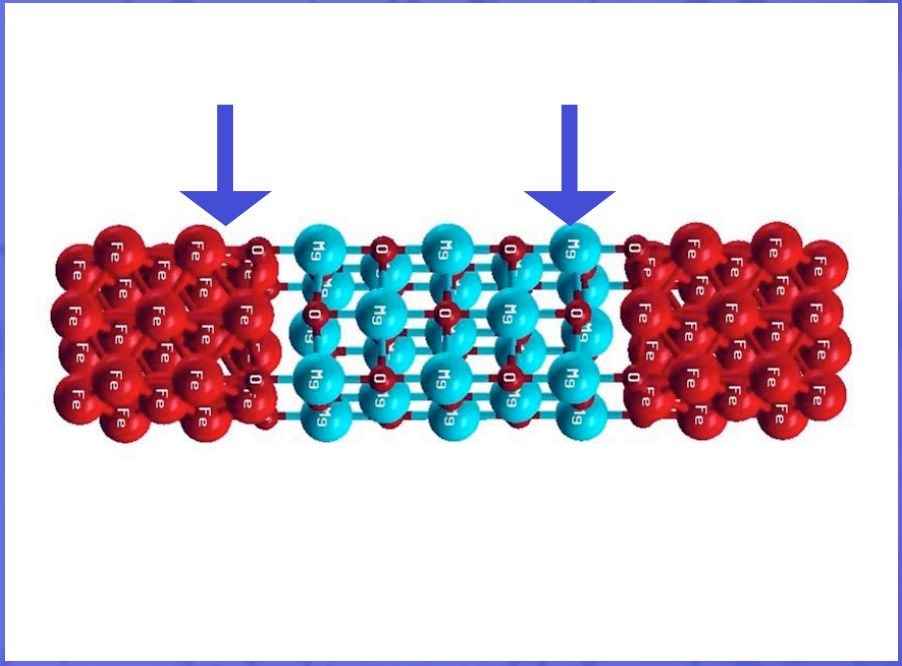
Theoretical results: ~3700%.

Possible reason: oxidizationlayer exists at the Fe/MgO interfaces.

Results:

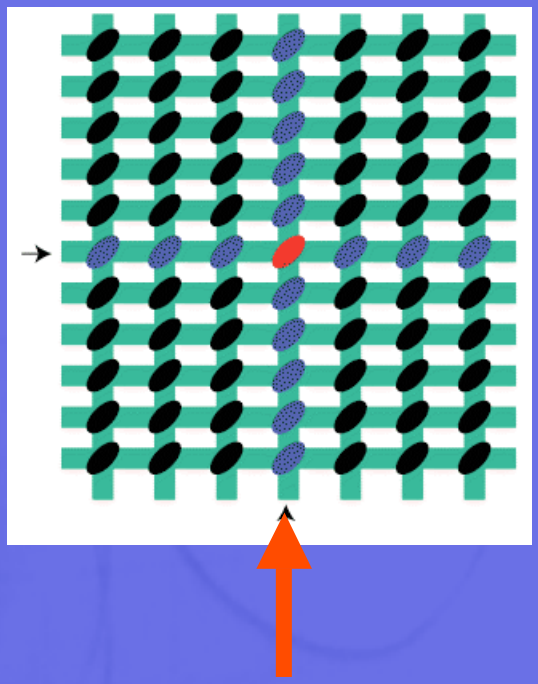
100% oxidization: TMR dropped to 169%. 50% oxidization: TMR dropped to 1040%.

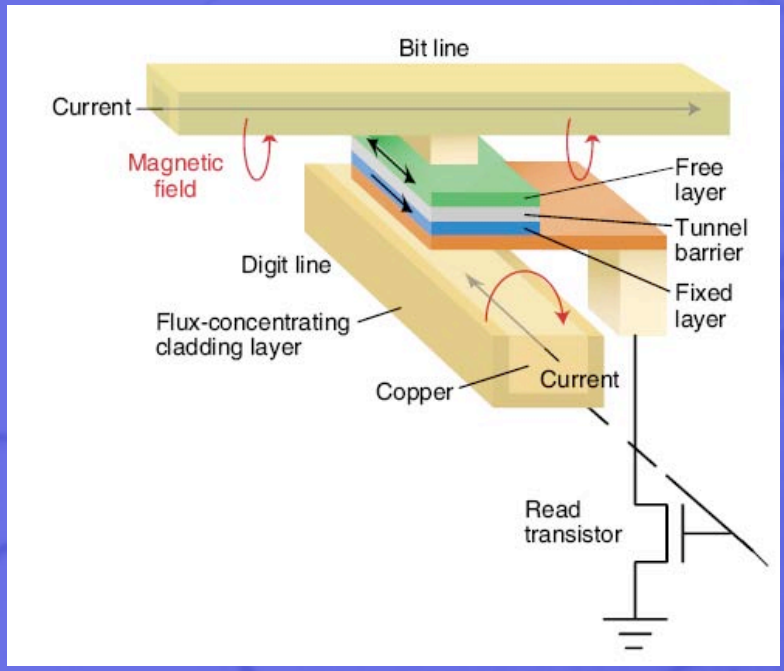
Experimental structure: 60% oxidization (Meyerheim etal, PRL 87, 076102 (2001).



D. Waldron etal, PRL, 97, 226802 (2006).

How to switch the device from PC to APC ?





- This is rather difficult to do from fabrication point of view.

J. Akerman, Science, 308, p508 (2005).

The phenomenon of spin transfer torque (STT):

STT is the torque exerted on the magnetization by spin polarized electric current. It has important implications on MRAM technology.

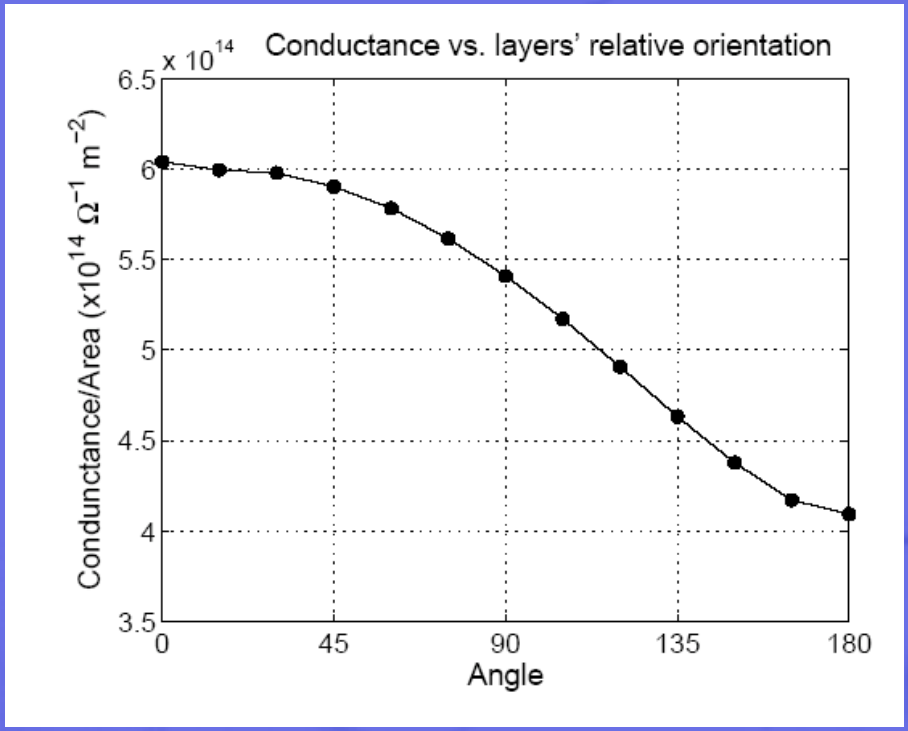
$$\frac{d\mathbf{s}_i}{dt} = \frac{1}{i\hbar}\sum_{i<j} \mathrm{Tr}\left[H^T_{i,j}\boldsymbol{\tau}G^<_{i,j} - \mathrm{h.c.}\right] + 2(\boldsymbol{\Delta}_i \times \mathbf{s}_i)$$

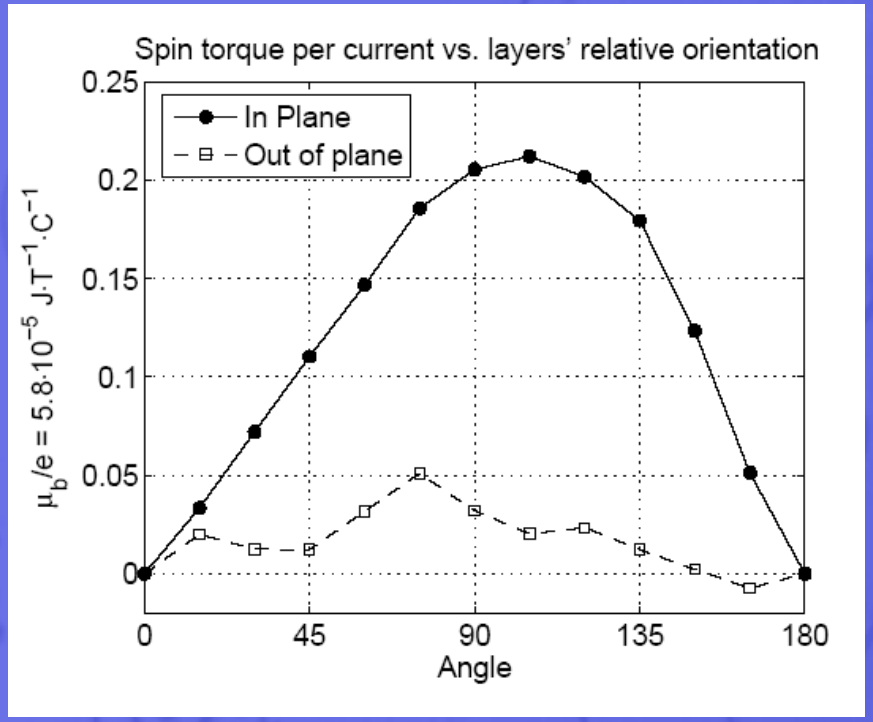
Spin current

precession

P. Haney etal., (2007).

Spin Transfer Torque Haney etal (2007)





The angular pre-factor of STT has been measured experimentally in PRL 84, 3149(2000). The calculated value is within a factor of 3 if assuming bulk Co damping factor, and agrees almost perfectly if assuming a reasonable value of thin film damping factor.

Summary of Fe-MgO-Fe:

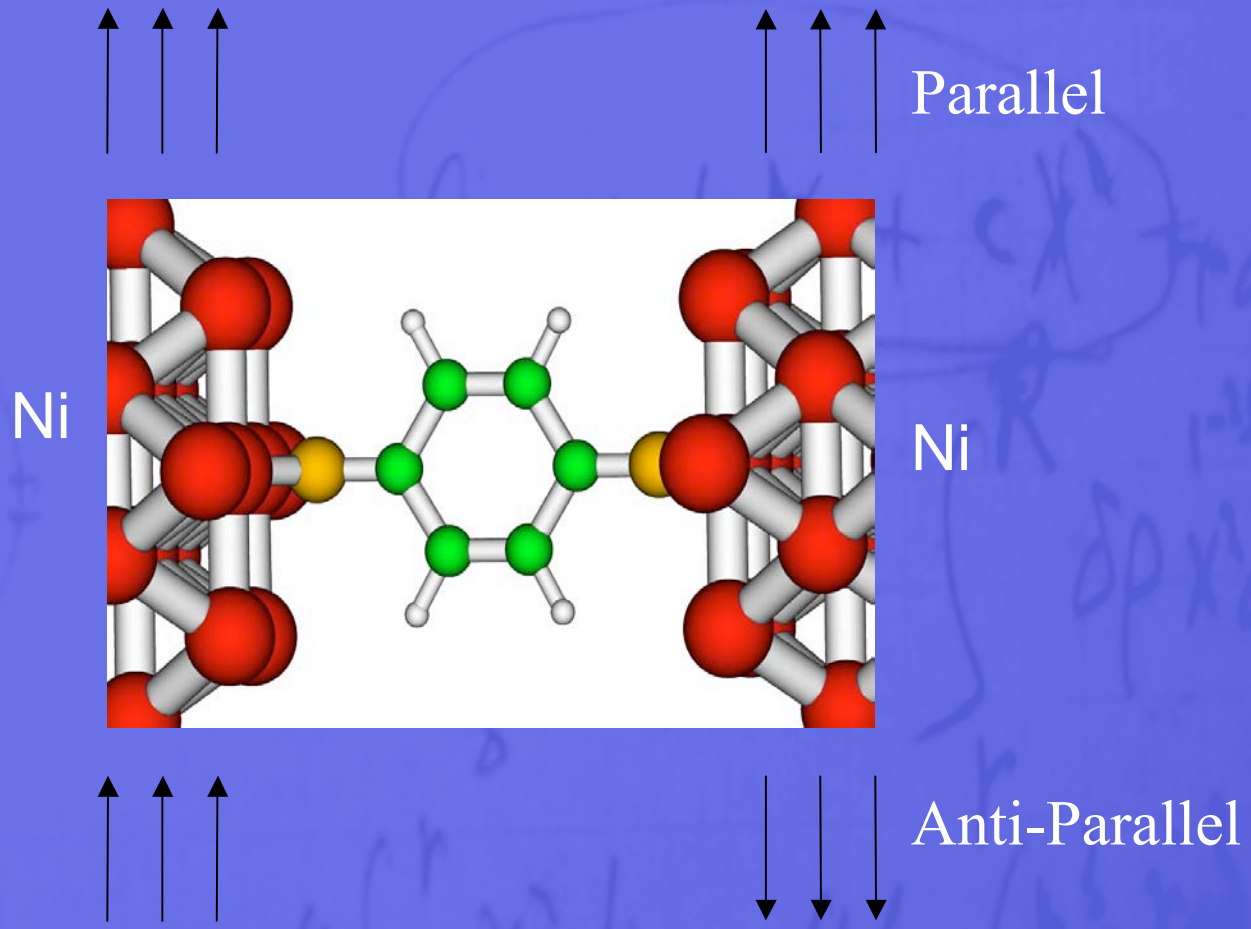
- Zero bias TMR: if there is a layer of FeO between the Fe and the MgO, the TMR value is drastically reduced. For 50% oxidization, TMR=1070%.
- Large TMR is due to small APC current. A finite bias increases APC current much faster than increasing PC current, causing TMR to drop.
- All voltage scales are consistent with experimental data.
- Remaining: how to reduce critical current for spin transfer torque?

Molecular TMR junction:

Ni leads: infinite cross-section in the transverse direction, extend to $z = \pm\infty$

We wish to compute spin-current:

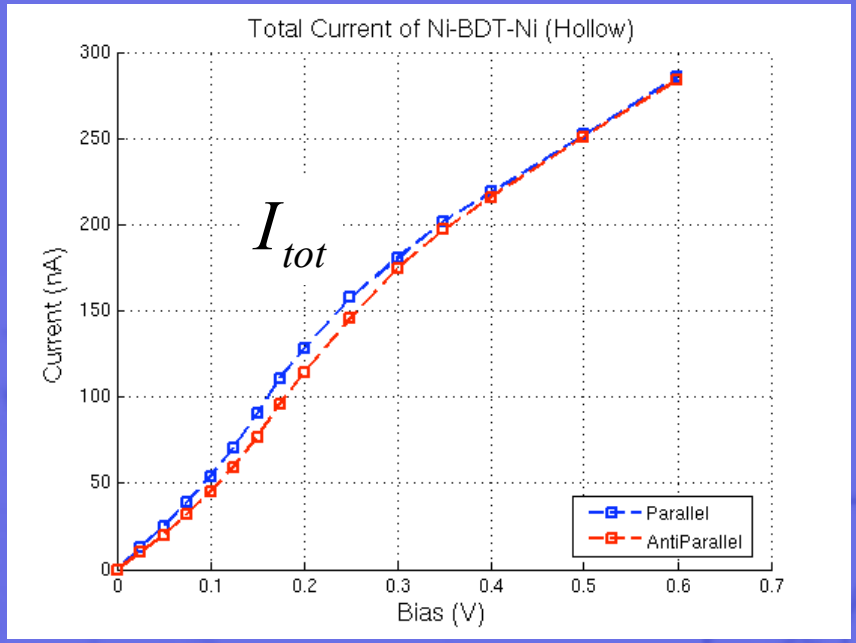
$$I_{\uparrow}, I_{\downarrow}$$

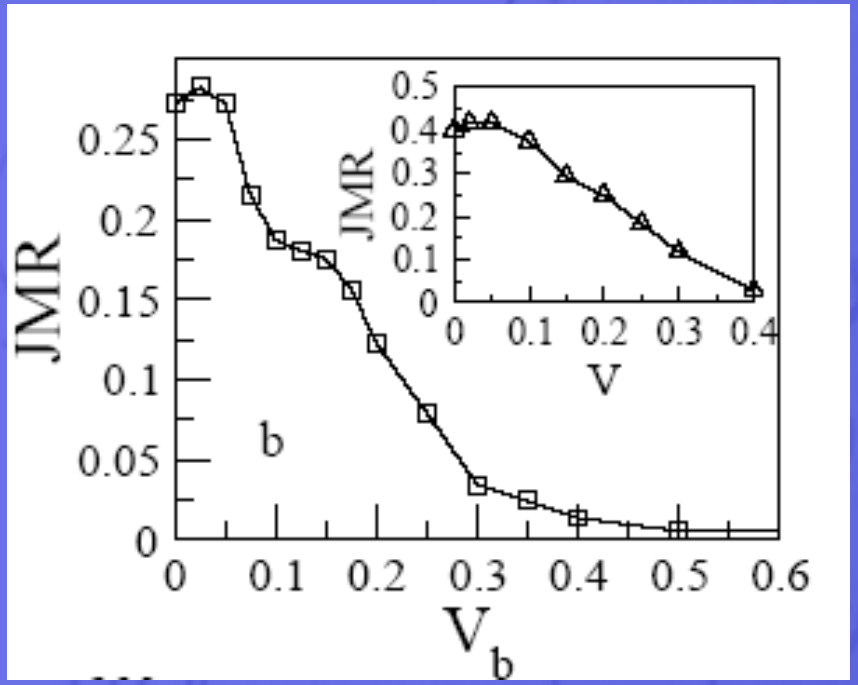


Waldron etal PRL 96, 166804 (2006)

