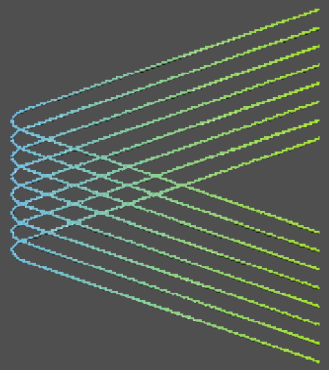
Dresden: 23.01.08



CRANN

Computing electron transport in nano- and bio-devices

Stefano Sanvito
School of Physics and CRANN, TCD

Trinity College
The University of Dublin

SEVENTH FRAMEWORK PROGRAMME

HEA
Higher Education Authority
An tÚdarás um Ard-Oideachas

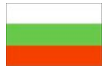
sfi

Transport: Can theory get in right?

- Has it got a solid theoretical foundation ?
- Is it predictive ?
- Is it practical ?

Once we know how a device is made at the atomic scale, can we predict its transport properties ?

Our Team

Cormac Toher		*(Spin-transport in organic)*
Ivan Rungger		*(Spin-injection, TMR, Smeagol)*
Das Pemmaraju		*(Diluted Magnetic semiconductors, ASIC)*
Maria Tsoneva		*(Dynamical magneto-transport effects)*
Ruairi Hanafin		*(MC for magnetic semiconductors)*
William Rodger Lee		*(Inelastic spin-transport in organic)*
Akinlolu Akande		*(Novel XC potential for Transport)*
Sankar Kesanakurthi		*(Spin-transport in organic)*
Nuala Caffrey		*(Multiferroic Tunnel Junctions)*
Andrea Droghetti		*(Diluted and defective oxides)*
Dr. Tom Archer		*(LDA+U and LDA+SIC methods)*
Dr. Nadjib Baadji		*(Spin-polarized STM for organics)*
Dr. Alex Reily Rocha		*(Smeagol, transport in large molecules)*

Acknowledgment

Friends

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Tchavdar Todorov (Queen's)

Oleg Mryasov (Seagate)

Olle Heinonen (Seagate)

Daniel Sanchez-Portal (San Sebastian)

Jose Soler (Madrid)

Smeagol fellows

J. Ferrer (Oviedo)

V. M. Garcia Suarez (Oviedo)

C.J. Lambert (Lancaster)

S. Bailey (Lancaster)

Resources

TCHPC

ICHEC

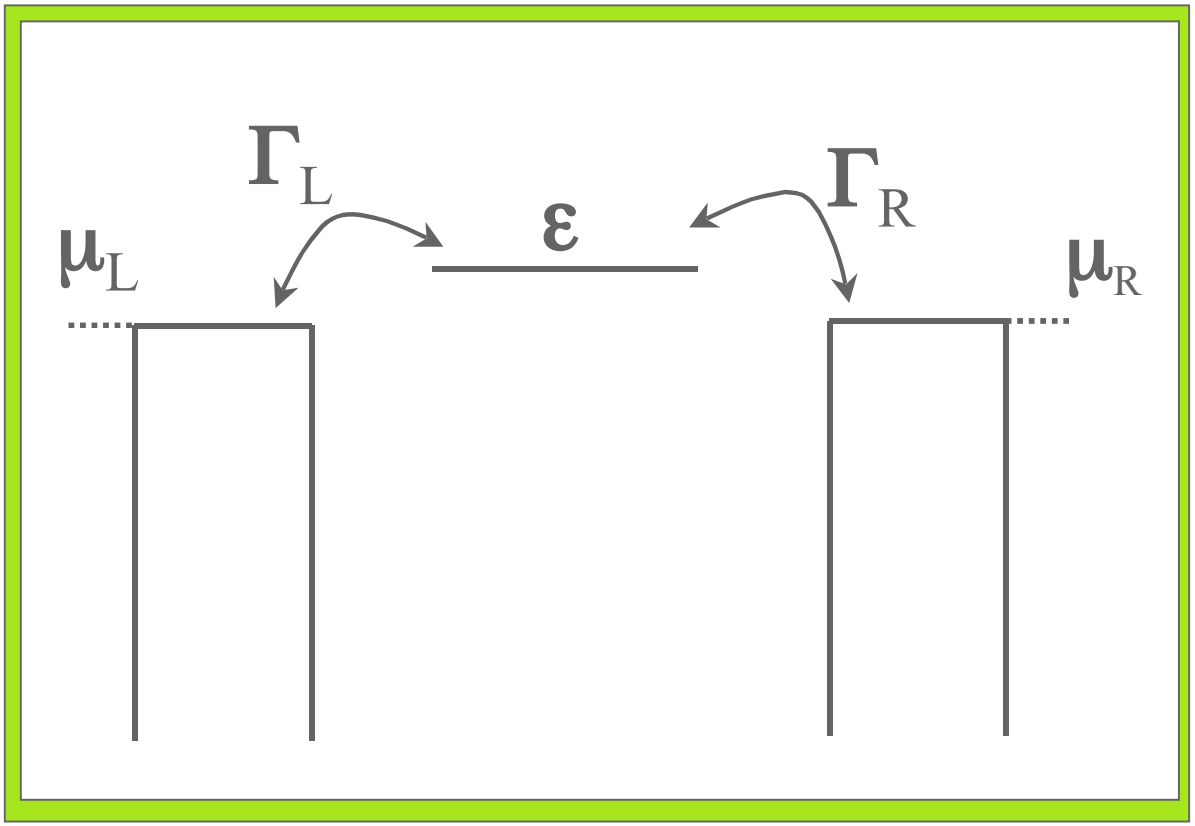
EUROPA

Outline

- Quantum transport: the concept
- The *Smeagol* project
- Nano-magnetism
  - Mn_{12} molecules
- Nano-Bio-science:
  - DNA transport
  - DNA sequencing
- Conclusions

Quantum Transport: the concept

Quantum Transport

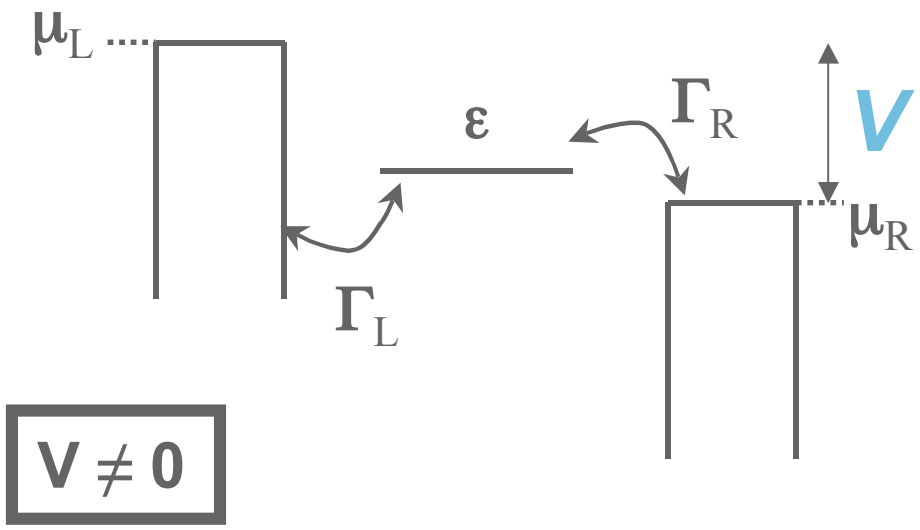


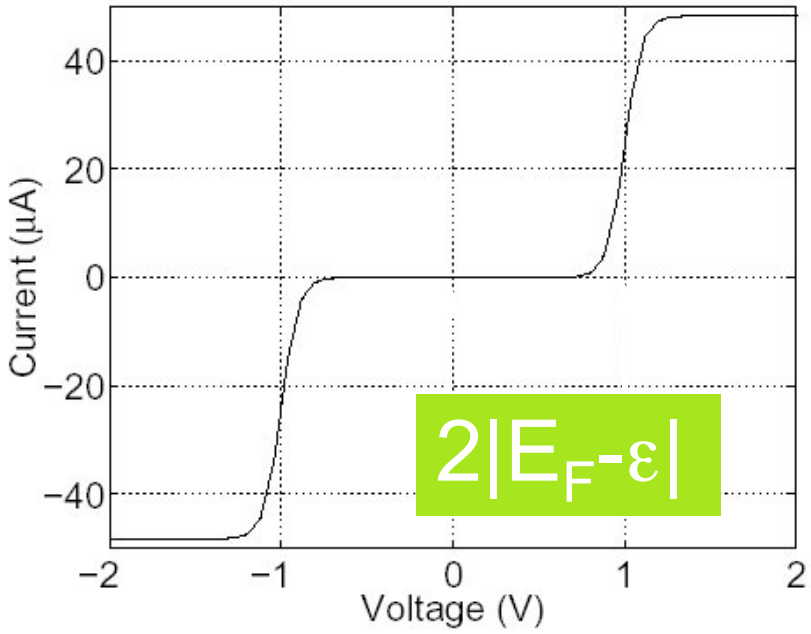
V = 0

Quantum Transport

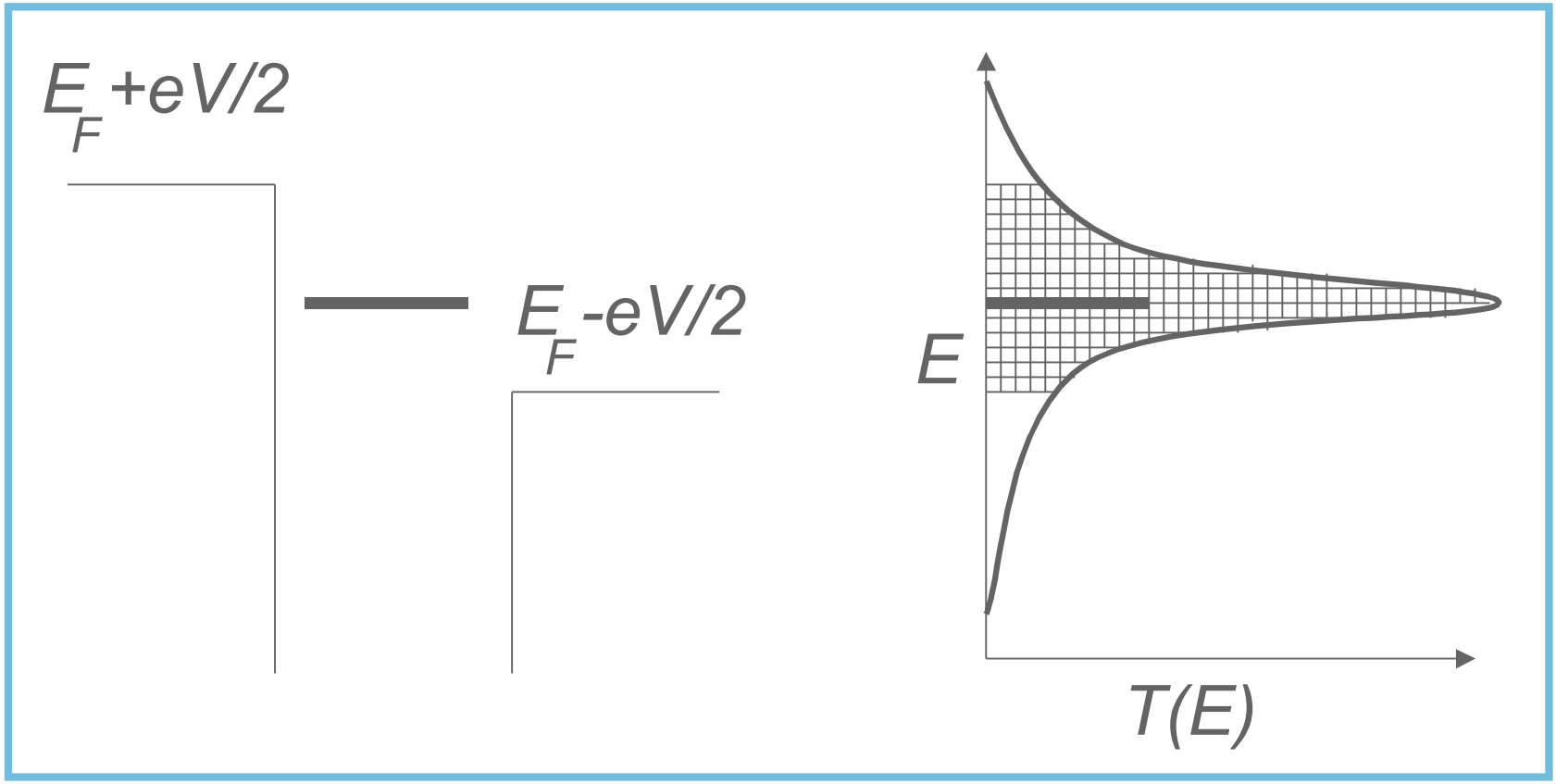
$$N = 2\,\frac{\Gamma_L f(\epsilon-\mu_L)+\Gamma_R f(\epsilon-\mu_R)}{\Gamma_L+\Gamma_R}$$

$$I = \frac{2e}{\hbar}\frac{\Gamma_L\Gamma_R}{\Gamma_L+\Gamma_R}[f(\epsilon-\mu_L)-f(\epsilon-\mu_R)]$$





Quantum Transport



$$I^{\sigma} \approx \frac{e}{h} \int_{E_{\mathrm{F}}-eV/2}^{E_{\mathrm{F}}+eV/2} T^{\sigma}(E;V)\, dE$$

The *Smeagol* project

Smeagol

Non-equilibrium Electronic Transport

http://www.smeagol.tcd.ie/

Mailing list http://lists.tchpc.tcd.ie/listinfo/smeagol-discuss

A. R. Rocha et al., Phys. Rev. B **73**, 085414 (2006); Nature Materials **4**, 335 (2005)

The *Smeagol* project

Idea:

To construct a solid, flexible and efficient quantum transport package for simulating detailed *I-V* characteristics of

Molecules

Nanodevices

Point contacts

Bio-sensors

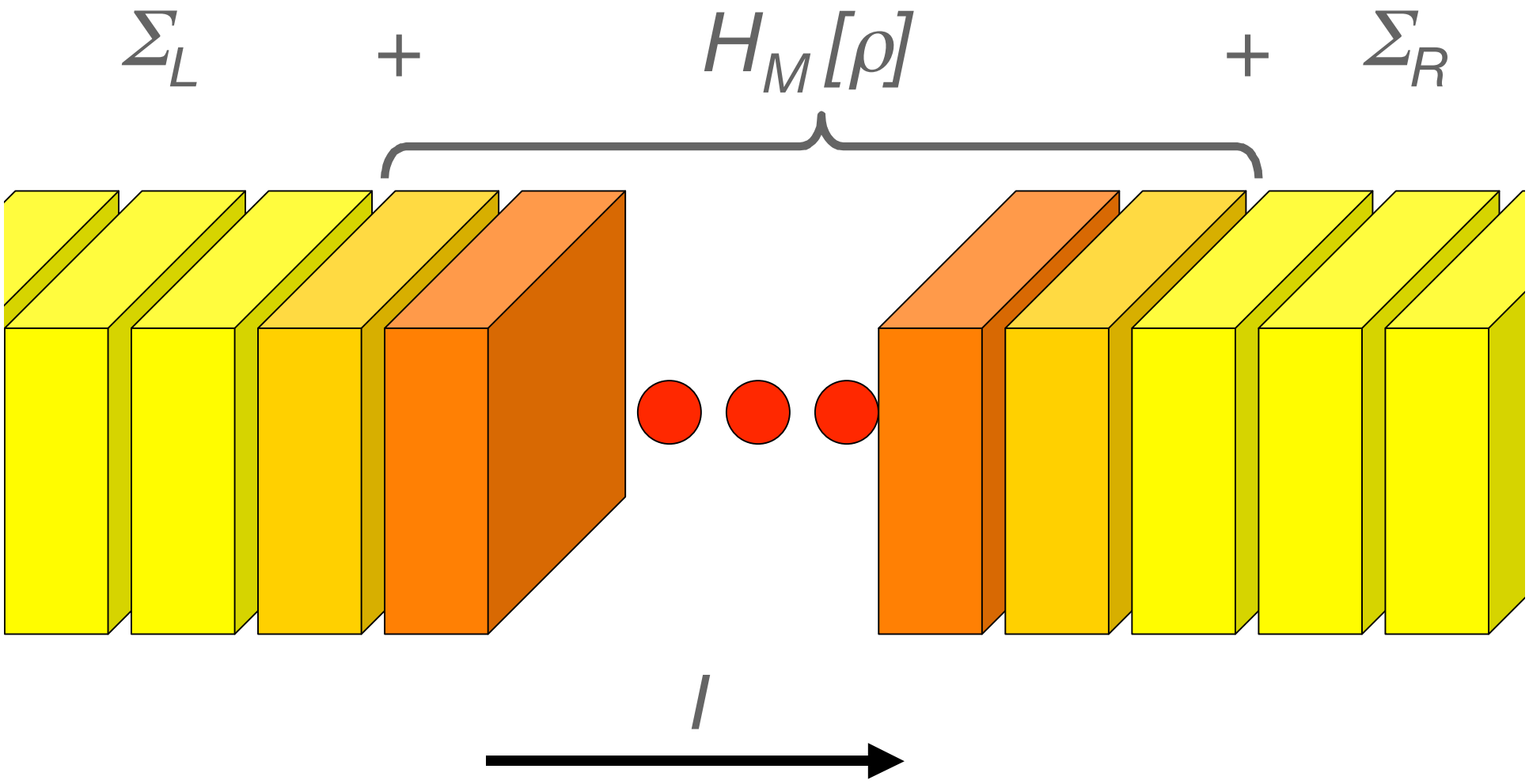
Transistors

Quantum Devices

Goal:

To achieve in quantum transport the same level of prediction capabilities than DFT has for electronic structure