Ni-BDT-Ni: Magneto-resistance ratio

$$\frac{I_{tot}^{\uparrow\uparrow} - I_{tot}^{\uparrow\downarrow}}{I_{tot}^{\uparrow\downarrow}}$$

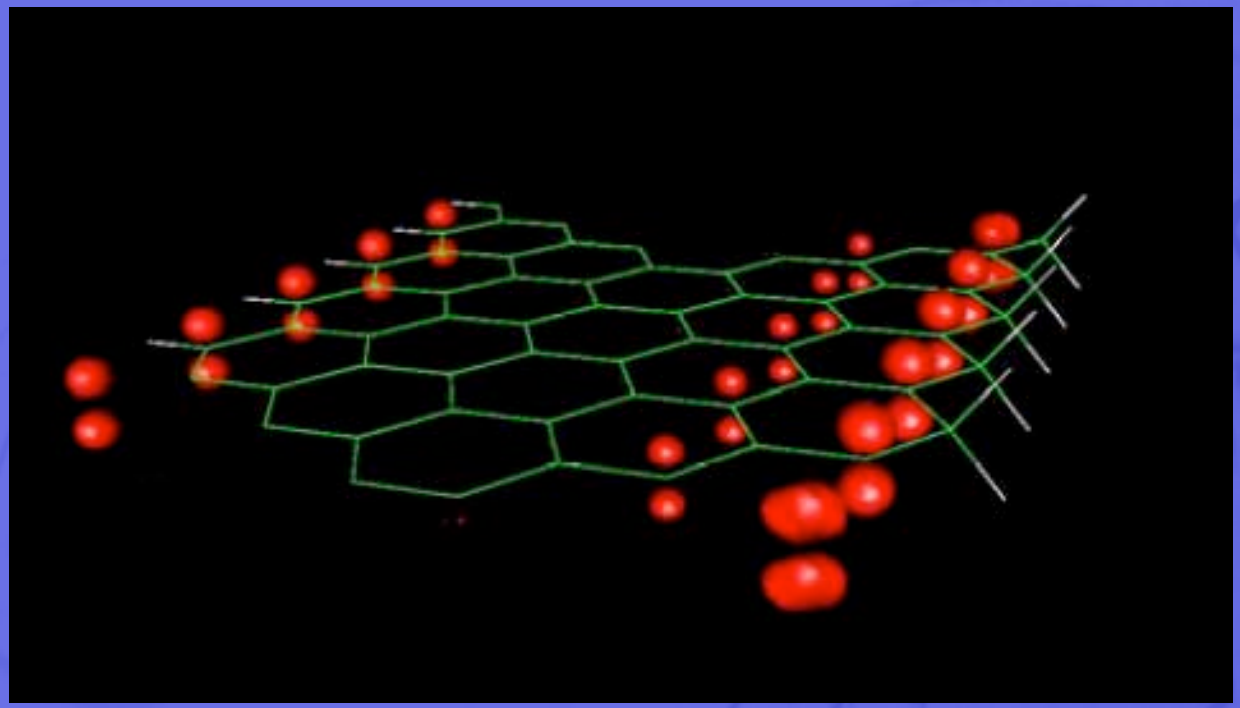




Although spin-currents are very different for up-up or up-down leads configurations, the total currents are rather close to each other!

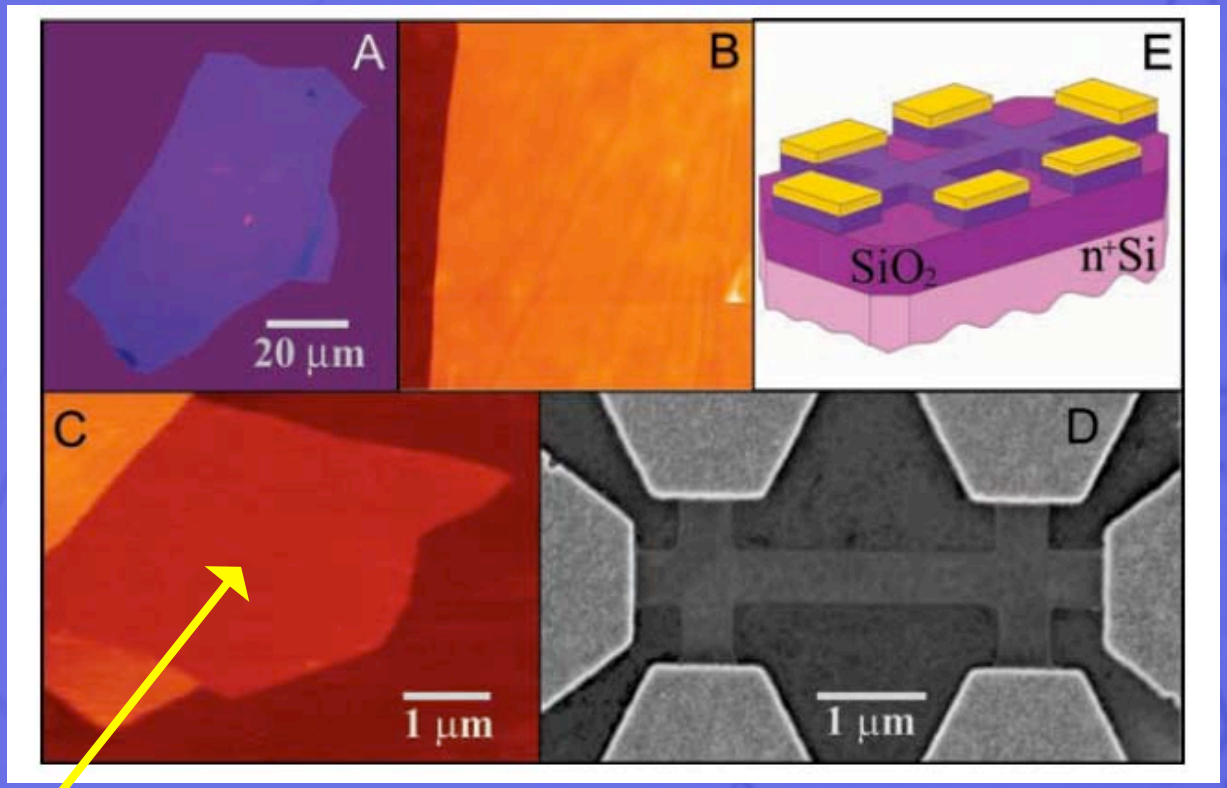
This gives rise to TMR ~ 28%.

Applicaoin: graphene spintronics:



On the zig-zag edges of a graphene ribbon, there is some “edge magnetism” due to localized electronic states. One may exploit this for graphene spintronics.

Graphene can now be produced experimentally



Single layer graphene

Mobility: 2.5m^2/V has been reported !

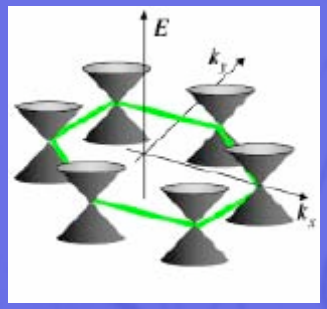
Novoselov etal Science, 306, 666 (2004); Zhang etal Nature, 438, 201 (2005).

Transport theory for bulk graphene sheets:

PRL 98, 076602 (2007) PHYSICAL REVIEW LETTERS week ending 16 FEBRUARY 2007

Quantum Transport of Massless Dirac Fermions

Kentaro Nomura and A. H. MacDonald



$$H_K = \hbar v \boldsymbol{\sigma} \cdot \mathbf{k} = v\hbar \begin{pmatrix} 0 & k_x - ik_y \\ k_x + ik_y & 0 \end{pmatrix},$$

$$[-i\hbar v \boldsymbol{\sigma} \cdot \nabla + V(\mathbf{r})]\psi = E\psi,$$

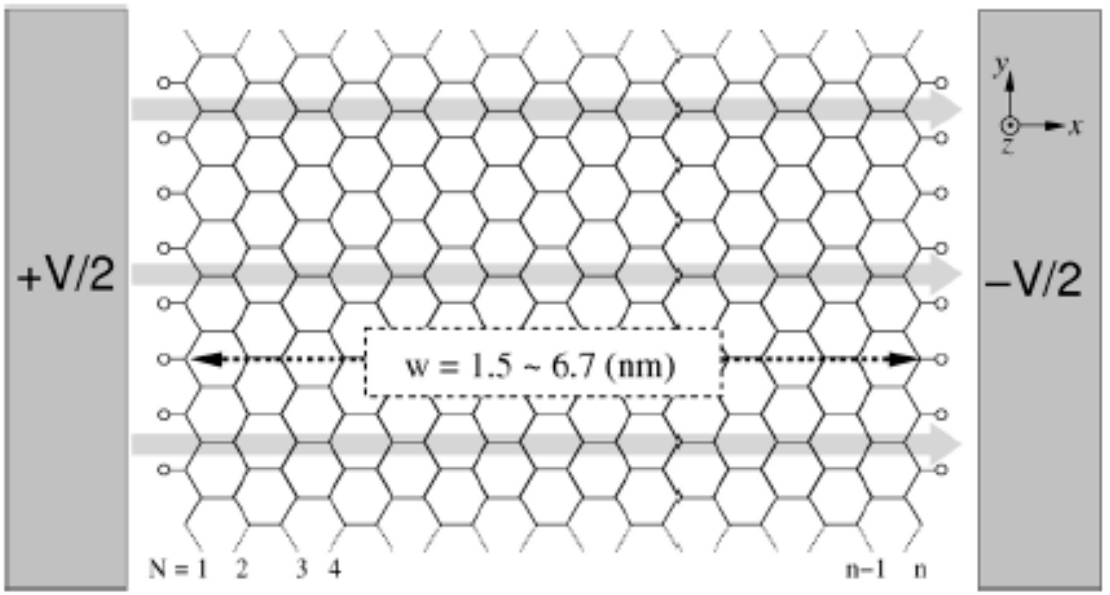
For charged impurity scattering V(r), Boltzmann theory gives transport properties. The massless fermion theory works near the Dirac point.

Half-metallic graphene nanoribbons

Young-Woo Son[1], Marvin L. Cohen[1,2] & Steven G. Louie[1,]

Zig-zag along y-axis (transport direction).

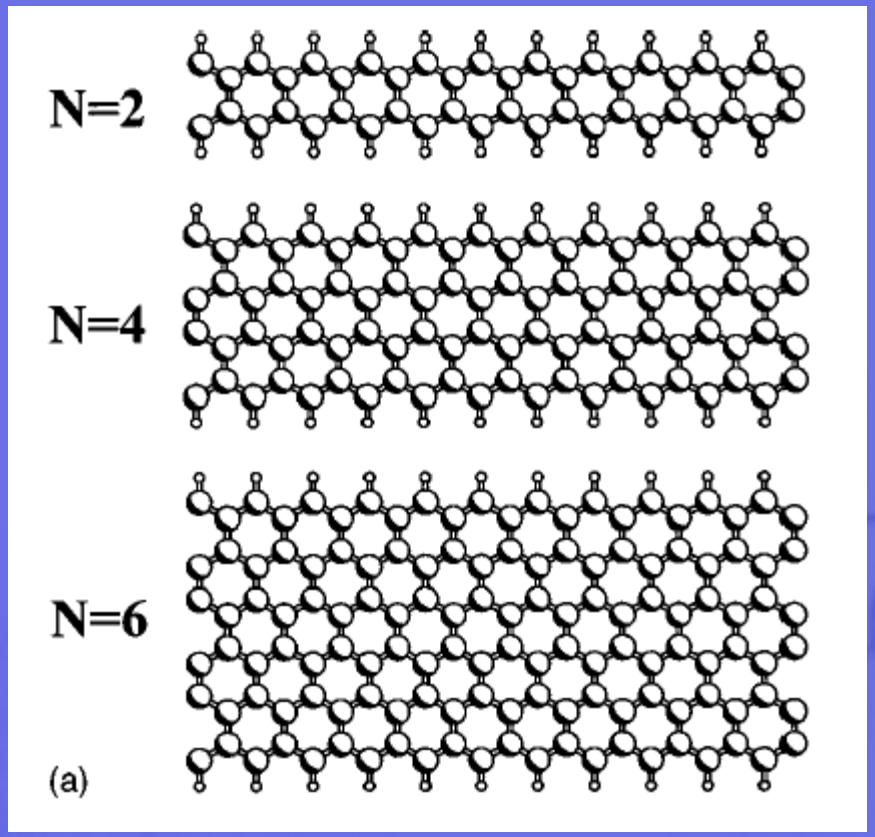
Electric field along x-axis, shifting spin resolved DOS relative to the Fermi level, producing a half-metallic behaviour.

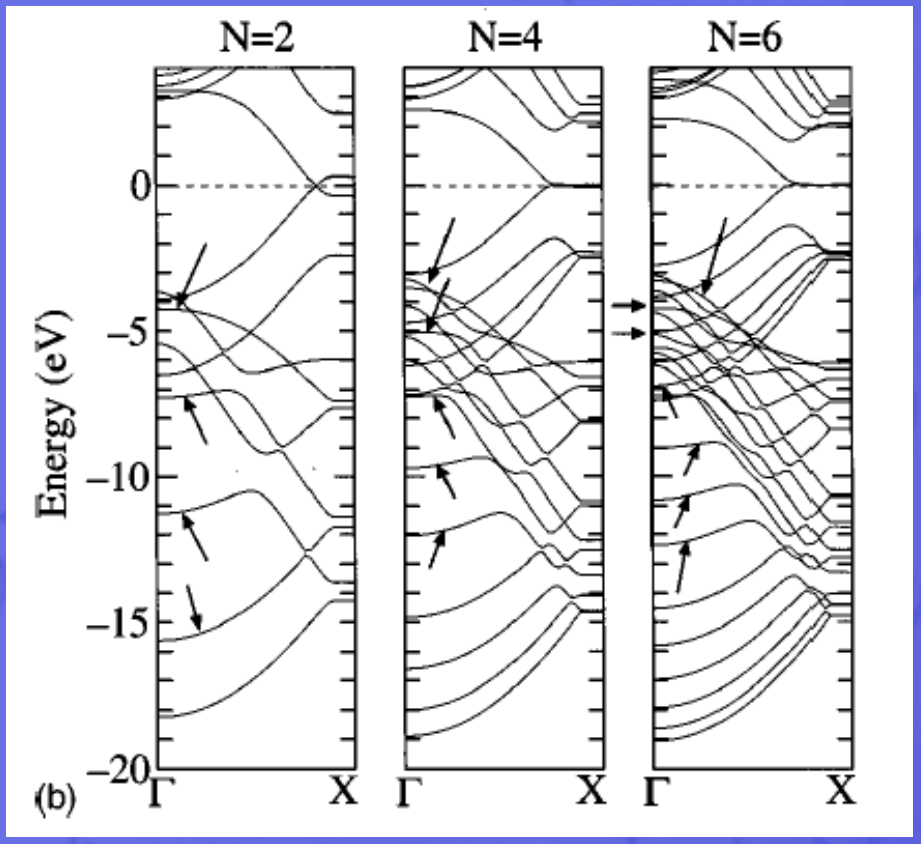


Beautiful descriptions of zigzag graphene nano-ribbons (ZGNR).

Son, Cohen and Louie, Nature (2006).

“Edge” states from DFT-LDA:





Miyamoto etal PRB 59, 9858 (1999).