The *Smeagol* project



The *Smeagol* project

$$\Sigma_\alpha = H_{\mathrm{M}\alpha} g_\alpha H_{\mathrm{M}\alpha}^\dagger$$

$$\Gamma_\alpha = i(\Sigma_\alpha - \Sigma_\alpha^\dagger)$$

A. R. Rocha and S. Sanvito, PRB **70**, 094406 (2004)

$$G(E) = [E - H_{\mathrm{M}} - \Sigma_{\mathrm{L}} - \Sigma_{\mathrm{R}}]^{-1}$$

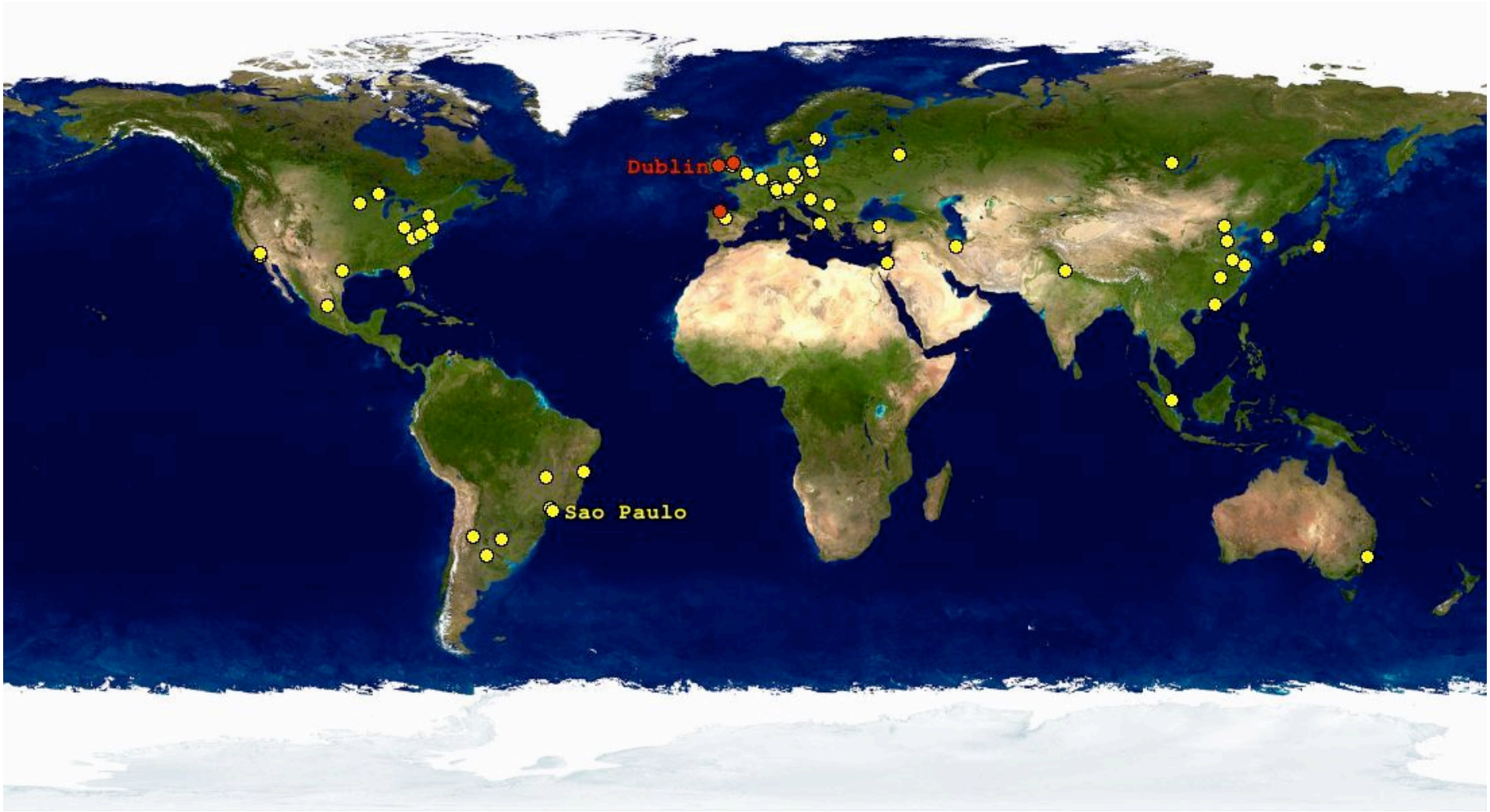
$$n_{ij}^\sigma = \frac{1}{2\pi} \int dE [G\Gamma_L f(E,\mu_L) G^\dagger + G\Gamma_R f(E,\mu_R) G^\dagger]_{ij}^\sigma$$

$$I^\sigma = \frac{e}{h} \int dE [\mathrm{Tr}(\Gamma_L G \Gamma_R G^\dagger)(f(E,\mu_L) - f(E,\mu_R))]^\sigma$$

The *Smeagol* project

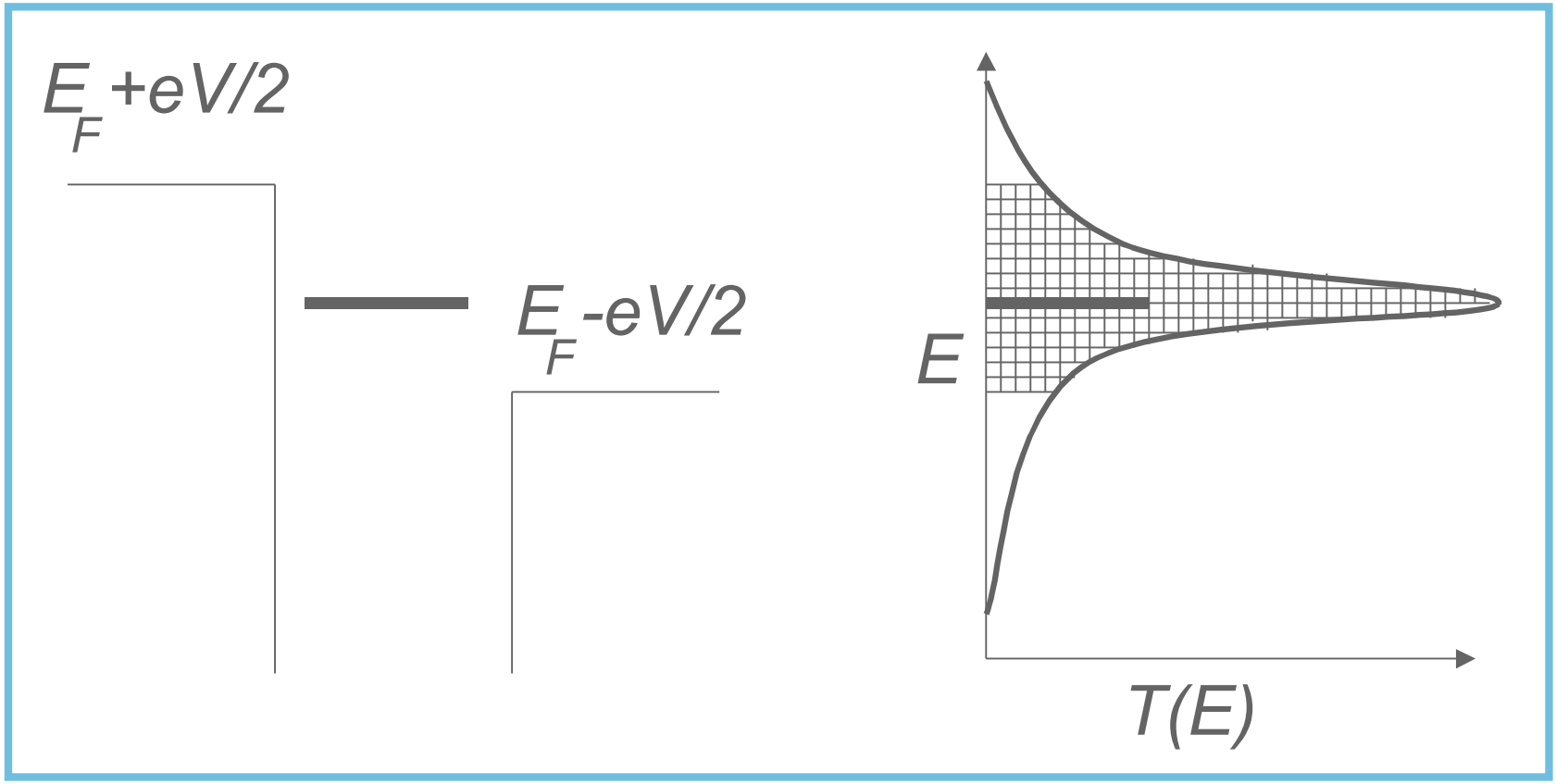
- It converges !! New adaptive mesh
- It can use leads with complicated electronic structure. New GF algorithm
- Both finite and periodic systems
- Parallel in *k*, *E and* χ_α*: Large scale demonstrated*
- It is spin-polarized
- It is non-collinear
- LDA/GGA …
- **LDA+SIC** and **LDA+U**
- **Spin-orbit**

Distribution



Warning!! Use DFT sensibly

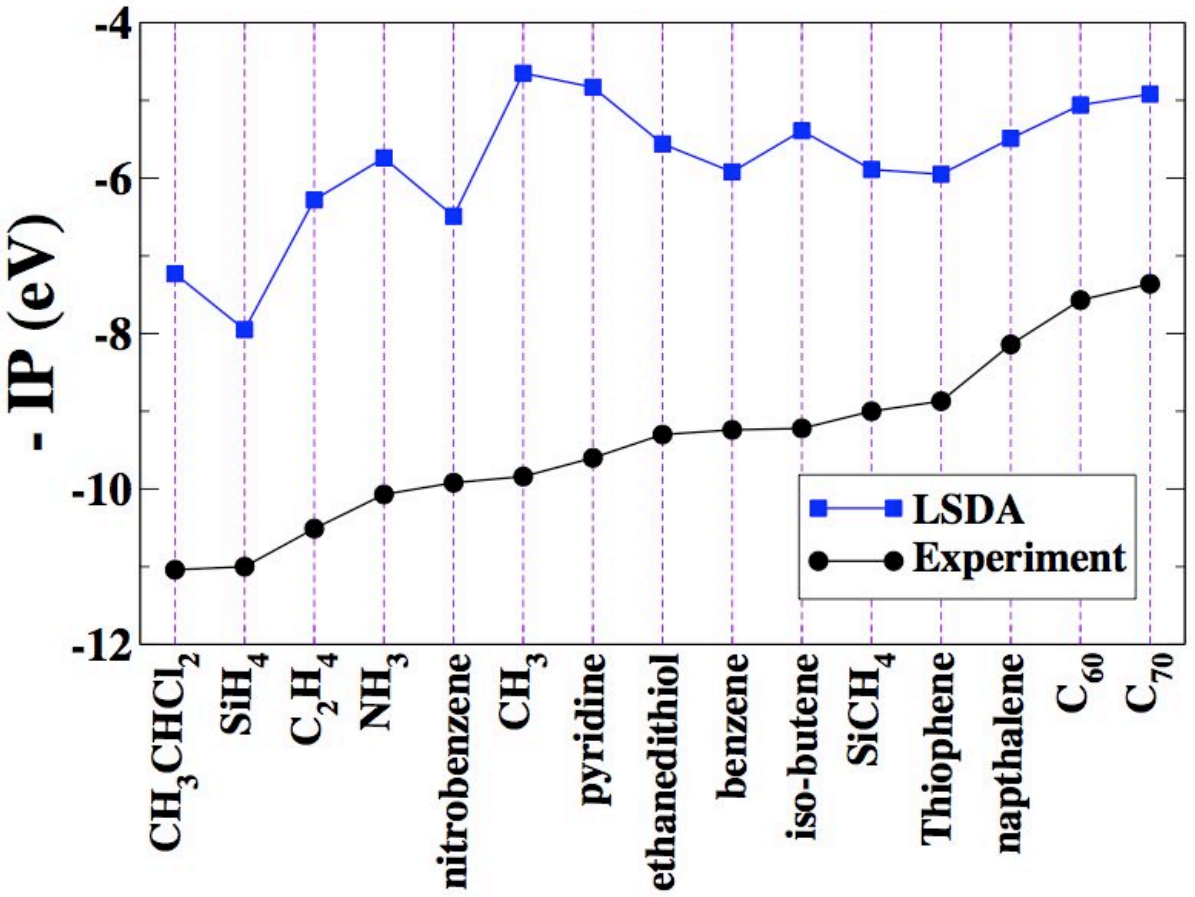
Warning!! Use DFT sensibly



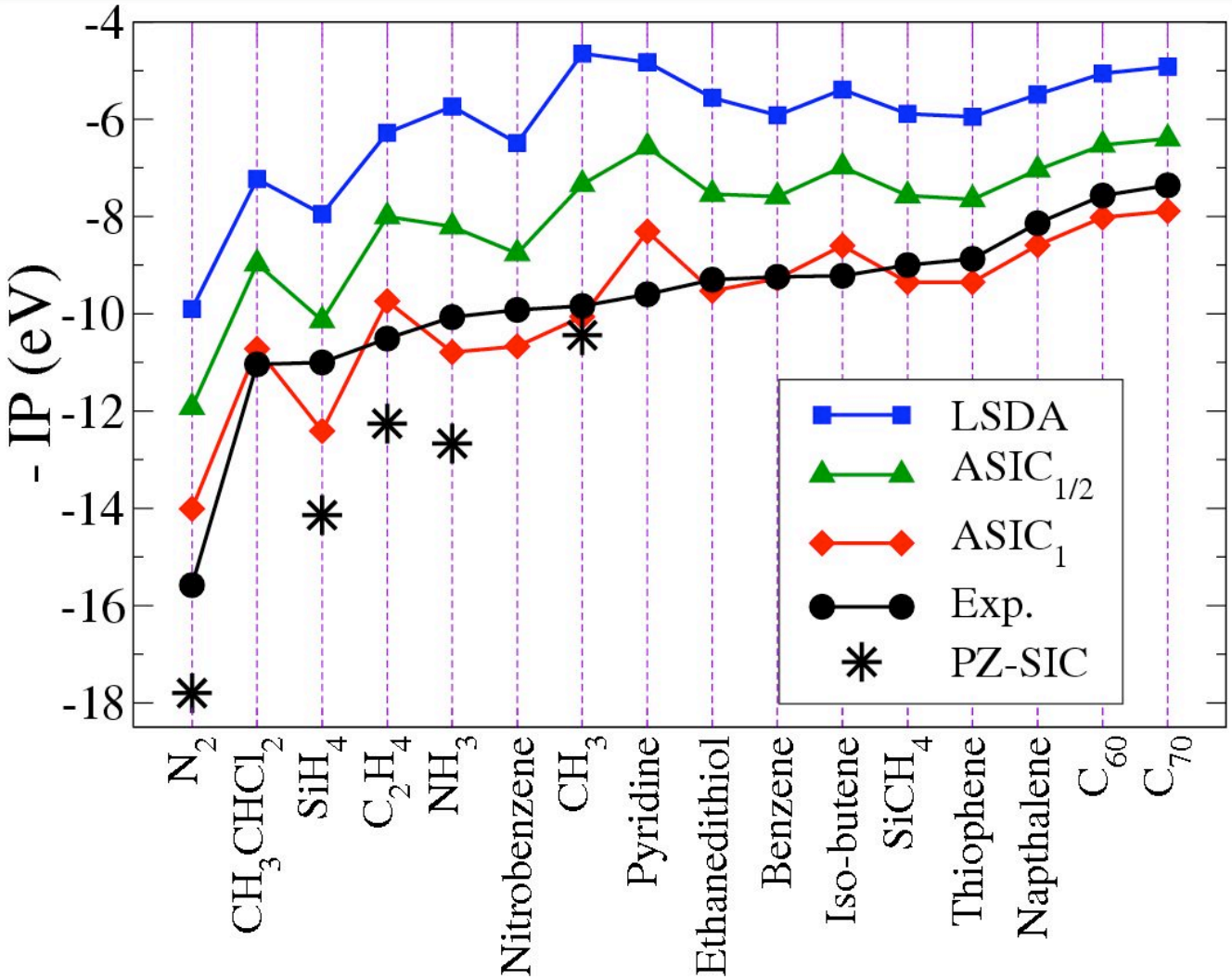
$$I^{\sigma} \approx \frac{e}{h} \int_{E_{\mathrm{F}}-eV/2}^{E_{\mathrm{F}}+eV/2} T^{\sigma}(E;V)\, dE$$

Warning!! Use DFT sensibly

$\varepsilon_{HOMO} \neq -I_N$

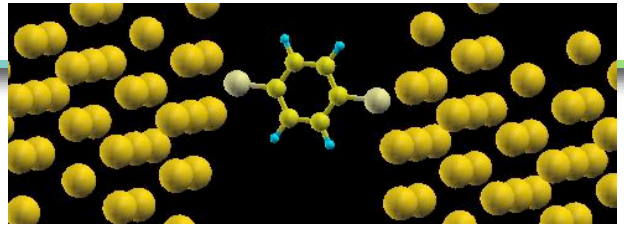


Warning!! Use DFT sensibly

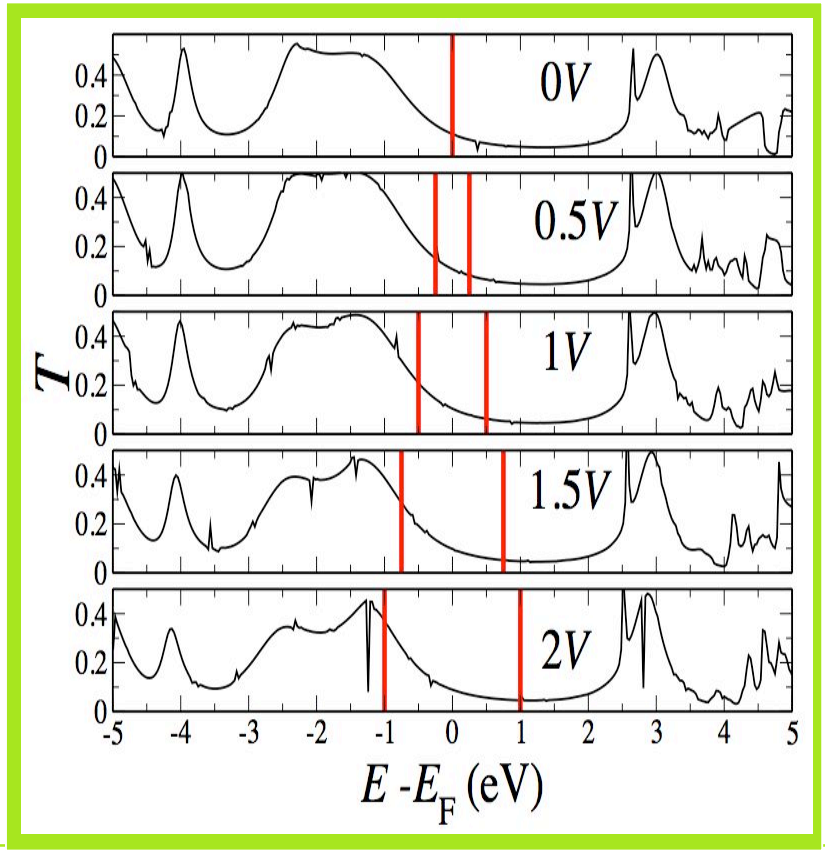


C. Das Pemmaraju, T. Archer, D.Sanchez-Portal and S. Sanvito, PRB **75**, 045101 (2007)

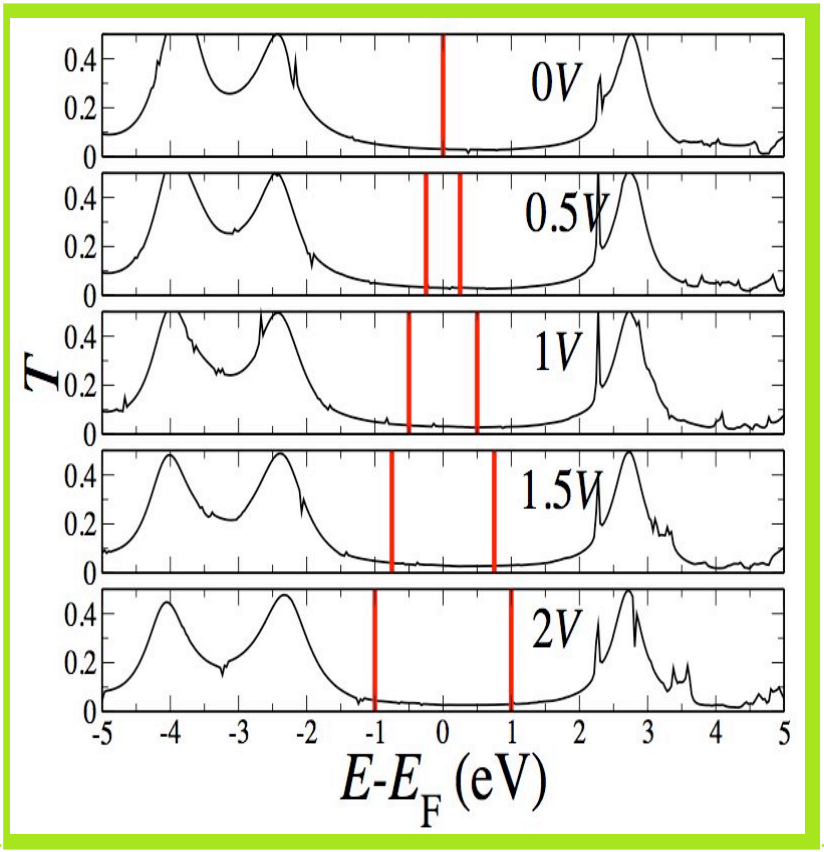
C. Toher and Sanvito, PRL **99**, 056801 (2007); PRL **95**, 146402 (2005)