Magnetic edges from DFT-LSDA:

PHYSICAL REVIEW B **67**, 092406 (2003)

Magnetic nanographite

Koichi Kusakabe* and Masanori Maruyama†
Graduate School of Science and Technology, Niigata University, Ikarashi, Niigata 950-2181, Japan
(Received 2 October 2002; revised manuscript received 11 December 2002; published 28 March 2003)

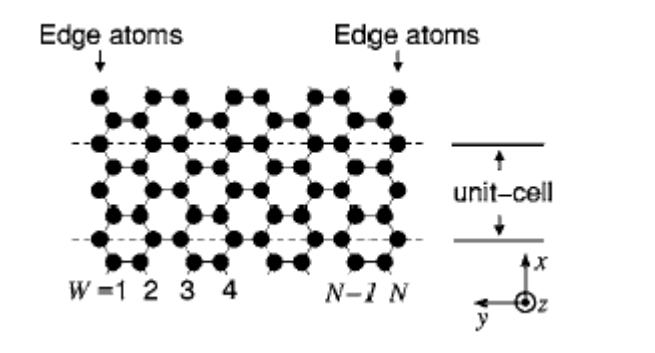
PHYSICAL REVIEW B **72**, 174431 (2005)

Magnetic ordering at the edges of graphitic fragments: Magnetic tail interactions between the edge-localized states

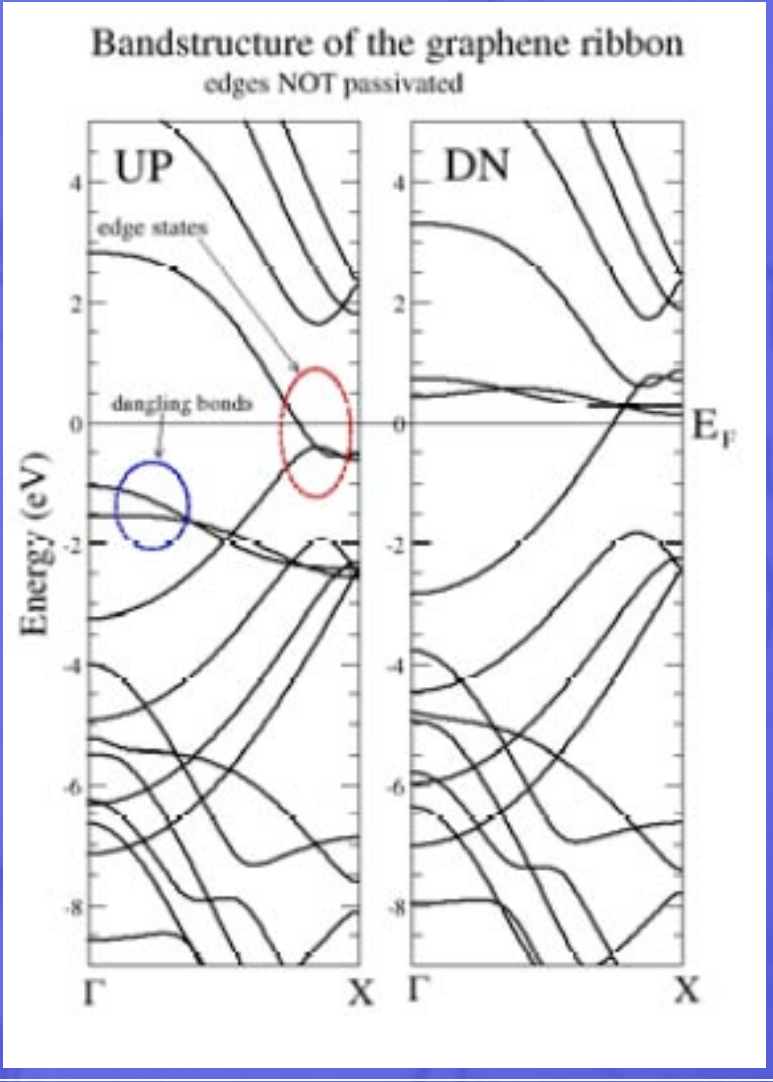
Hosik Lee,[1] Young-Woo Son,[1] Noejung Park,[2] Seungwu Han,[3] and Jaejun Yu[1,*]
[1]*School of Physics and Center for Strongly Correlated Materials Research, Seoul National University, Seoul 151-747, Korea*
[2]*Department of Applied Physics, Dankook University, Seoul 140-714, Korea*
[3]*Department of Physics, Ewha Womans University, Seoul 120-750, Korea*
(Received 23 May 2005; revised manuscript received 14 September 2005; published 30 November 2005)

Plus several other papers (some are earlier)

Dangling bonds and edge states:



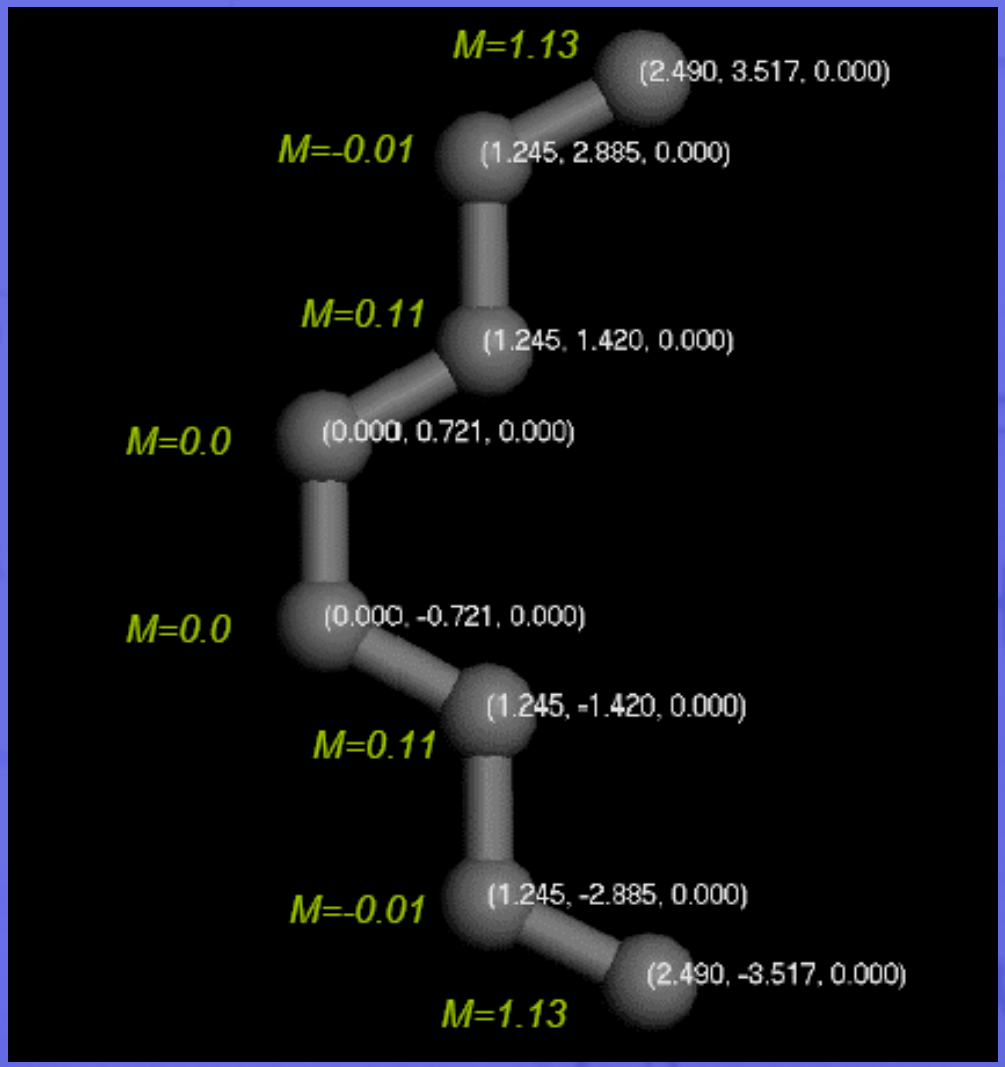
Lee etal, PRB 72 (2005)



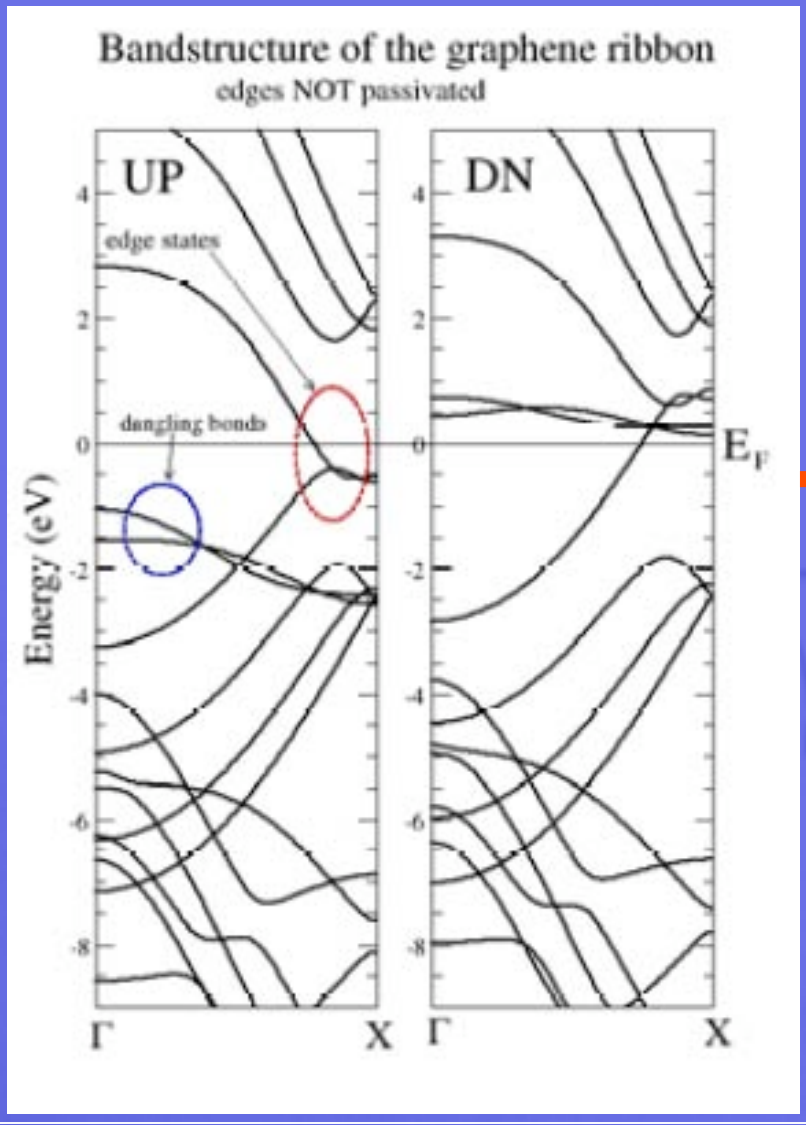
LAPW calculation by WIEN2K.

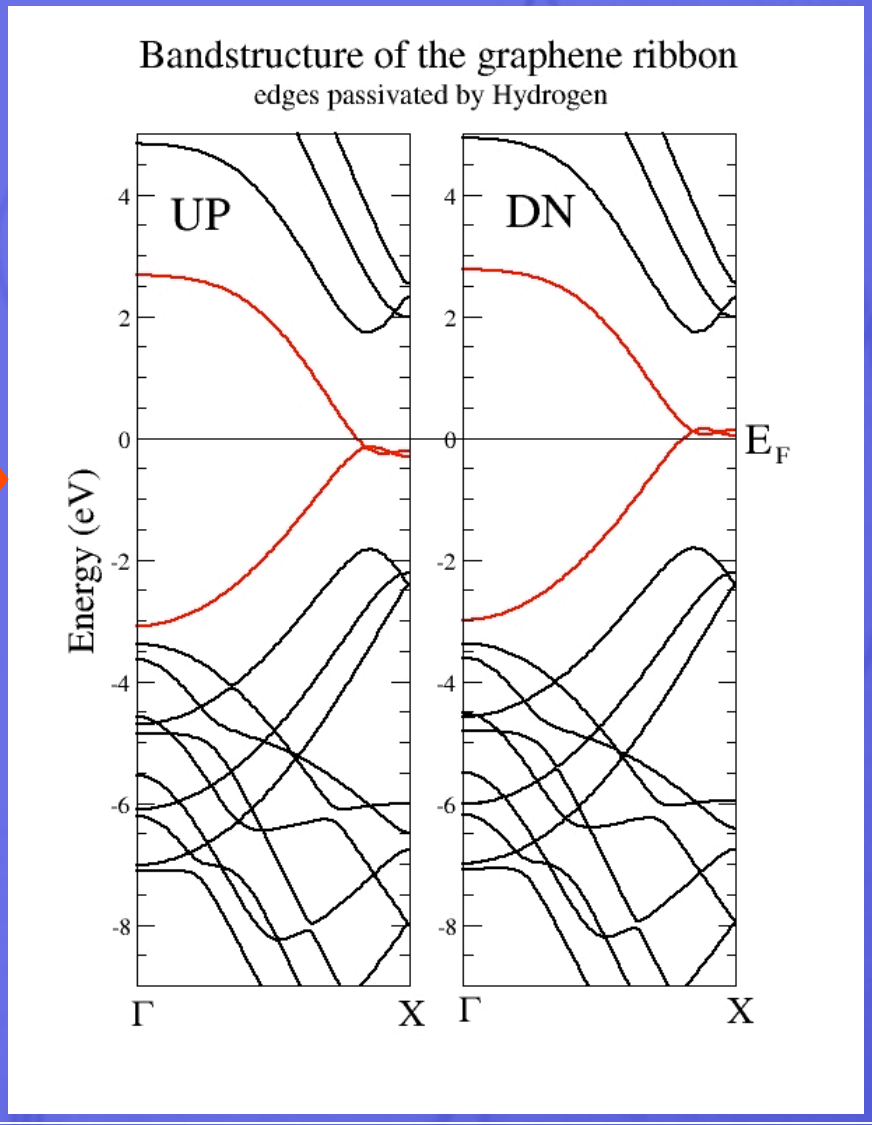
V. Timochevski (2006)

Magnetic moment per atom for pure ribbon:

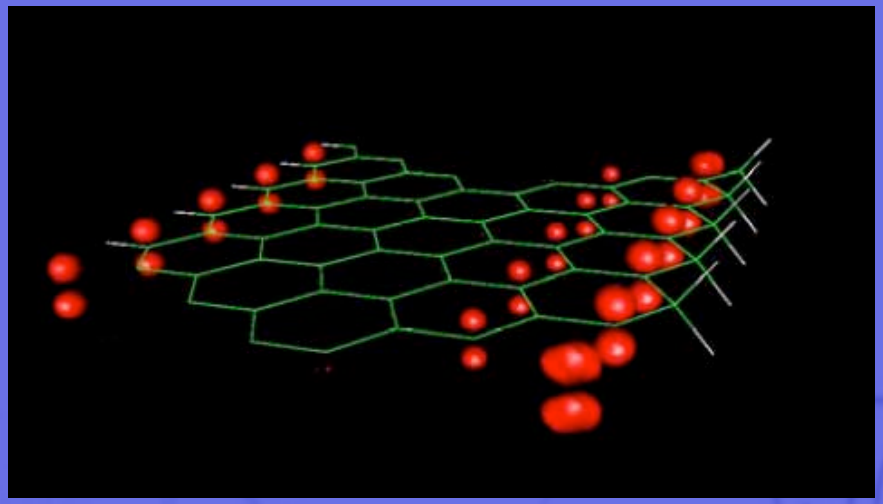


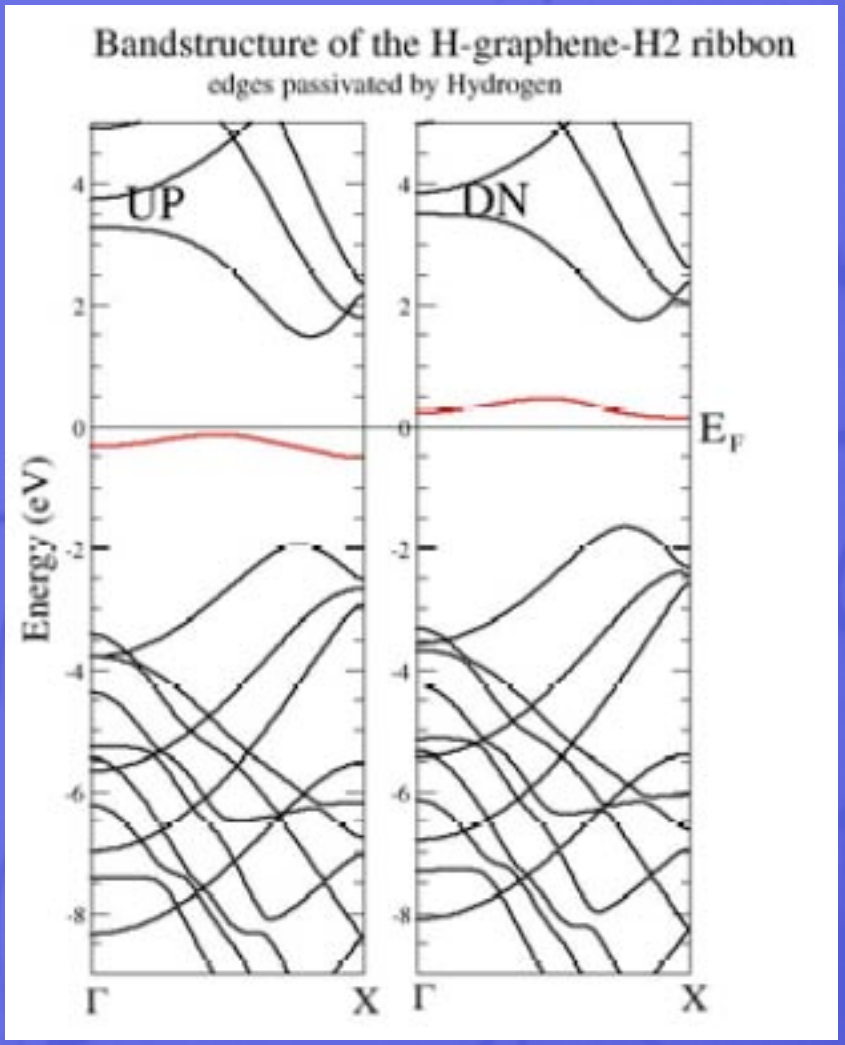
Saturating the dangling bonds, only edge state left:



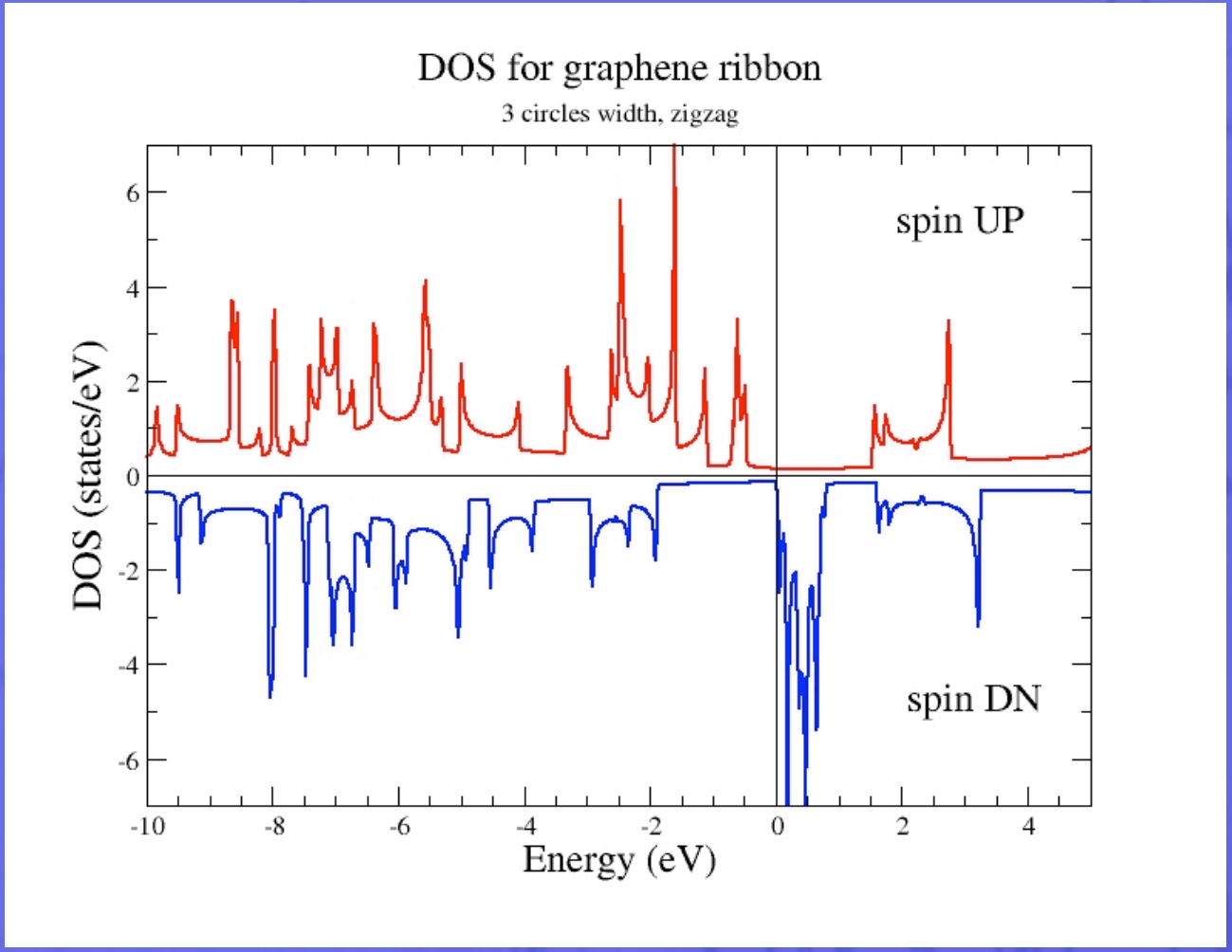


H-graphene-H2



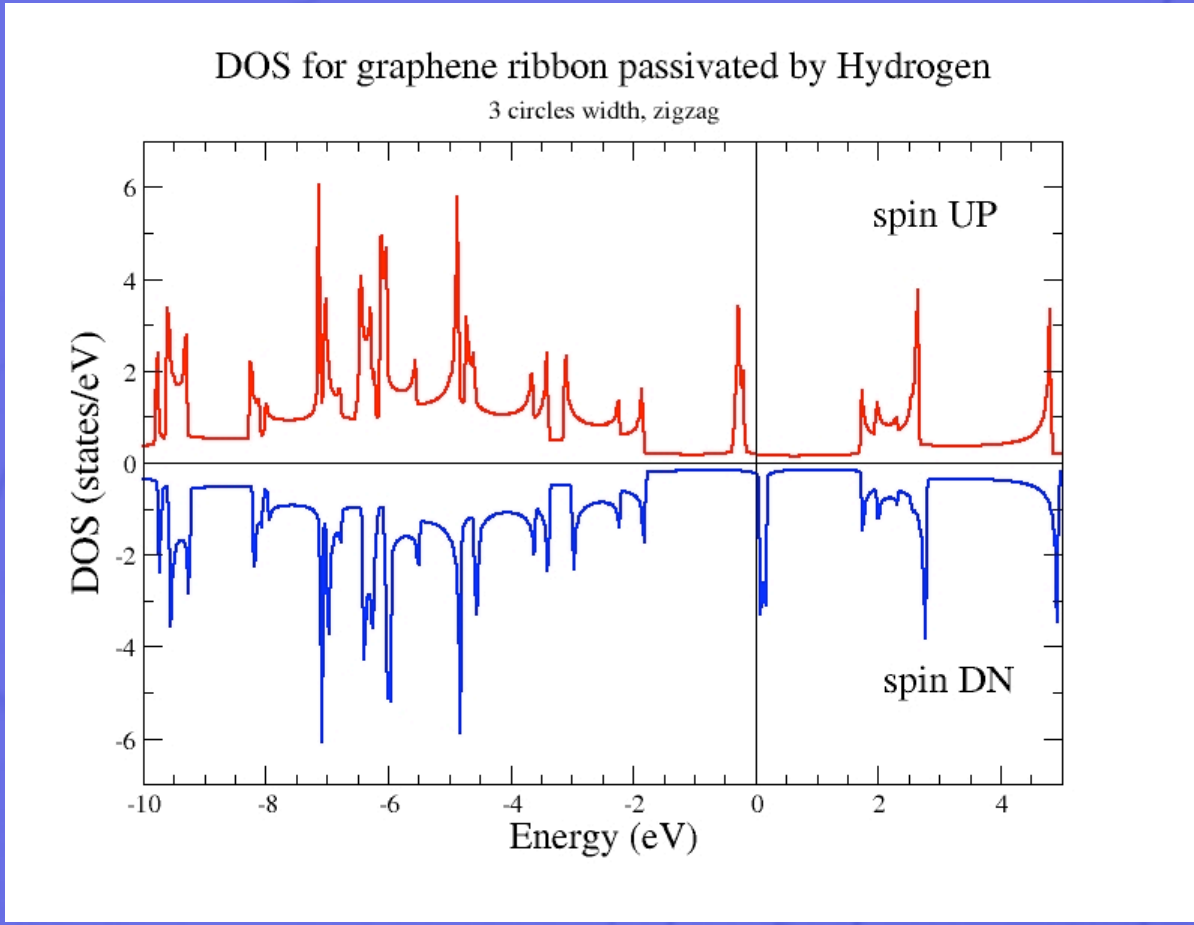


DOS: spin splitting for un-passivated edge



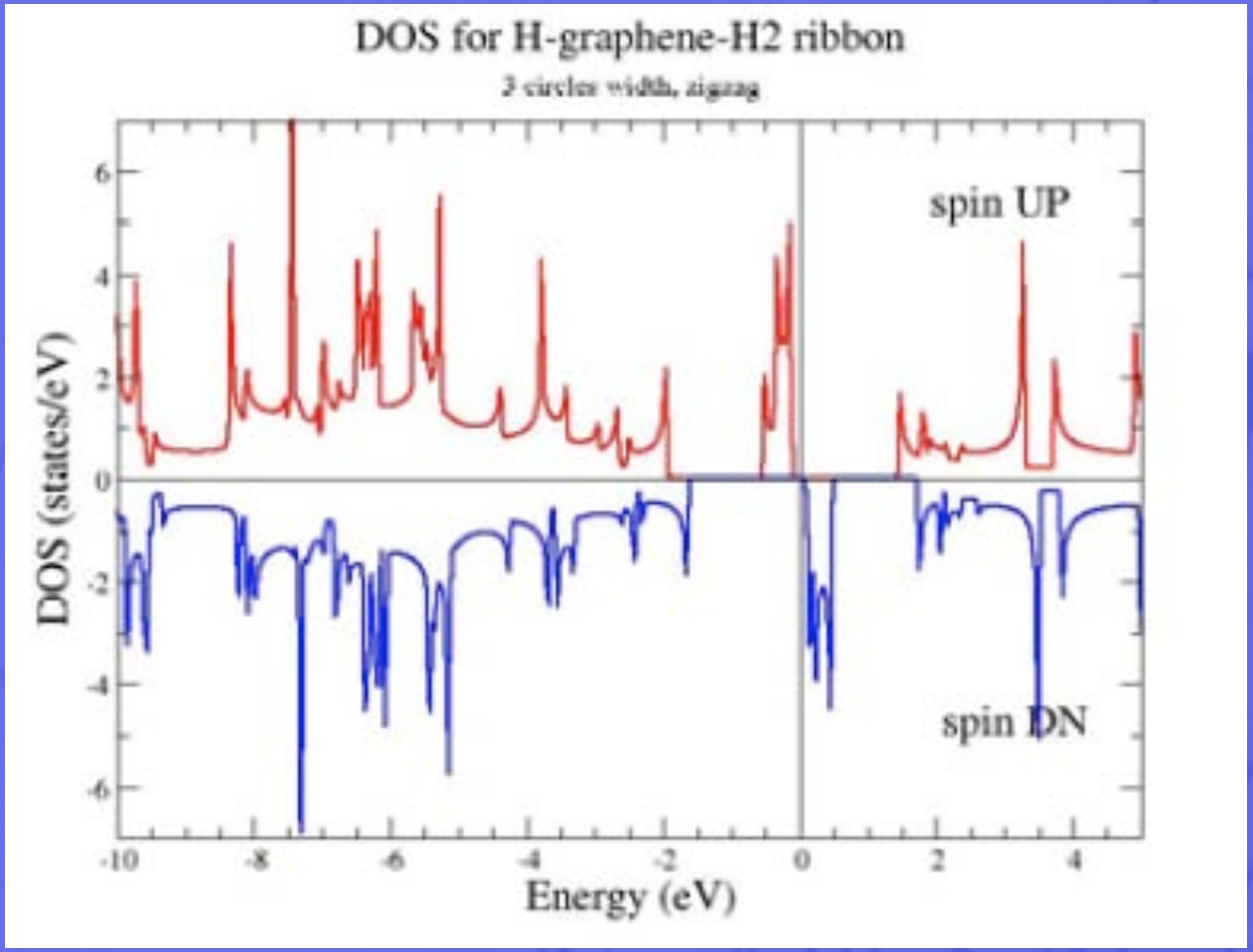
V. Timochevski (2006)

DOS: spin splitting for H-passivated edge



V. Timochevski (2006)

H-graphene-H2



V. Timochevski (2006)

Total energies:

SYSTEM	FM	AFM	(FM-AFM)/atom
graphene	-1235.817 eV	-1235.849 eV	+4.0 meV
H-graphene-H	-1272.713 eV	-1272.716 eV	+0.3 meV
H-graphene-H2	-1288.321 eV	-1287.954 eV	-4.5 meV

Along each edge FM is more stable than AFM across the width of ribbon. The FM and AFM are almost degenerate. Recent report puts this energy difference as 1/W.

Are these correct ? Can one measure them ?

More Accurate Calculations?

The accuracy depends on the level of theory: but there are always some approximations in theory.

Magnetic Measurement?

Magnetic measurements, e.g surface magnetic optical Kerr effect (SMOKE) and/or electron cycle resonance (ECR) cannot provide spatial resolution down to the atomic scale.

Real Space Observations?

Real space local probe by spin polarized STM may be possible. Does the edge magnetism give enough spin contrast in STM?

→ **Simulation of STM spin contrast (Wei Ji etal, (2007)).**

Spin polarized STM images on single sheet ZGNR in vacuum

We justify this simulation by: (i) we have to start from a simple case; (ii) we wish to get a baseline result; (iii) There is a report on experimentally suspending graphene sheets in vacuum:

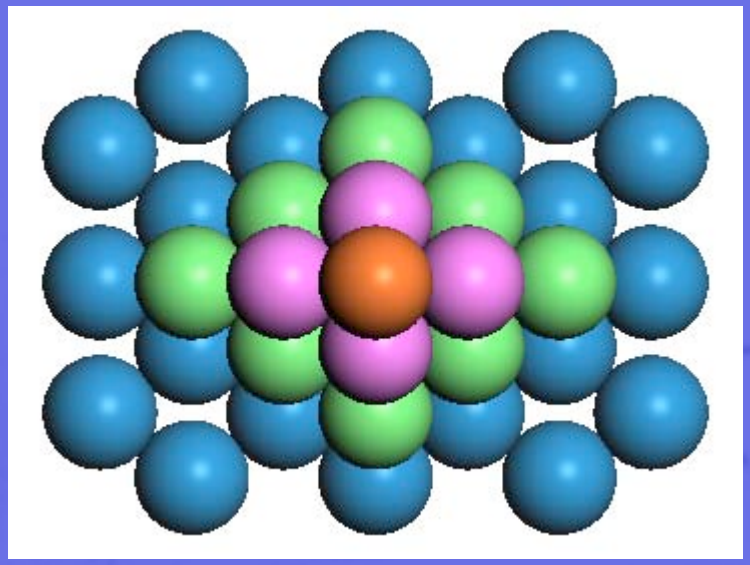
The structure of suspended graphene sheets

Jannik C. Meyer[1], A. K. Geim[2], M. I. Katsnelson[3], K. S. Novoselov[2], T. J. Booth[2] & S. Roth[1]

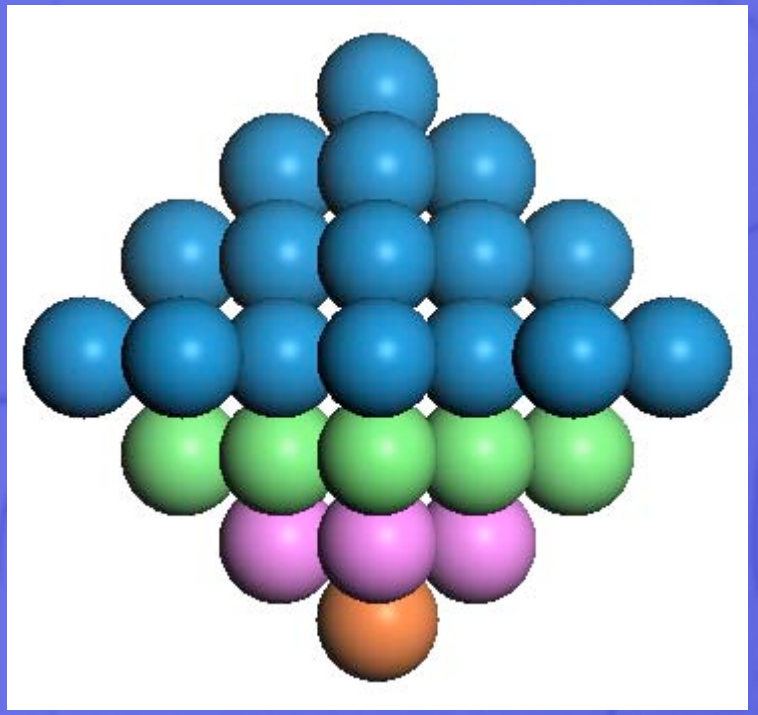
Nature, 446, 60 (2007).

We are also simulating double layer ZGNR and ZGNR sitting on SiC crystal surface.

W(110) tip

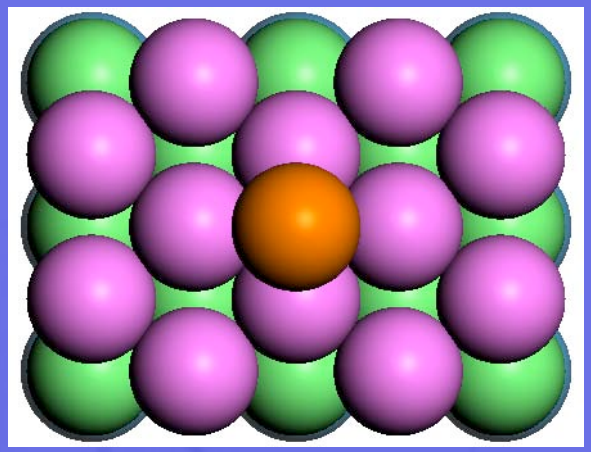


Bottom view



Side view

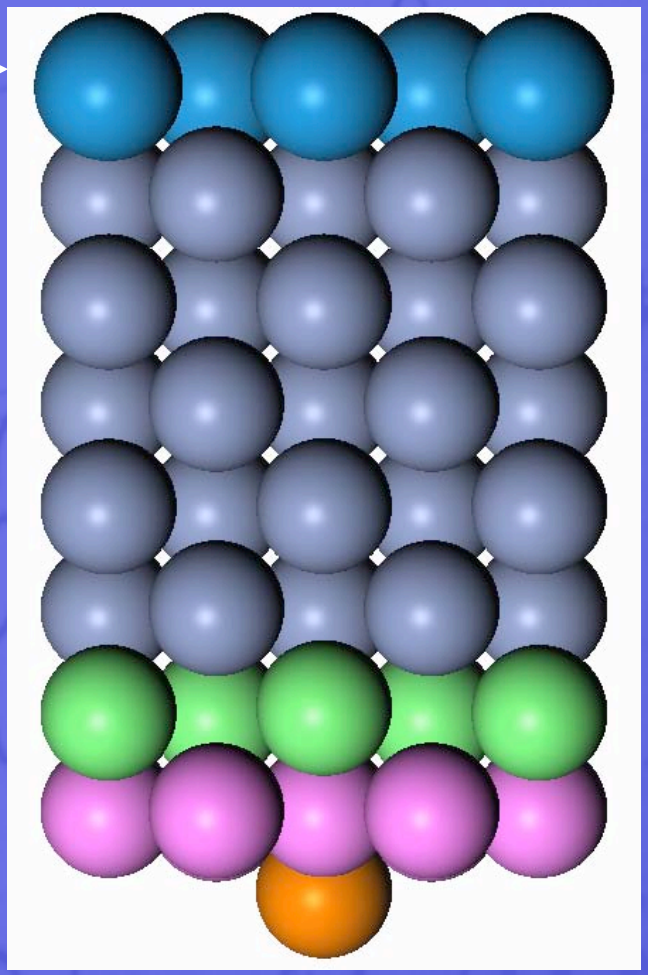
W(110)-Cr tip



Bottom view

W

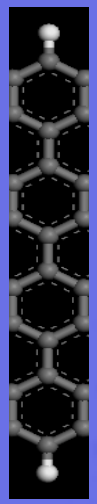
Cr

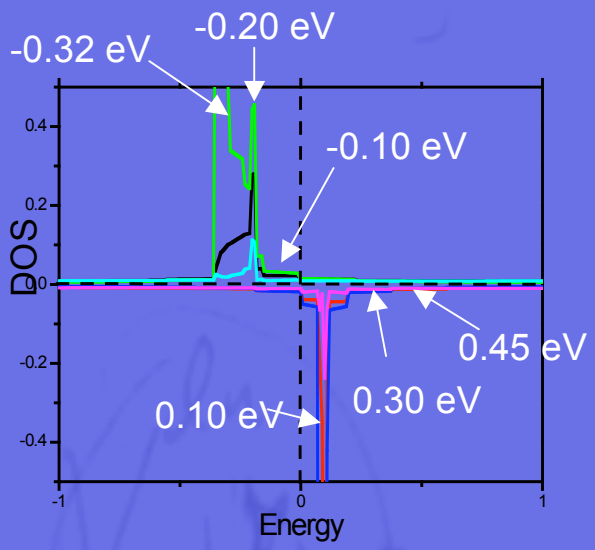


Side view

Simulation 1- spin polarized edge with W tip

Unitcell



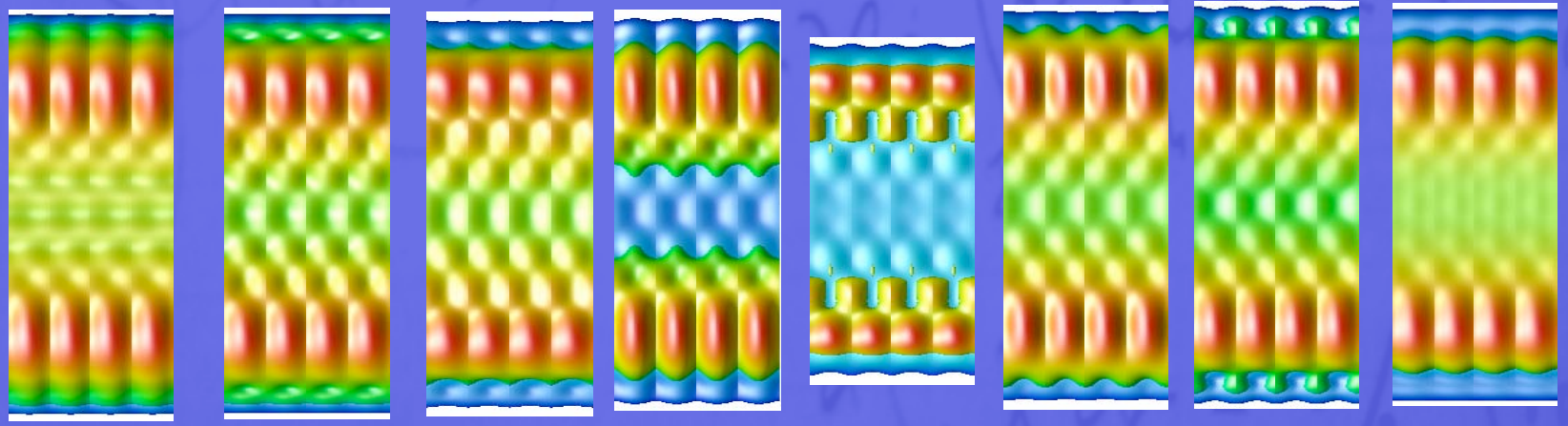


Interesting Levels:
-0.32 eV,
-0.20 eV,
-0.10 eV,
+0.10 eV,
+0.30 eV,
+0.45 eV,
Two contrasts:
-0.80 eV
+0.80 eV

Spin non-resolved
W110 Tip
I: 40 pA

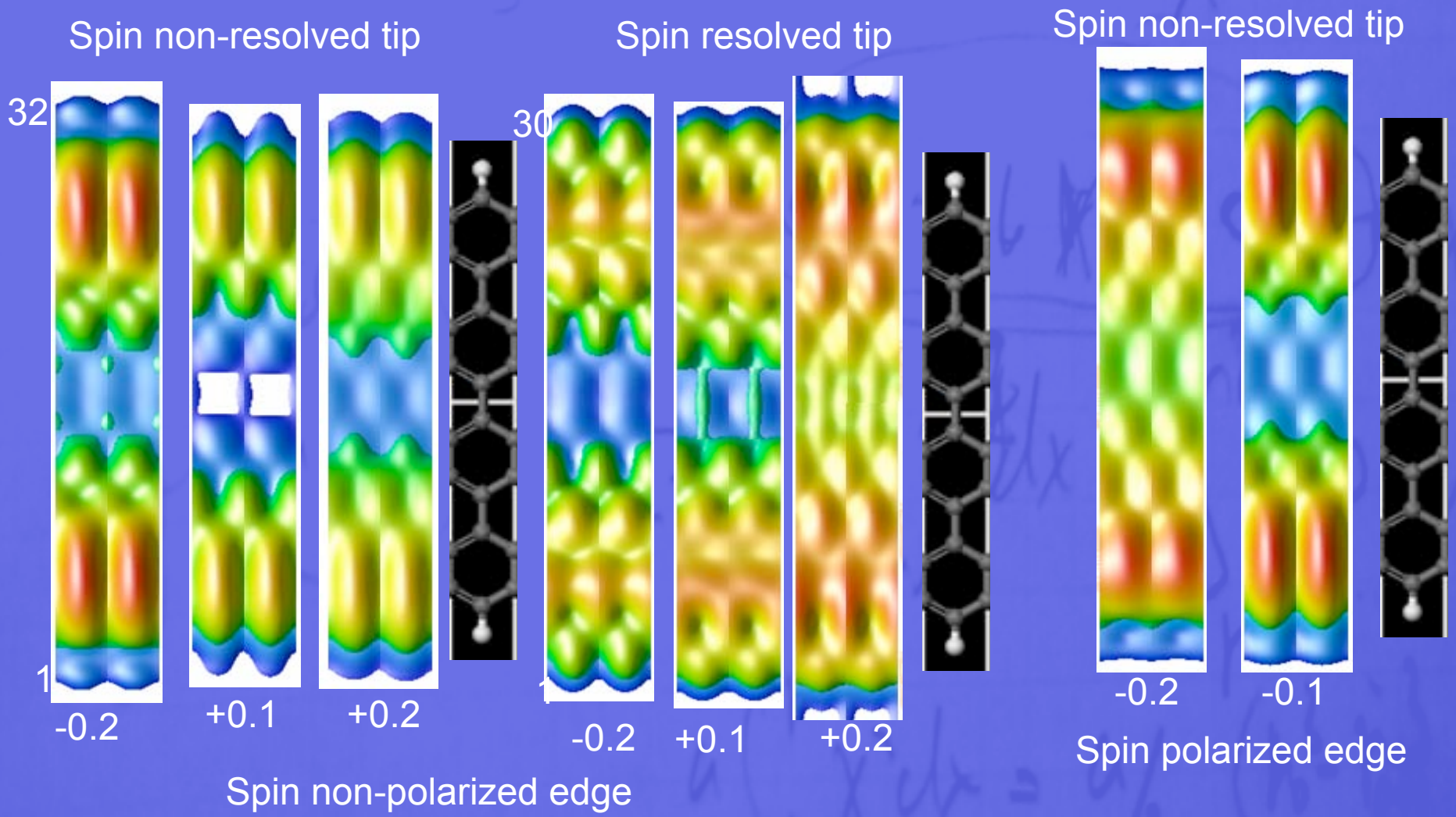
VASP+BSKAN, Hofer (2003).

Spin is not resolved.



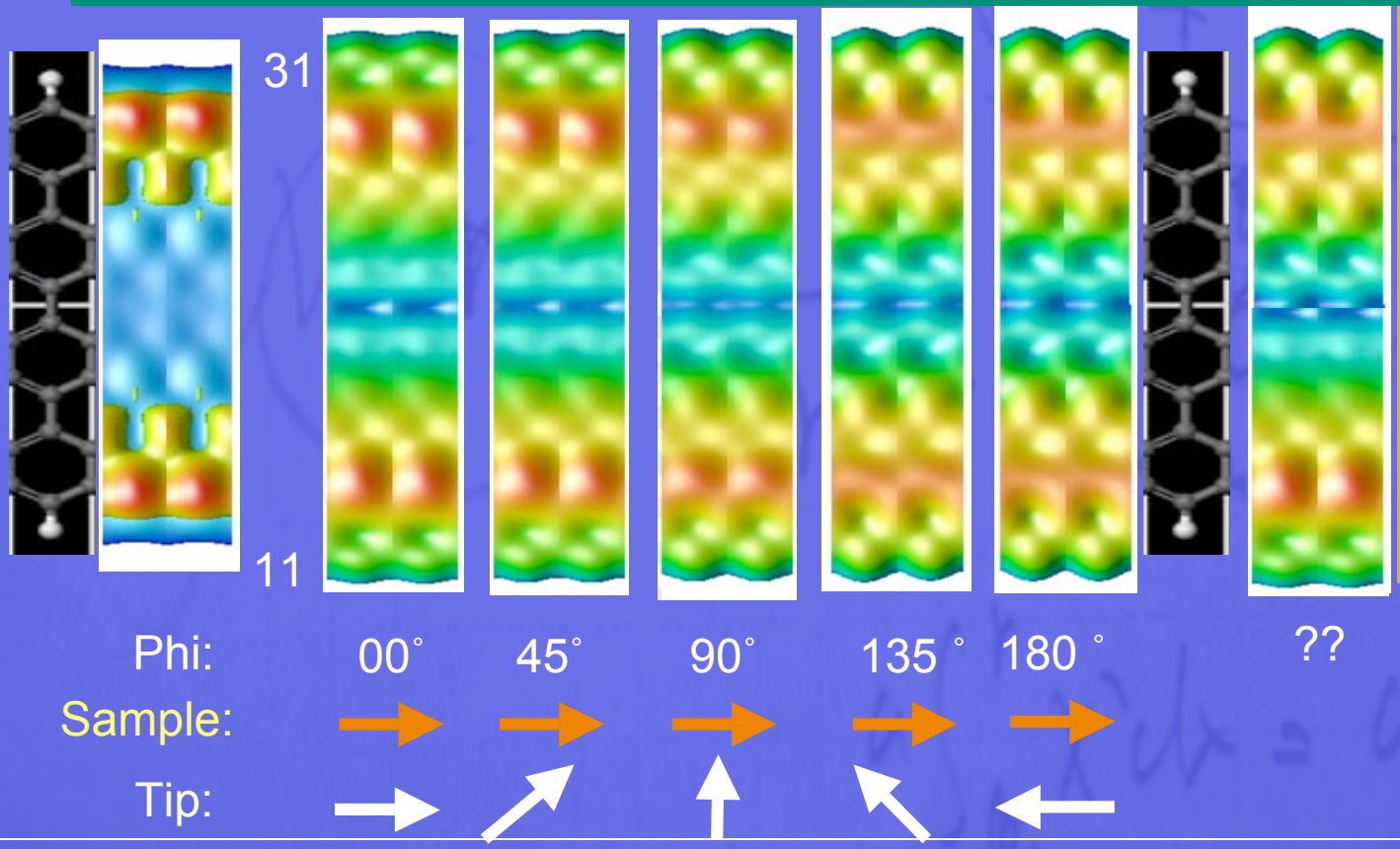
-0.80 V | -0.32 V | -0.20 V | -0.10V | +0.1 V | +0.3 V | +0.45 V | +0.80 V

Simulation 2- spin non-polarized edge with W & Cr tips



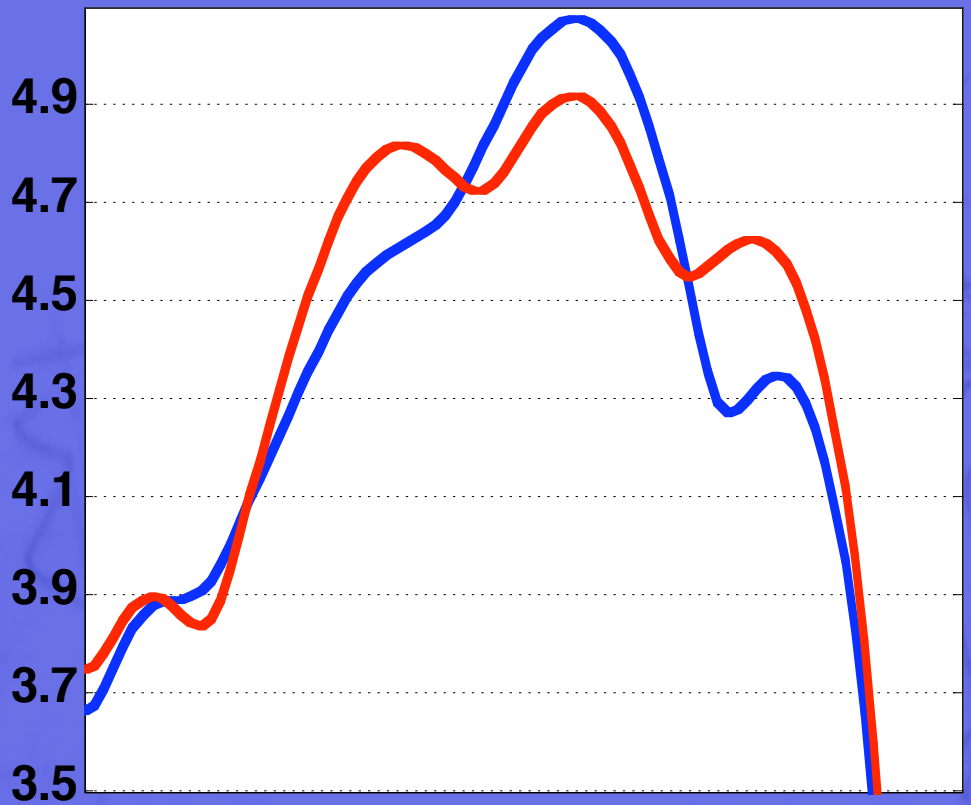
Simulation 3 - spin polarized edge with Cr tip

- Spin resolved Cr tip on W(110) base
- Bias Voltage: +0.1 V (Largest contrast among all interesting voltages)
- Tunneling Current: 40 pA (typical current for molecular systems at low T)
- Sample-tip Coupling: from FM to AFM (non-collinear spin polarization)



- Contrast reversal between FM and AFM coupling only occurs at edges
- The spin (non)-polarized edge states can be resolved by changing of tip polarizations.
- Features in the out side of edges

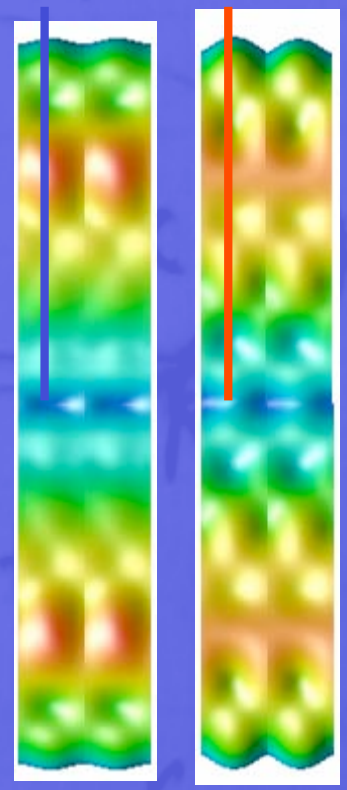
Corrugation height of spin-polarized image



AFM

FM

+0.1 V 2 pA



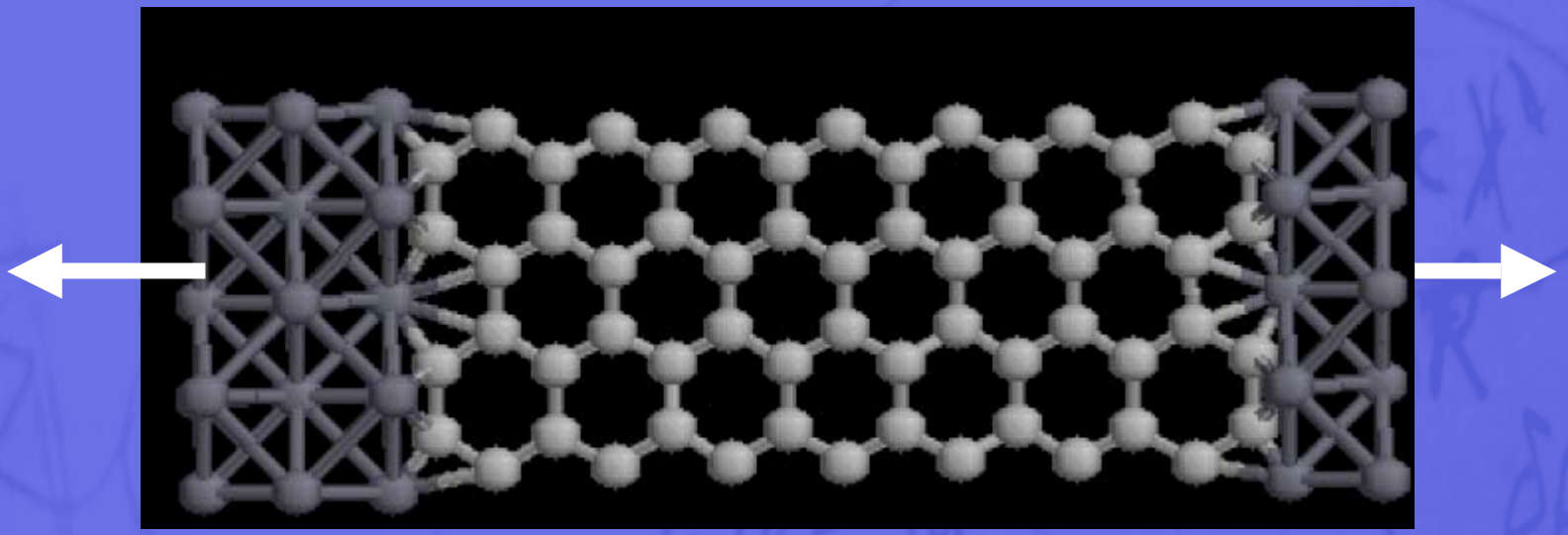
This height difference should be resolvable.