$G=0.23G_0$



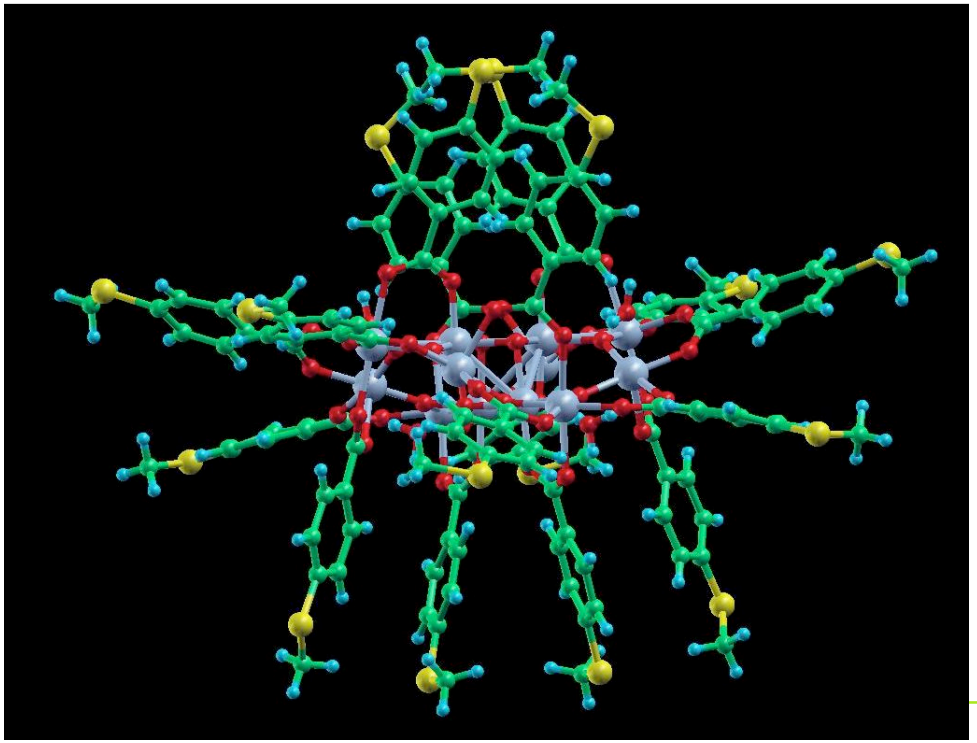
$G=0.06G_0$

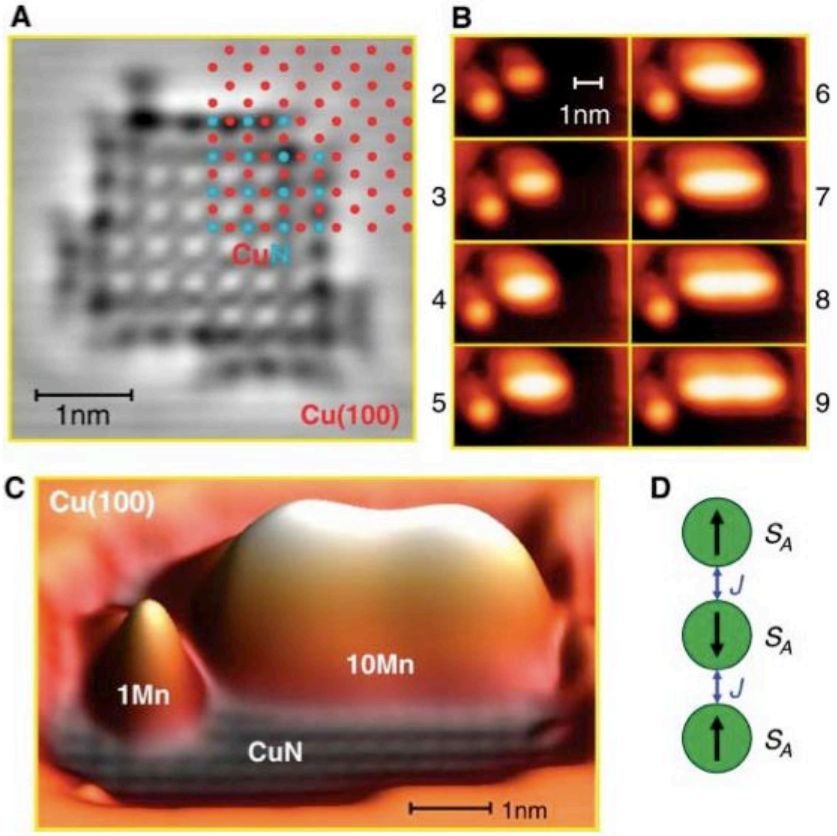


Transport across Mn_{12}

Transport across Mn_{12}

C.F. Hirjibehedin et al, Science **312**, 1021 (2006)

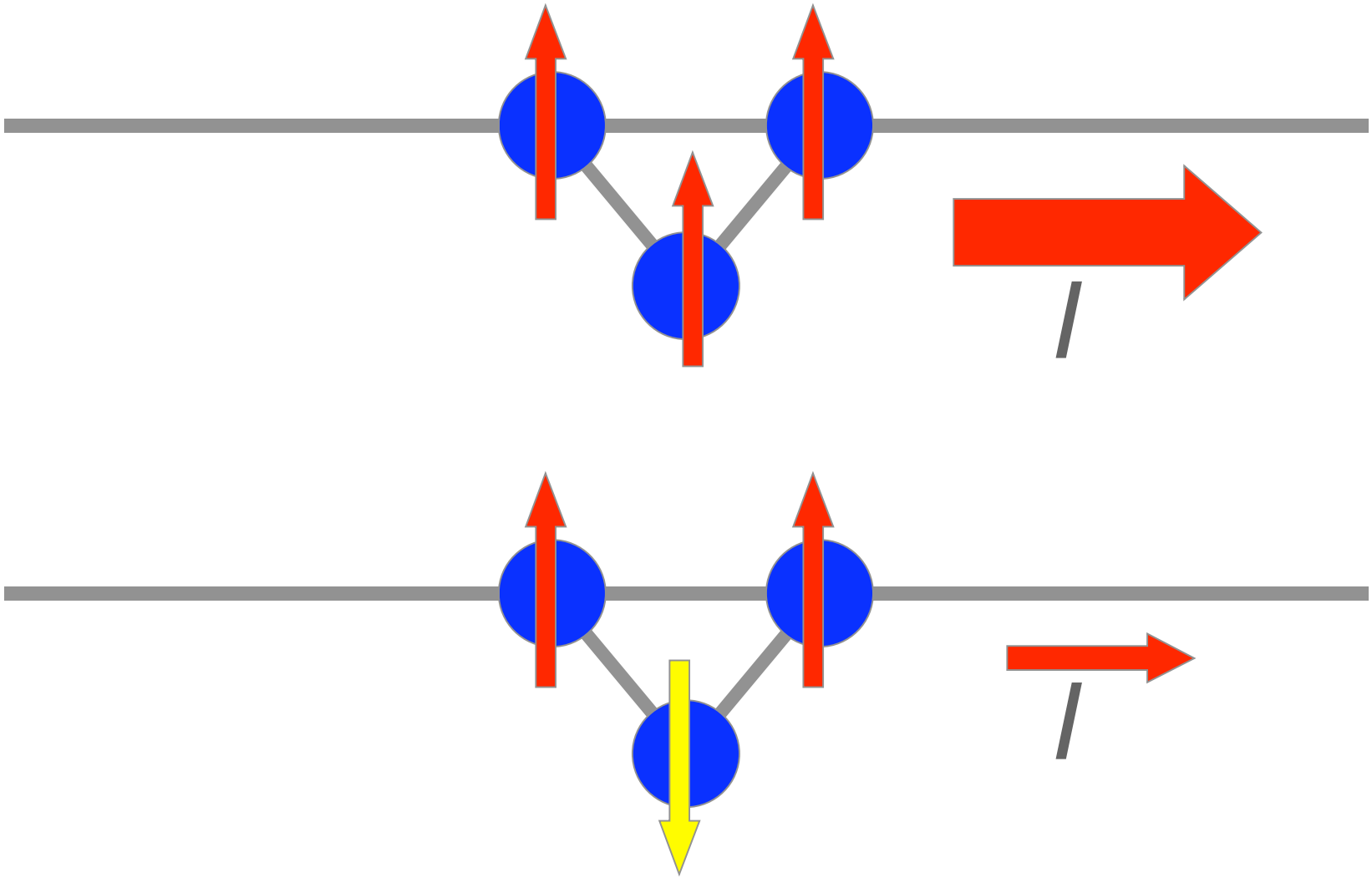




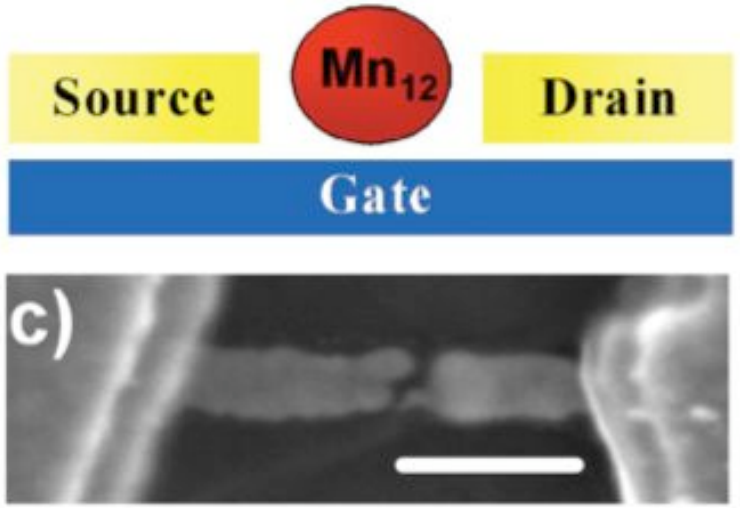
H.B. Heersche et al, PRL **96**, 206801 (2006)