Summary of single layer ZGNB:

- There appears to be large enough spin contrast, detectable using a good spin polarized STM in UHV at low temperature T.
- How low a T? We don't know yet, but we are trying to estimate (Tao Ji at McGill, suggested by Allan MacDonald).
- Experimental challenge: produce stable single layer ZGNB hanging in vacuum ☺

Graphene transport junction (GTJ):

Bin Wang etal. (2007).



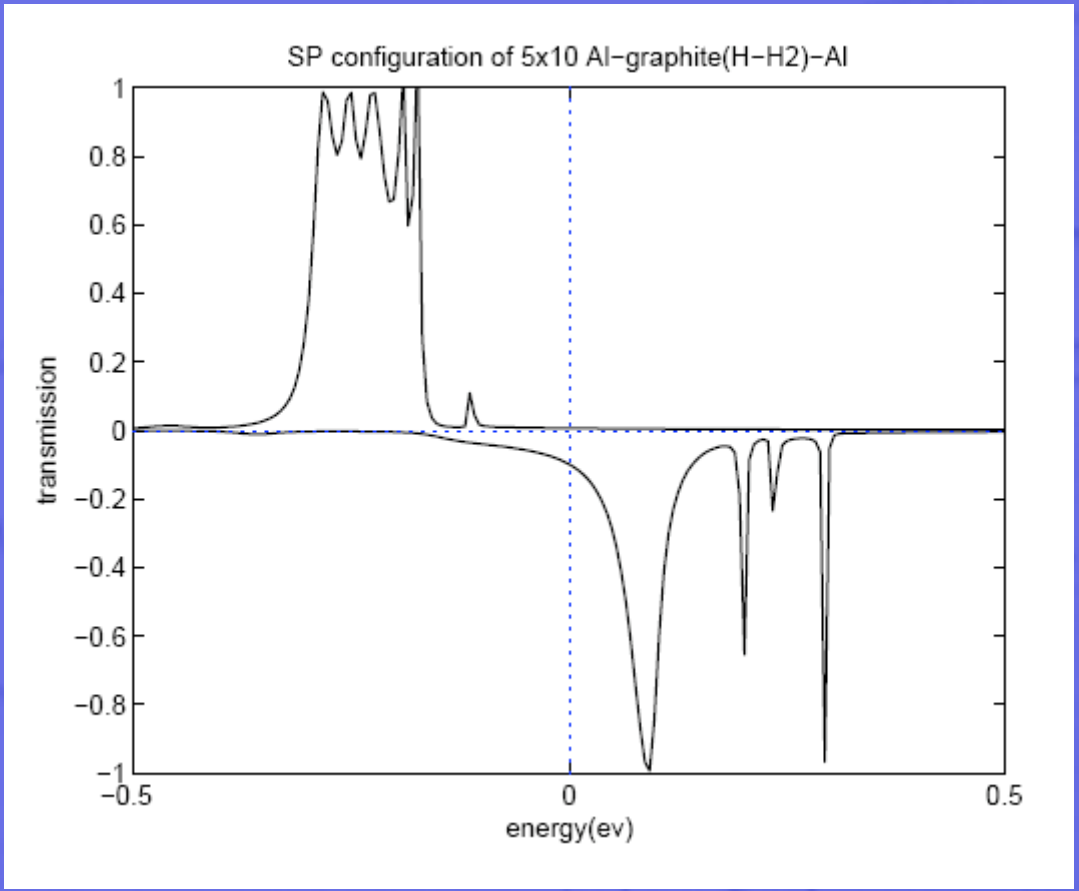
Normal metal lead

Graphene ribbon

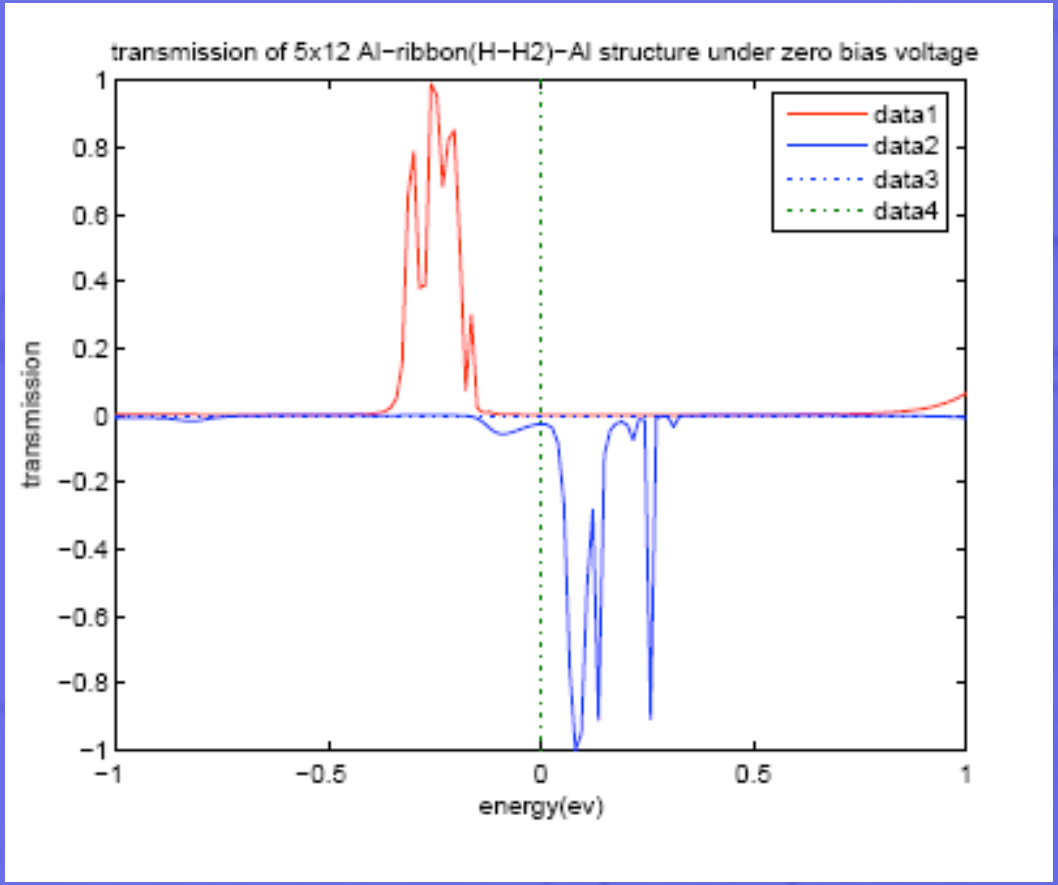
Normal metal lead

Let's compute spin polarized current through this transport junction.

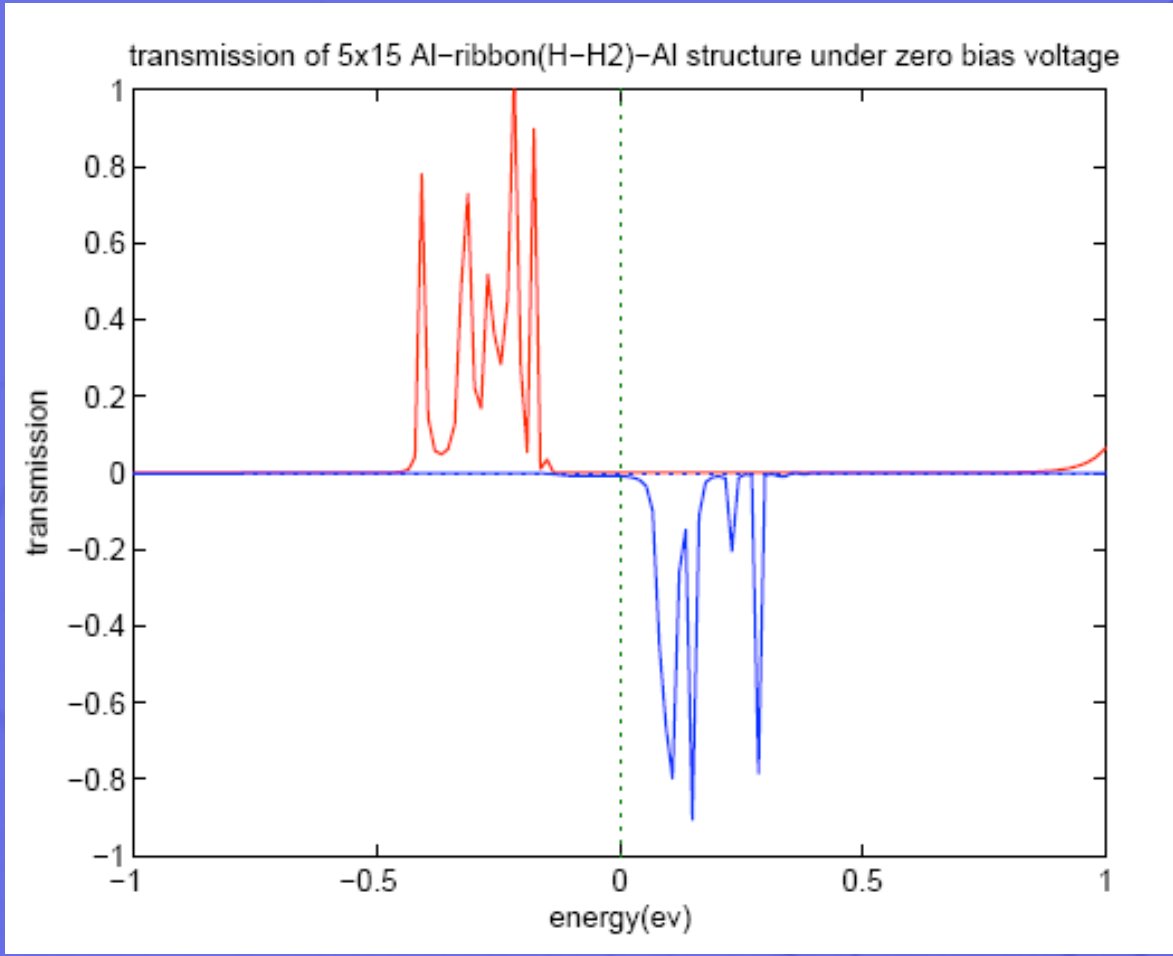
Ribbon with width 5, length 10 rings:



Width 5, length 12:

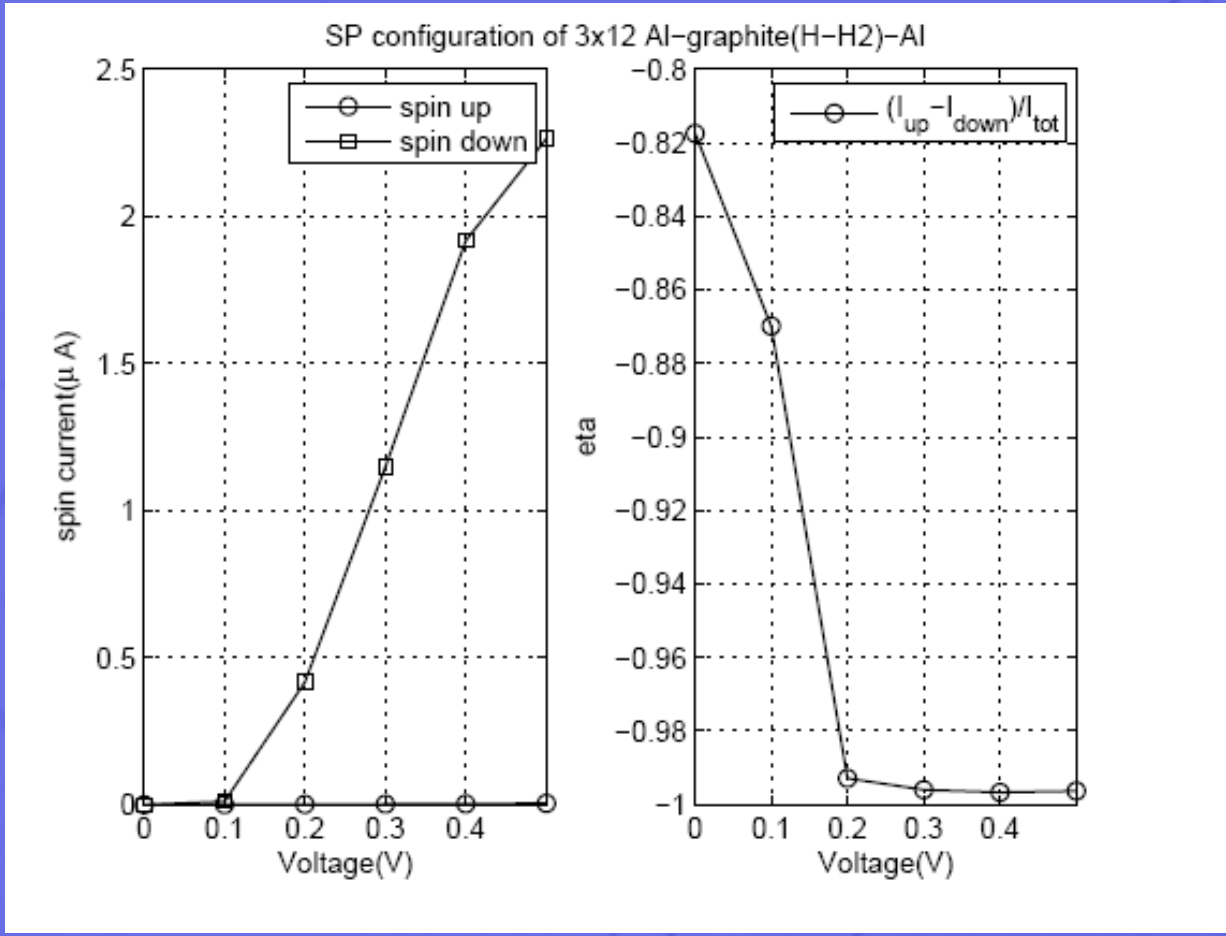


Width 5, length 15 rings:



Features become sharper as L is increased.

Only one spin channel contributes to I-V:

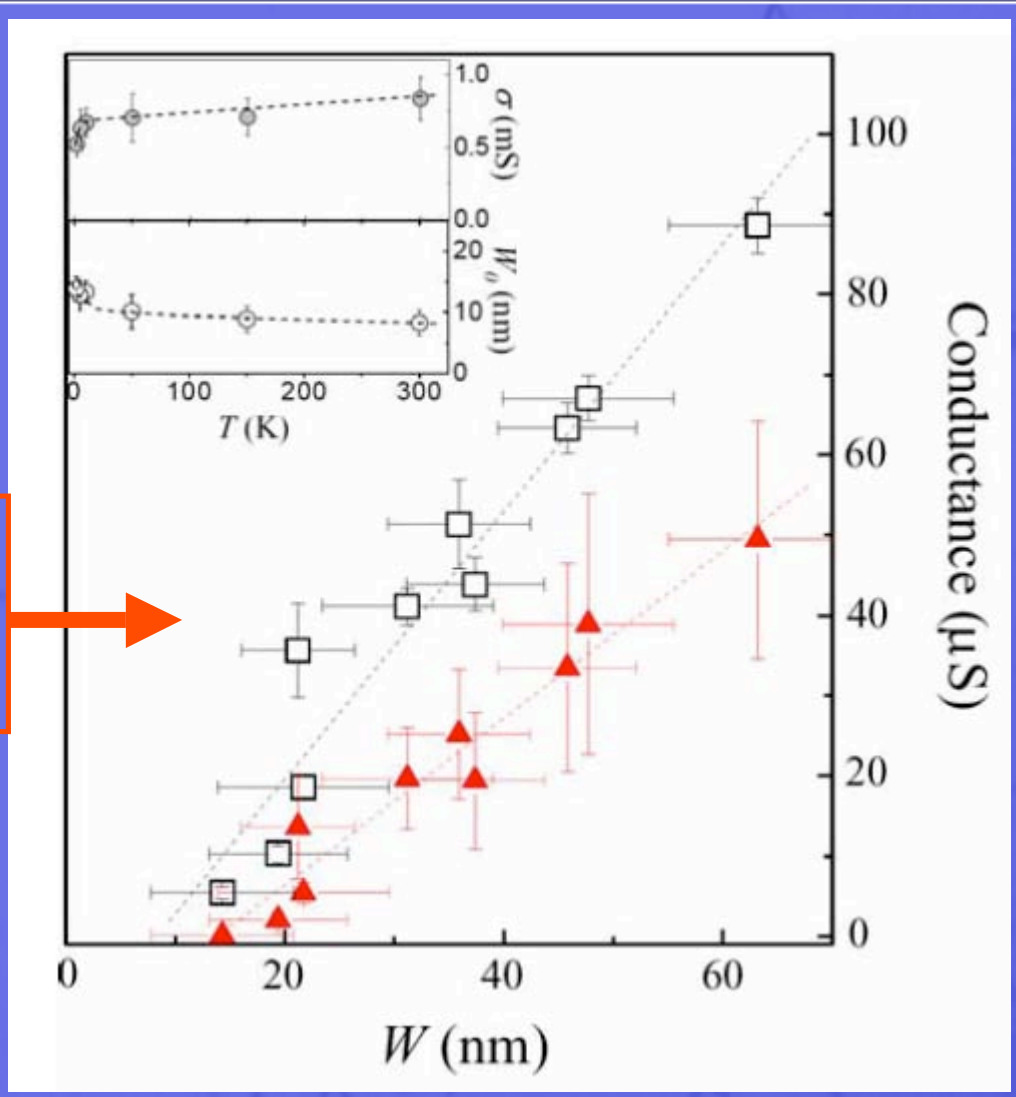


Almost half metallic: a good spin filter.

Experimental situation

Melinda Y. Han etal.
Preprint (2007).

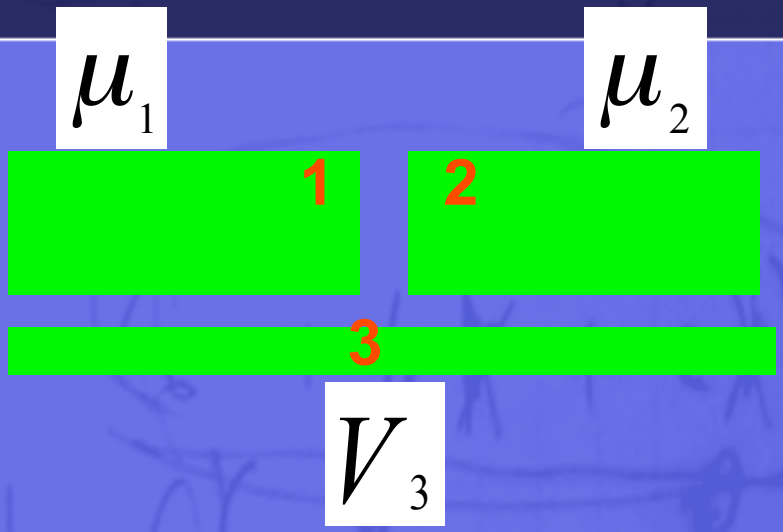
The corresponding resistance of these ribbons is 10^6 - 10^4 Ohm.



Summary of graphene spintronics

- DFT-LSDA predicts a magnetic edge for zigzag edged graphene ribbon at zero temperature. The exchange energy can be 1eV or more.
- Thermal fluctuation will destroy 1d magnetism in the thermal dynamic limit. But for a nanoscale (or mesoscale) system, one may still obtain some magnetic moment. Work needed to determine this length scale.
- Spin polarized STM suggests enough spin contrast.
- Interesting anyway!

Application: Non-equilibrium charge--- capacitance



$$\rho = \rho\left(\mu_1, \mu_2, V_3\right)$$

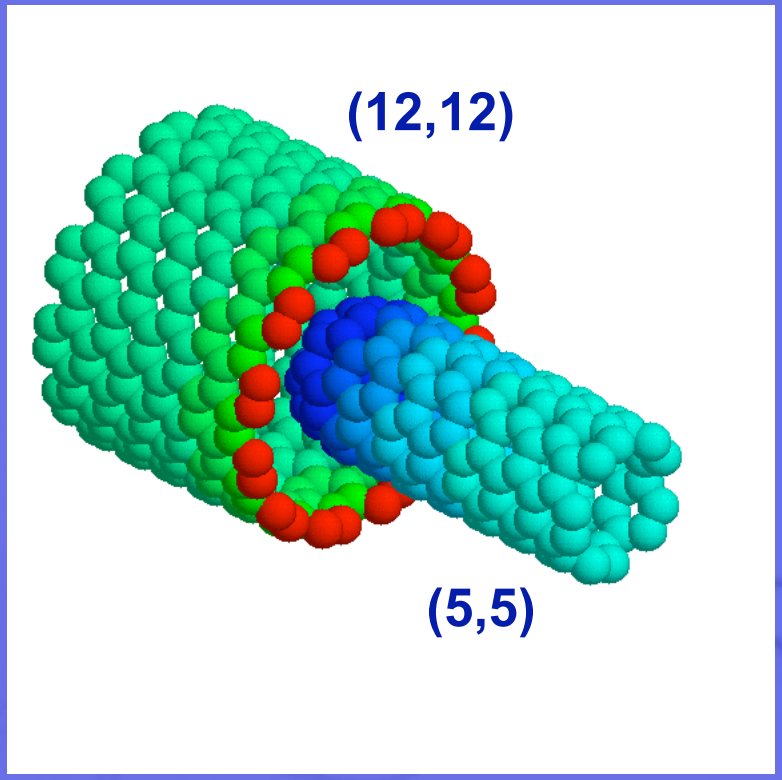
$$\Delta\rho_1 = C_{11}\Delta\mu_1 + C_{12}\Delta\mu_2 + C_{13}\Delta V_3$$

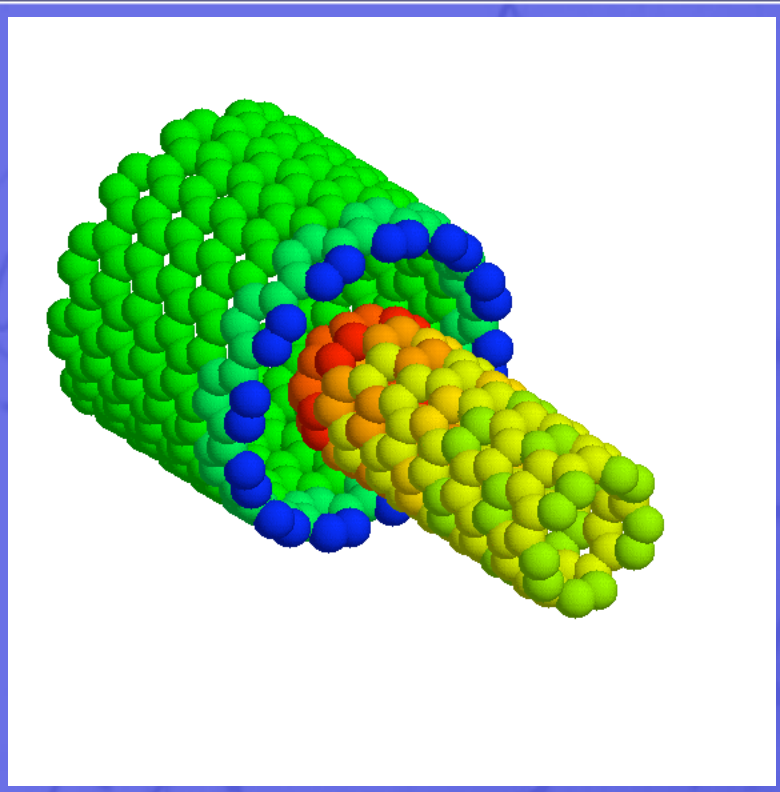
$$\Delta\rho_2 = C_{21}\Delta\mu_1 + C_{22}\Delta\mu_2 + C_{23}\Delta V_3$$

Note: charge is induced everywhere.

P. Pomorski etal. PRB (2003,2004).

Charging outer tube: **charging inner tube:**





$$C_{21} = -0.056aF$$

$$C_{11} = 0.160aF$$

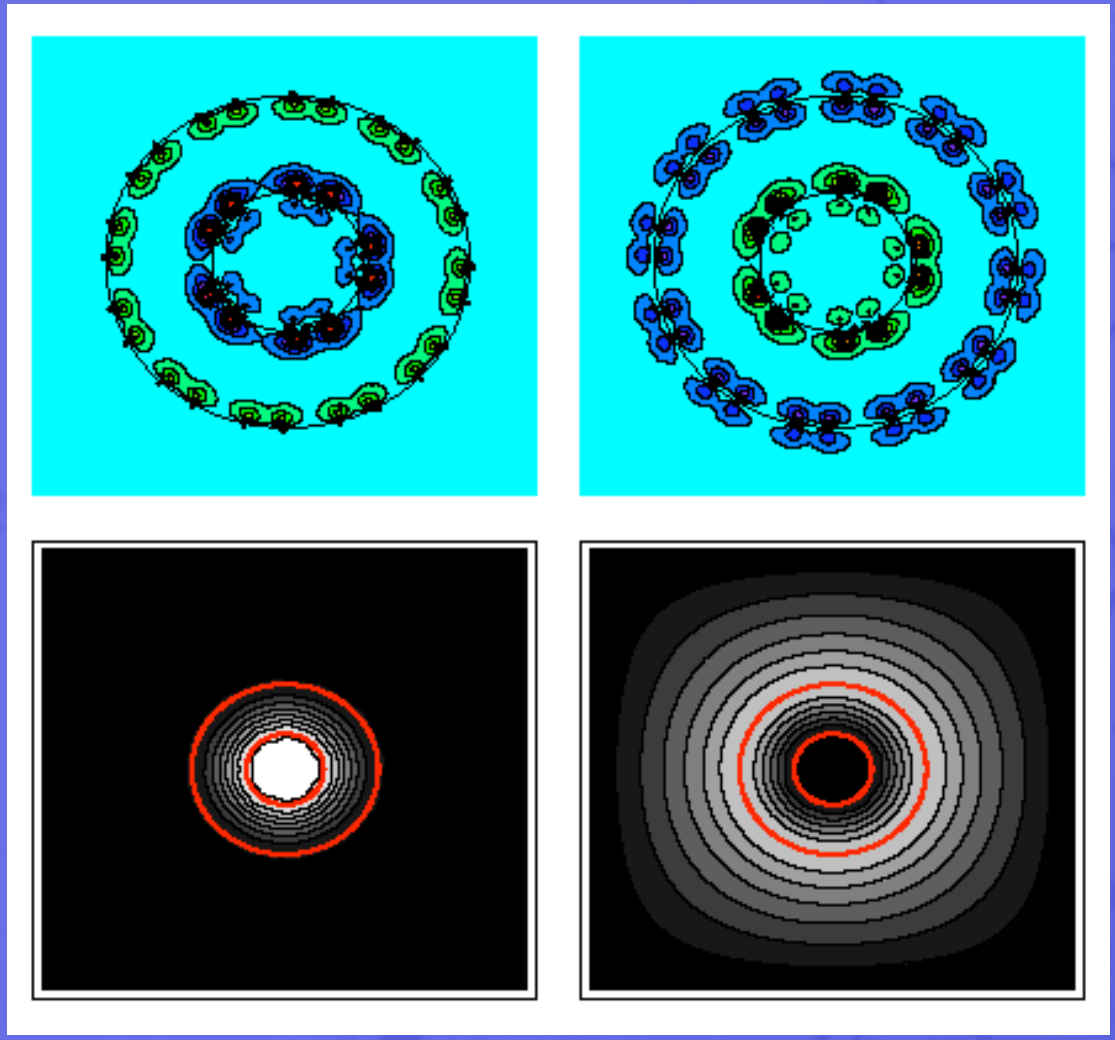
$$C_{12} = -0.058aF$$

$$C_{22} = 0.096aF$$

Charge and characteristic potential

charge

Potential

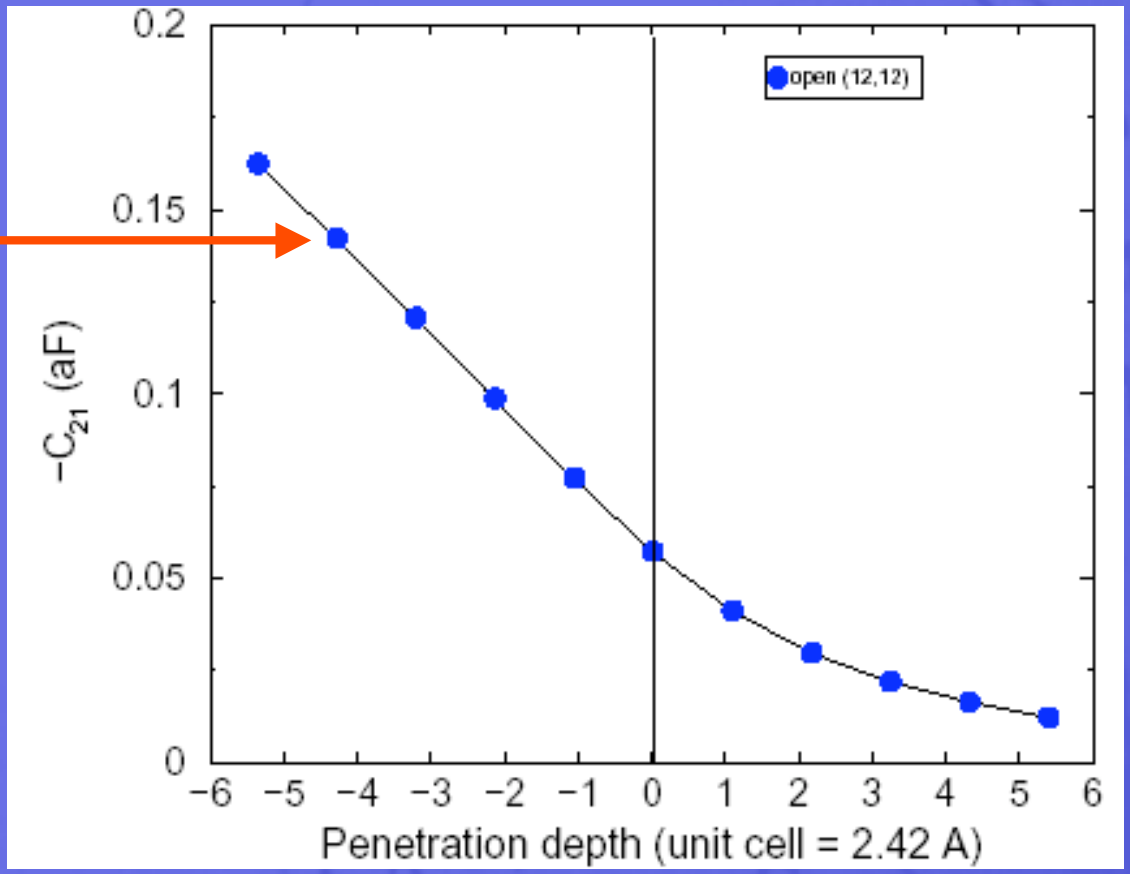


Capacitance as the two tubes approaching each other

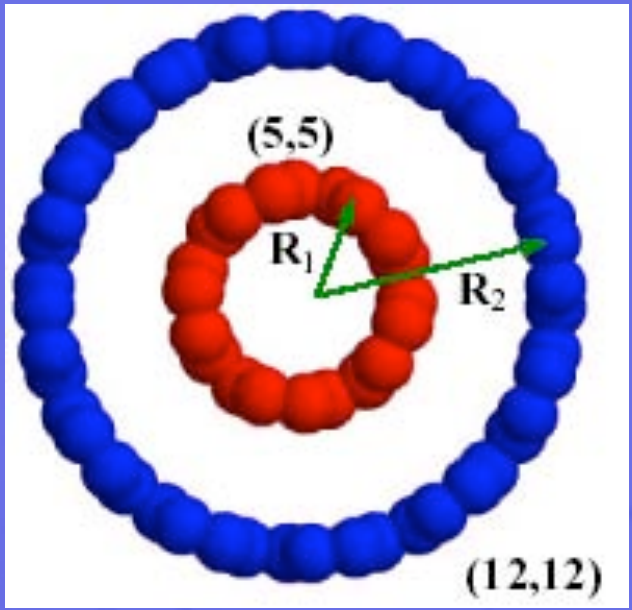
(12,12)-(5,5) nanotube junction

C21 per unit length at large penetration is 0.012aF.