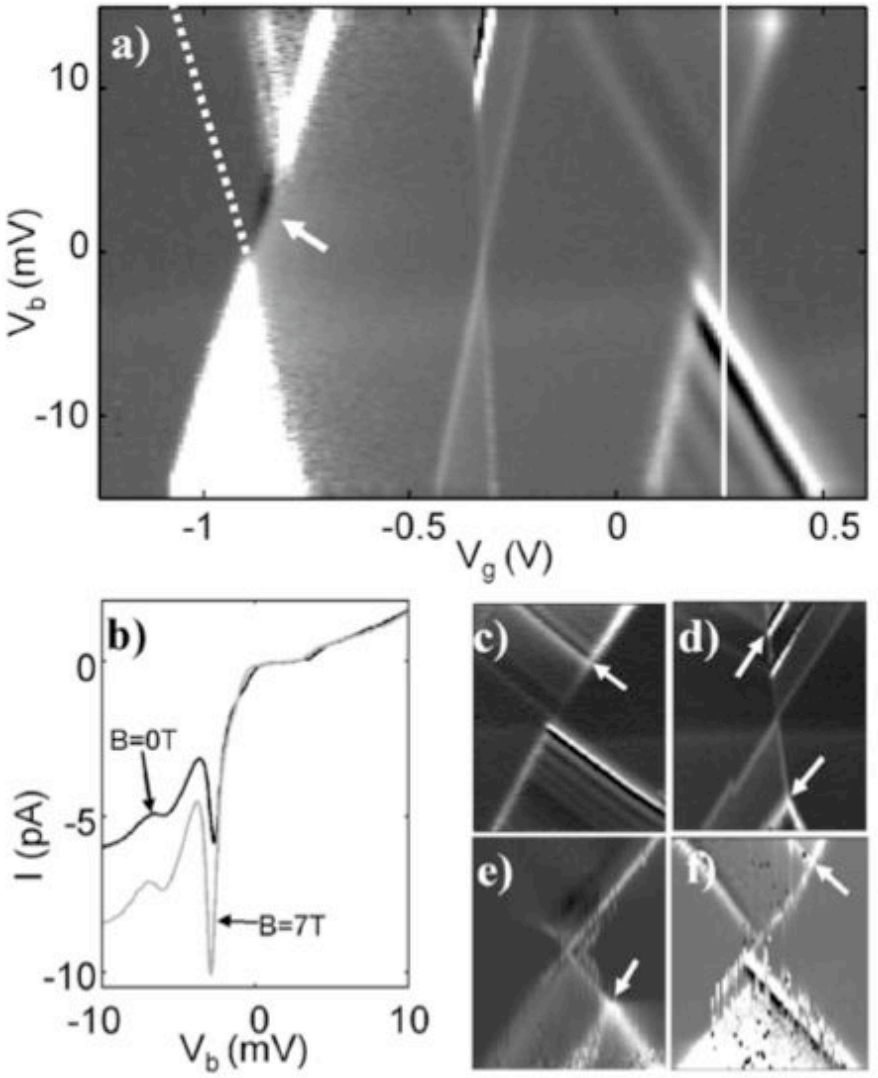
M.H. Jo et al, Nano Lett. **6**, 2014 (2006)

Transport across Mn_{12}



Transport across Mn_{12}

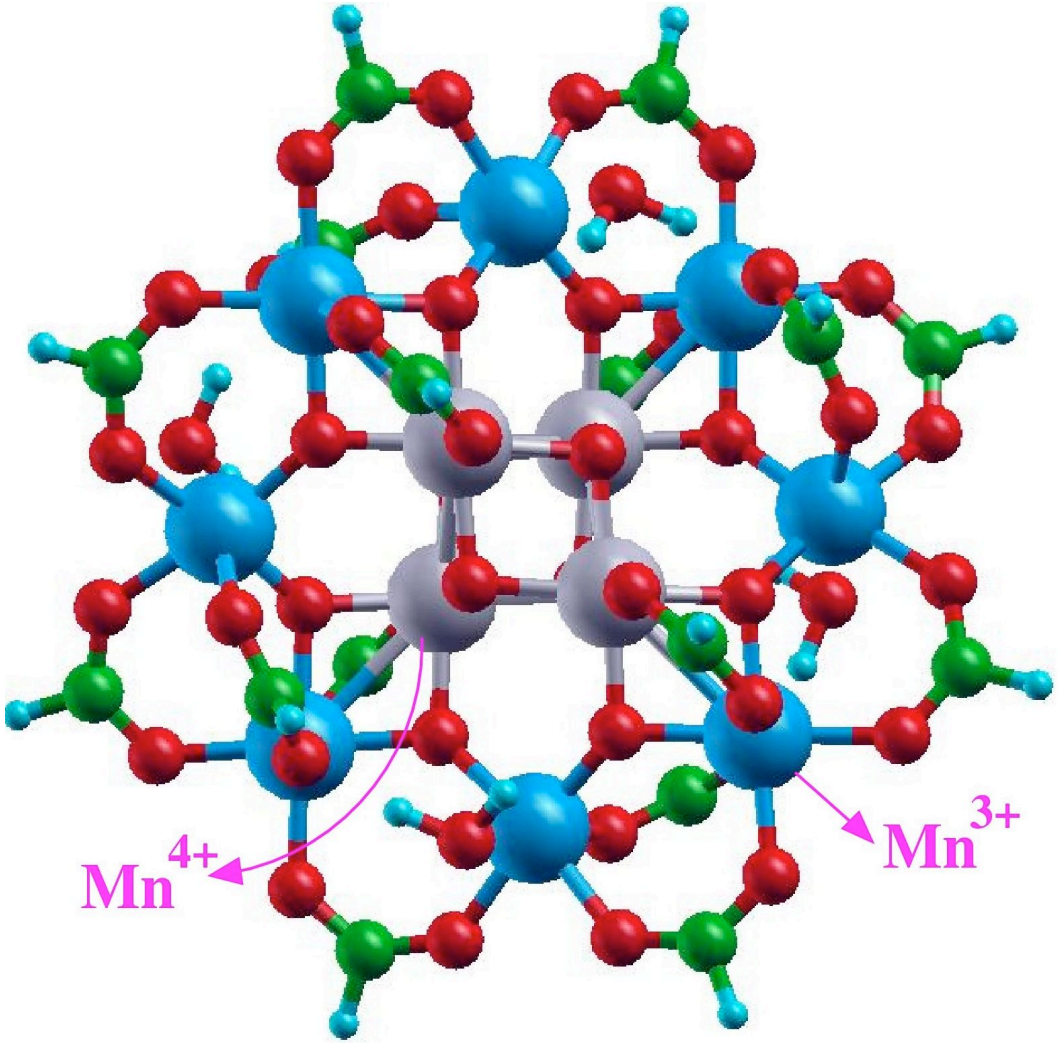




H.B. Heersche et al, PRL **96**, 206801 (2006)

M.H. Jo et al, Nano Lett. **6**, 2014 (2006)

Transport across Mn_{12}

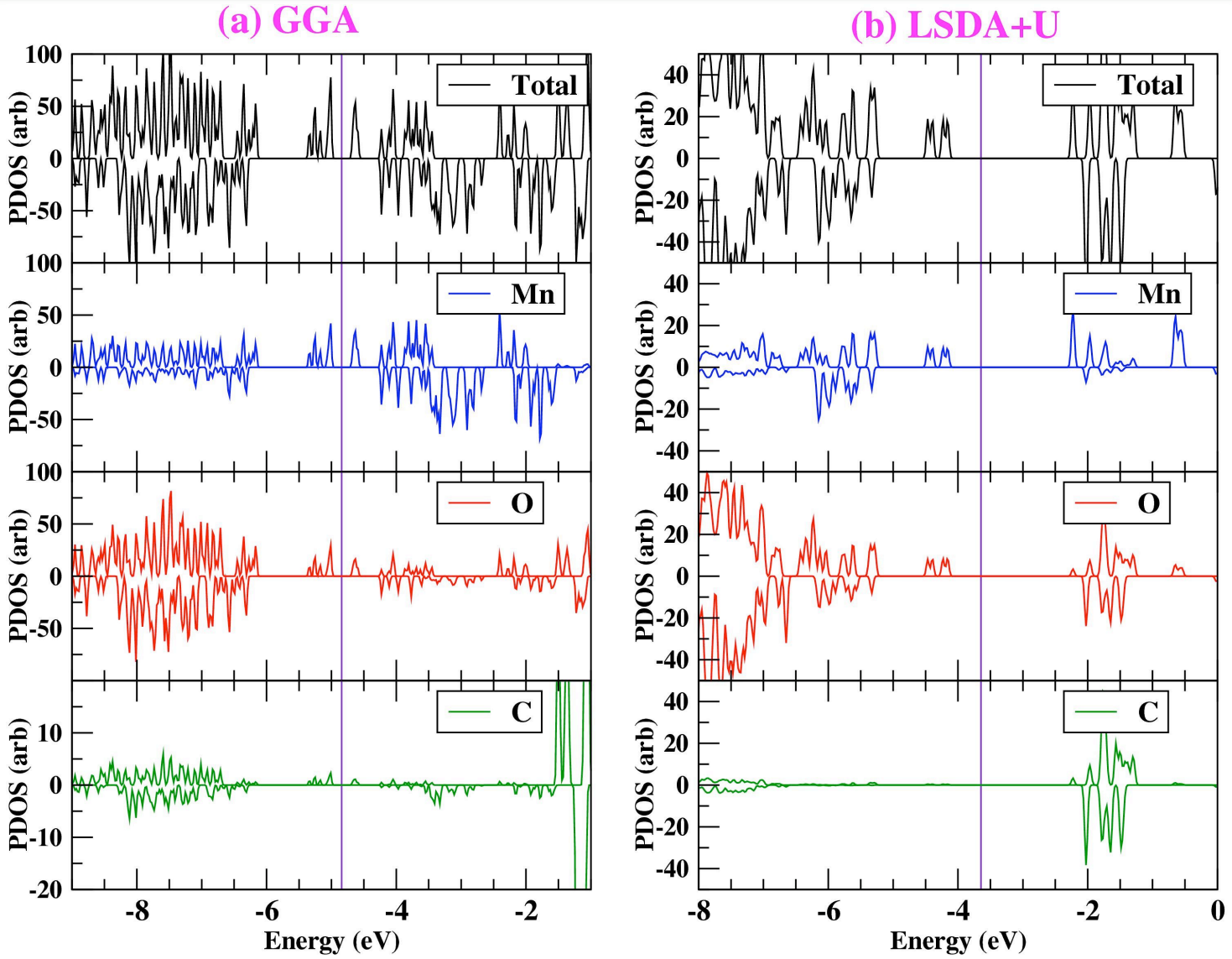


Mn^{3+} S=2

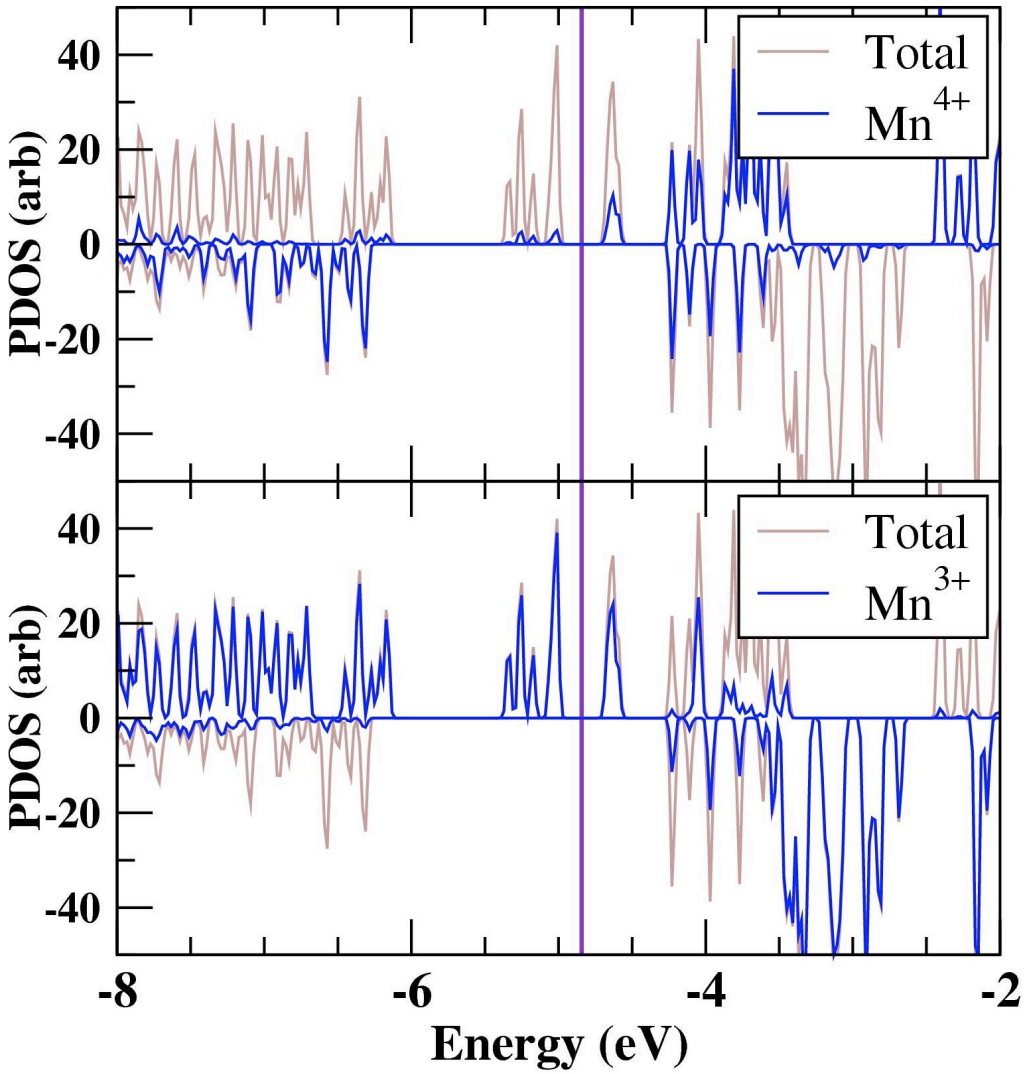
Mn^{4+} S=3/2

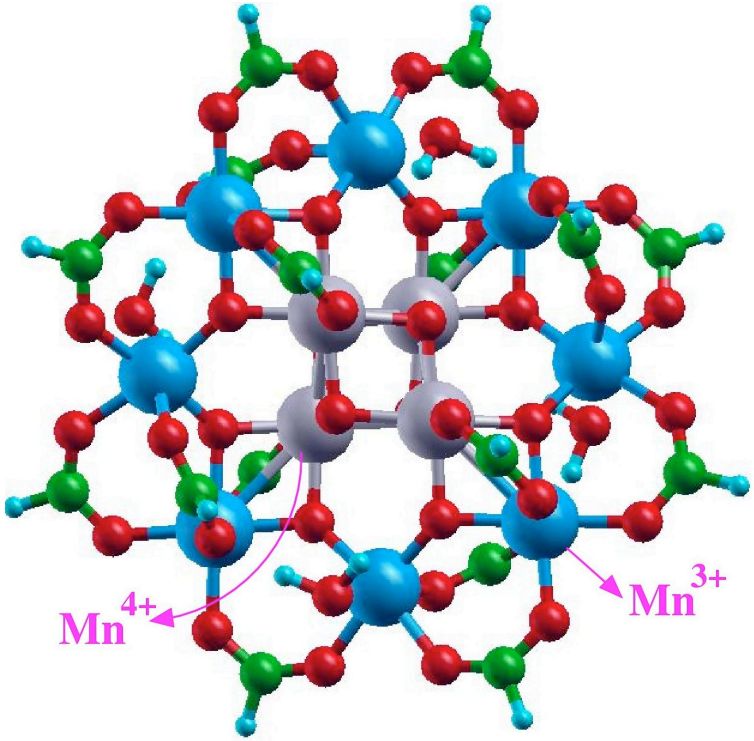
S_{GS}=10

Transport across Mn_{12}

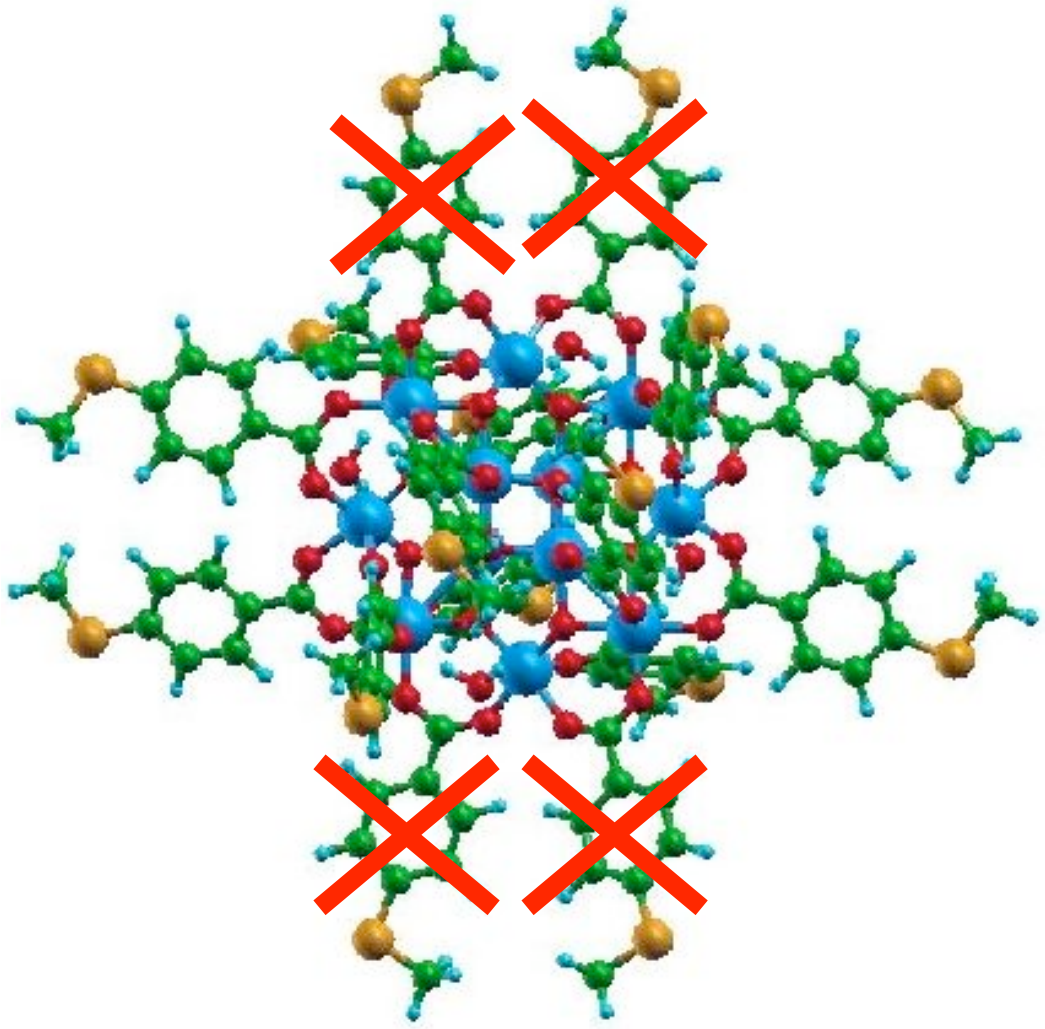


Transport across Mn_{12}

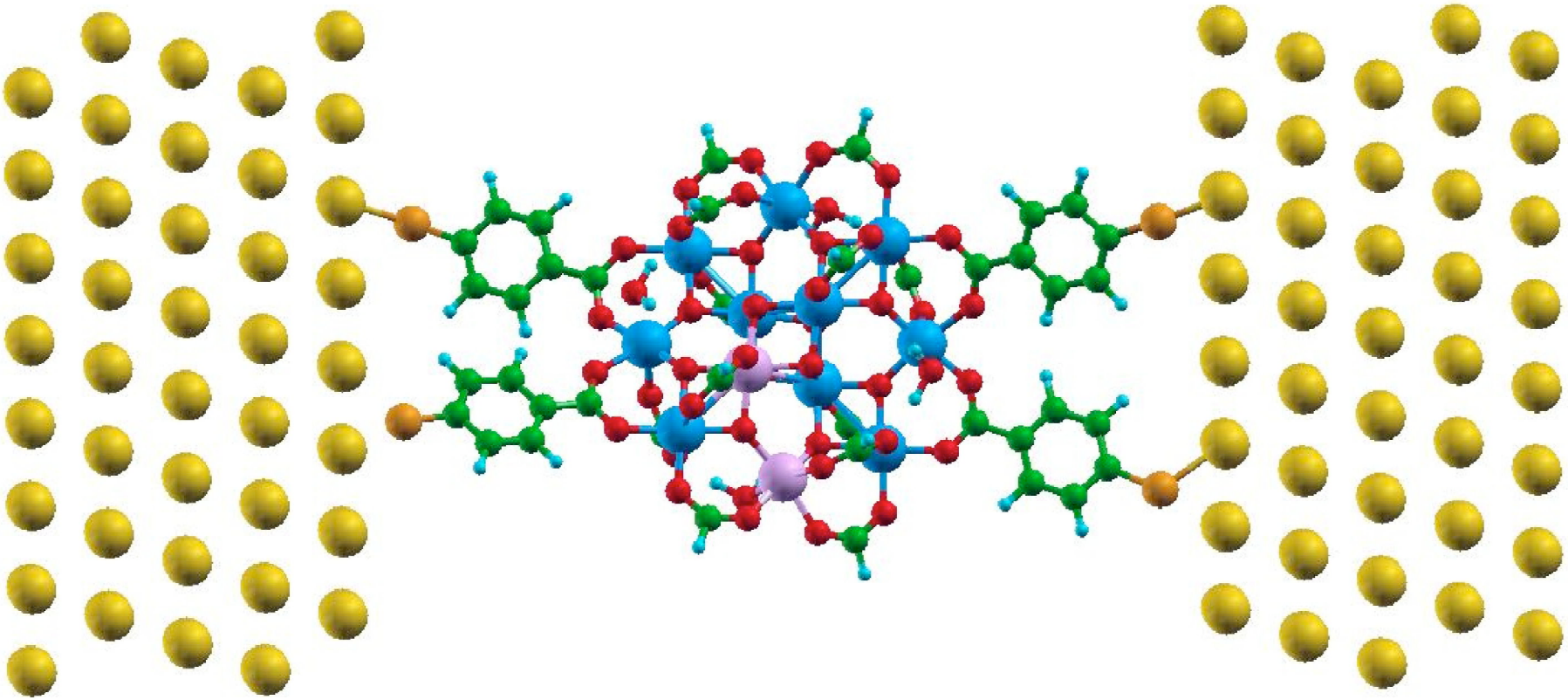




Transport across Mn_{12}