For (5,5)-in-(12,12) periodic two-wall system: C21=0.014aF.



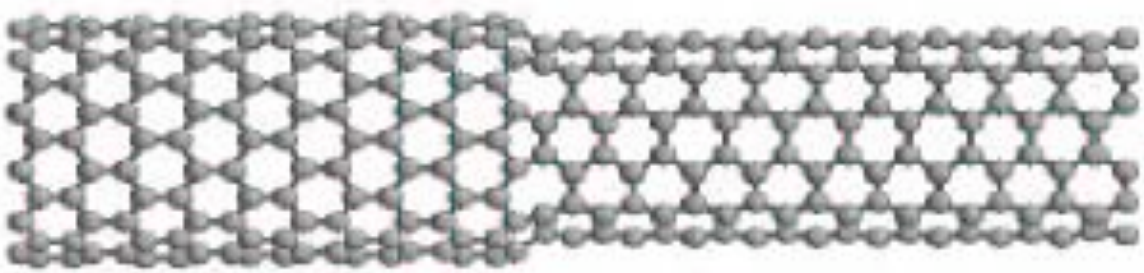
Classical values:



$$C_{21} = \frac{2\pi \varepsilon_0 L}{\ln(\frac{R_2}{R_1})}$$

Classical capacitance formula would predict 0.14aF or more, at least 10 times greater than quantum result --- very wrong indeed.

Junction with conductance gap:

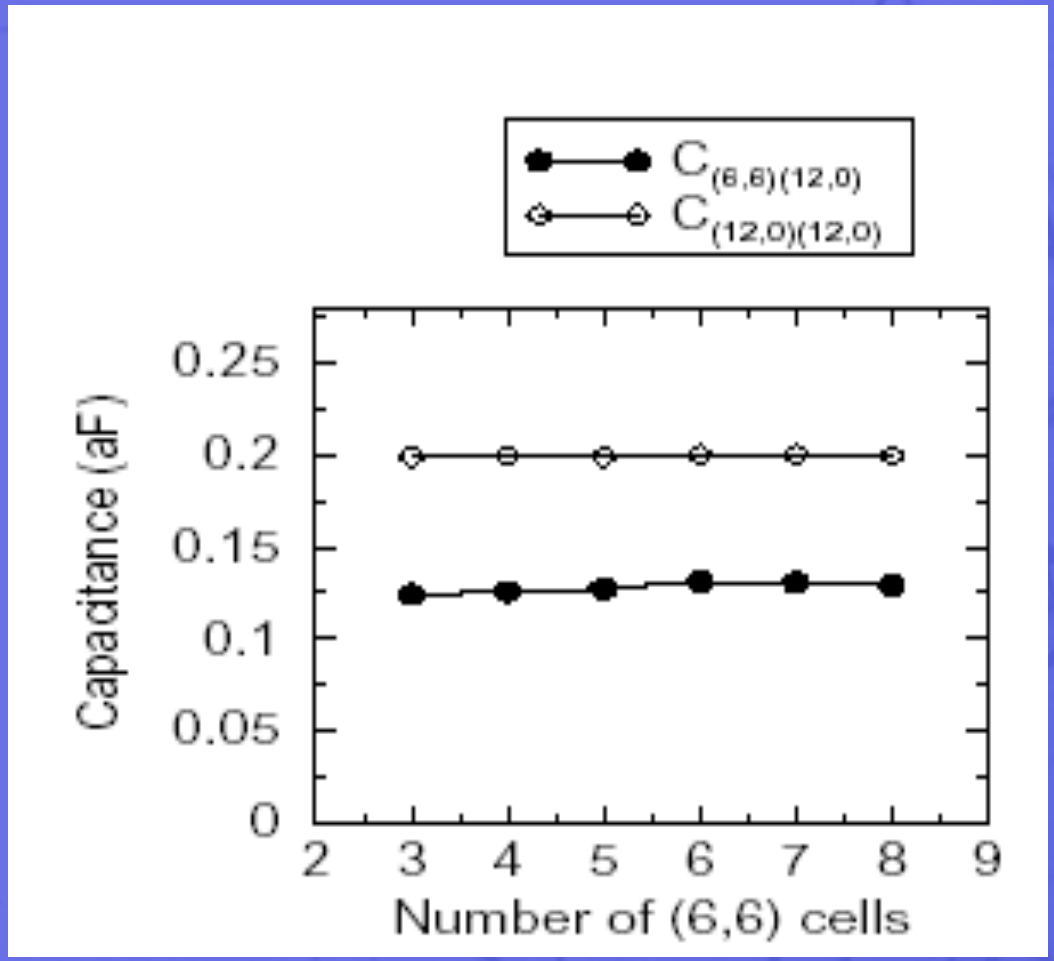


(12,0) tube **(6,6) tube**

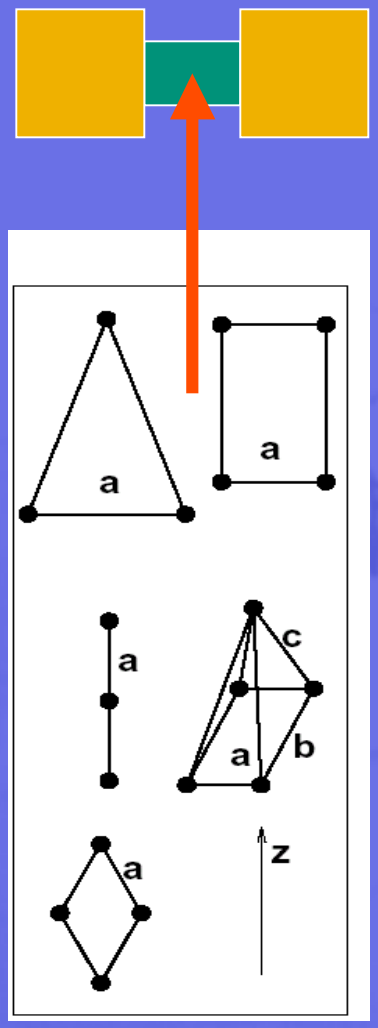
This is a strange junction: both tubes are metal, they contact perfectly, but conductance is zero due to wave-function mismatch.

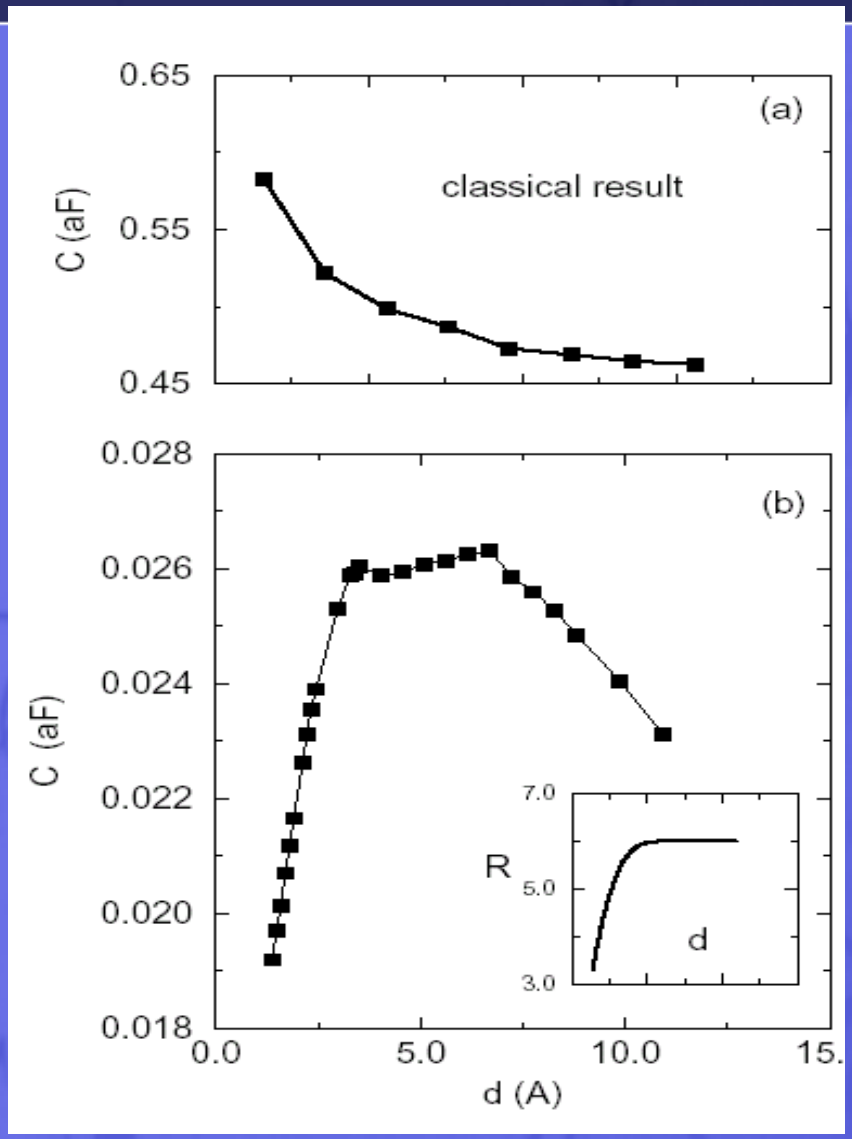
(12,0)/(6,6) junction:

Rather large capacitance---of course!



Example: C of tunnel junctions:





J.Wang etal PRL 80, 4277

Can we observe it ?

From WKB analysis, neglecting tunneling, Christen & Buttiker derived a formula:

$$C = \frac{R}{\frac{1}{C_e} + \frac{1}{C_q}}$$

$$C_e = \varepsilon \frac{A}{d}$$

usual electrostatic C

$$C_q \propto DOS$$

quantum C due to finite DOS of plates

For C(d) to increase with d, must have $\frac{\partial C}{\partial d} > 0$

$$\frac{\partial C}{\partial d} > 0$$

(e

We know $R(d) \propto 1 - \exp(-\frac{d}{L})$ where L depends on the barrier and other system parameters, and L is usually

a few angstroms. Our analysis concludes th $d < d^* = \alpha L$

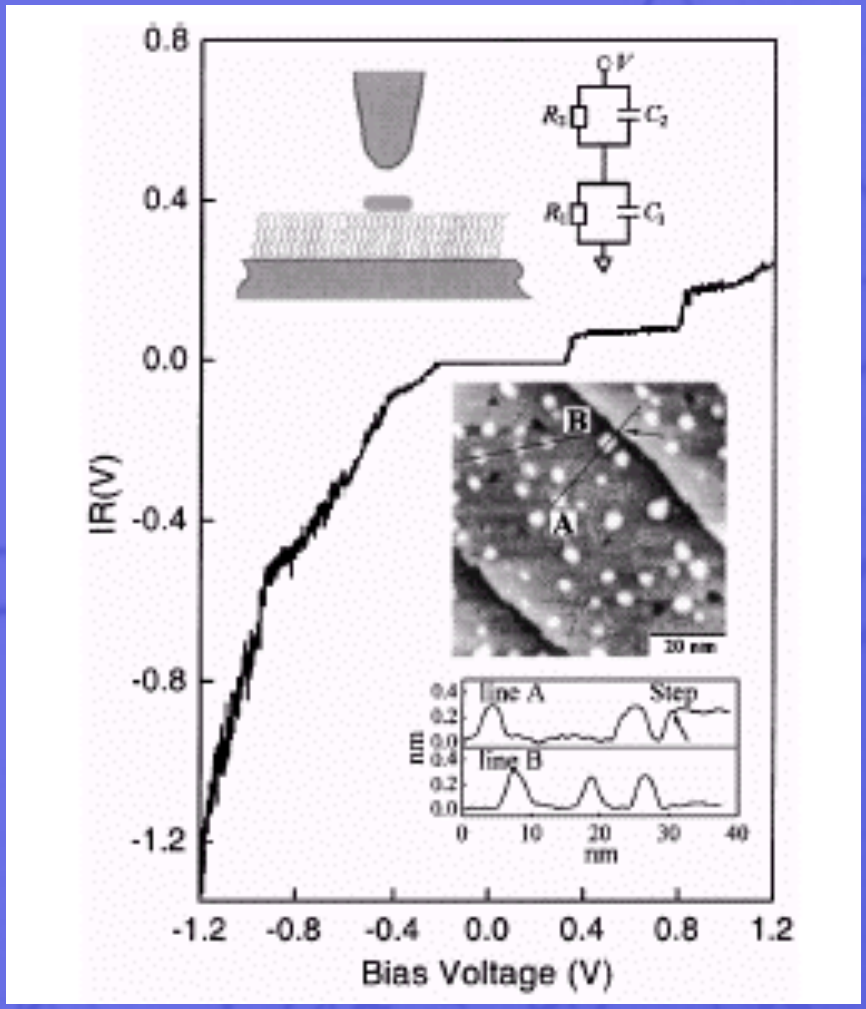
observe the non-classical phenomena when

$\alpha \approx O(1)$ **for atomic plates**

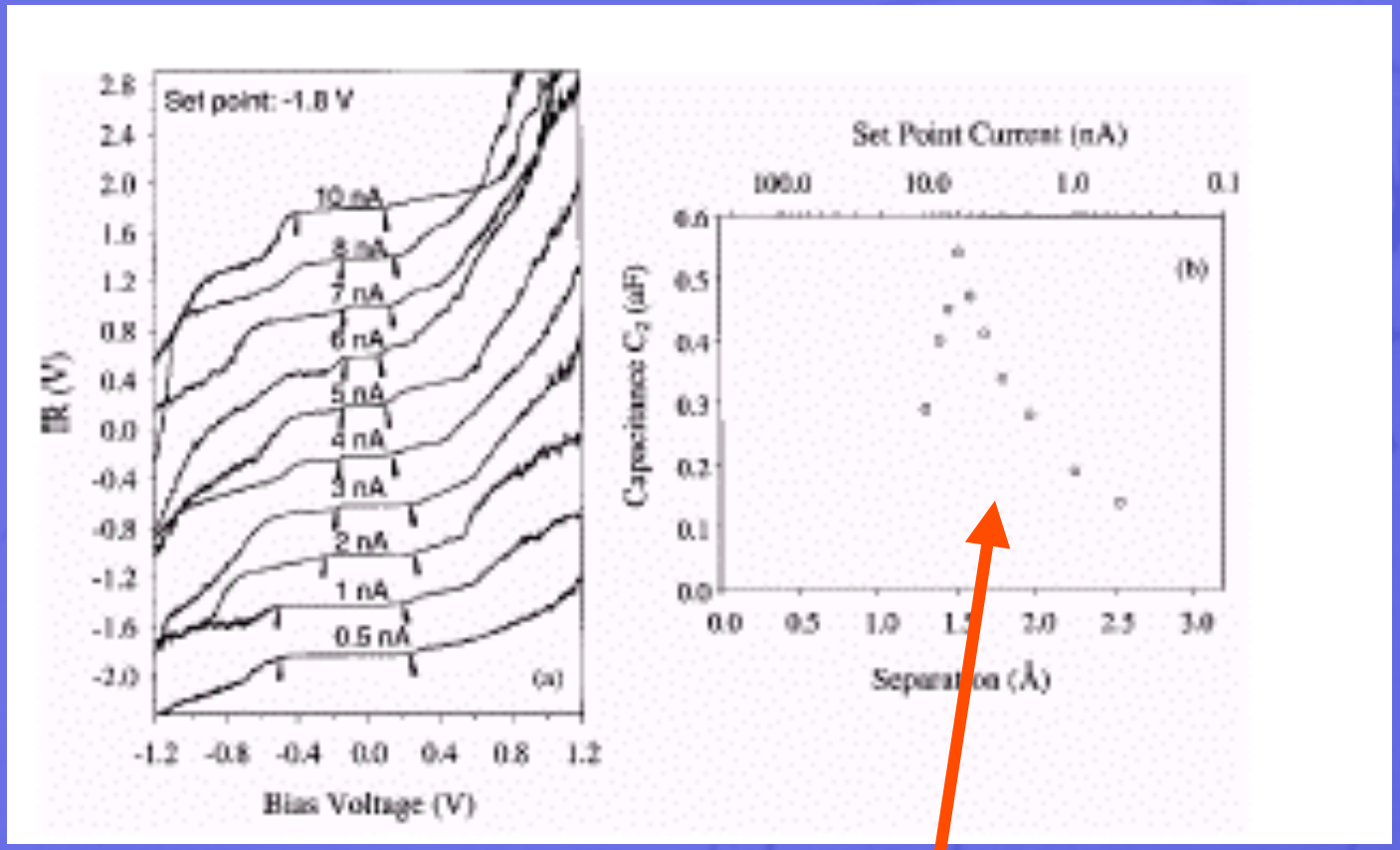
But $\alpha \approx 4 \times 10^{-3}$ for macroscopic plates

Experimental evidence: (J.G.Hou etal PRL 86, 5321 (2001))

Measure capacitance from charging energy in the Coulomb Blockade regime, for Au atomic clusters.



Experiments (Hou etal PRL 86, 5321(2001)



Non-classical behavior!

Summary of capacitance

- Quantum corrections to non-equilibirum charge can be very important at nano-scale due to small DOS.
- Electro-chemical capacitance of molecular scale systems has non-classical behavior due to DOS, tunneling, bias, and DC coupling.
- By measuring C=C(V) we found a way to deduce the local density of states of a nanosystem.
- Experimental work is possible, a direct dynamic measurement will be very much desired.