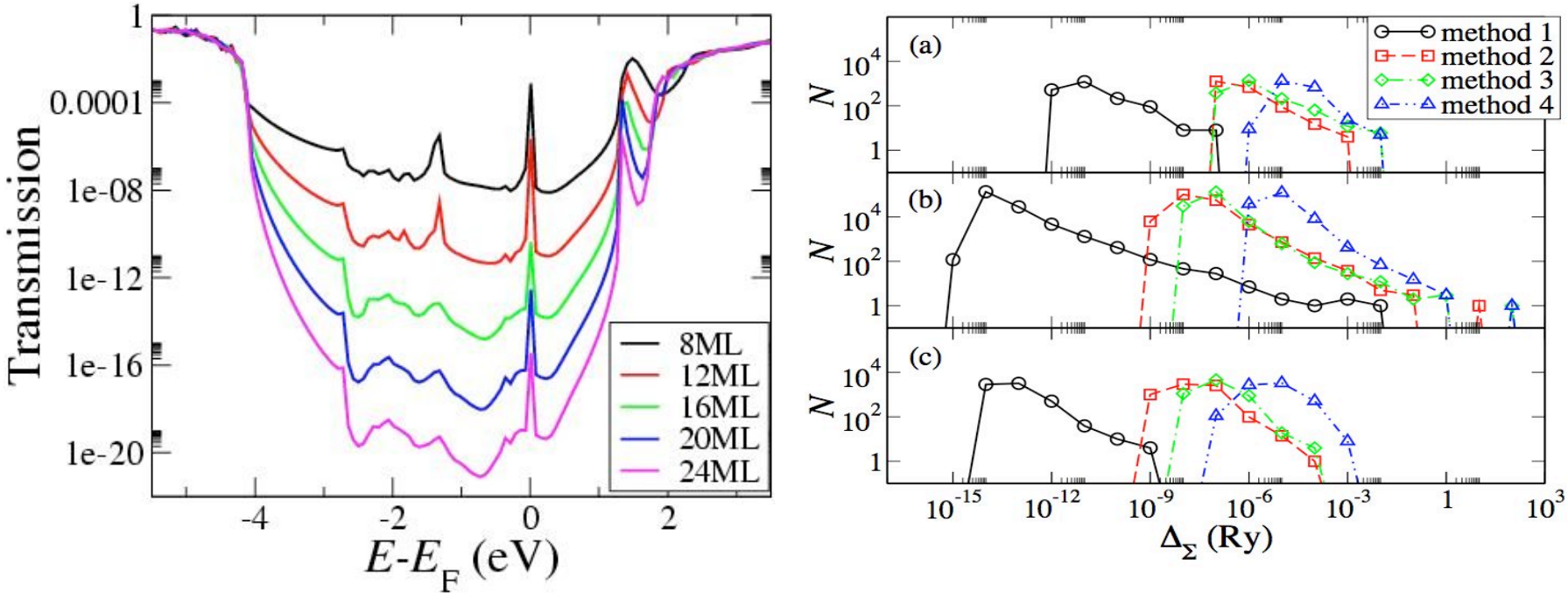
Transport across Mn_{12}



Why we can do it?

Transport across Mn_{12}

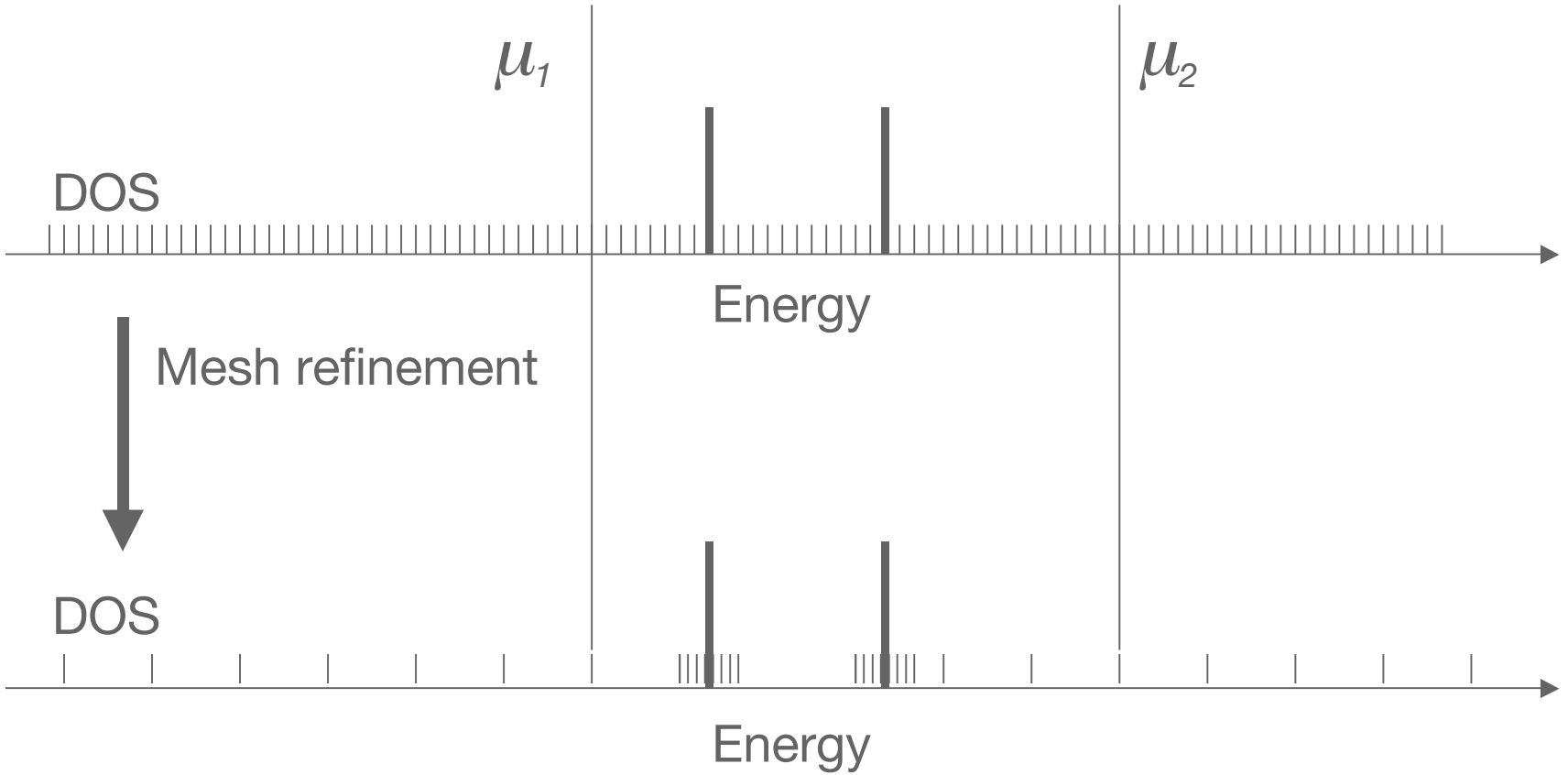
Extremely accurate transport scheme



I. Rungger *et al.*, cond-mat/0712.1369

Integration of the density matrix

$$n_{ij}^{\sigma} = \frac{1}{2\pi}\int dE[G\Gamma_L f(E,\mu_L)G^{\dagger} + G\Gamma_R f(E,\mu_R)G^{\dagger}]_{ij}^{\sigma}$$

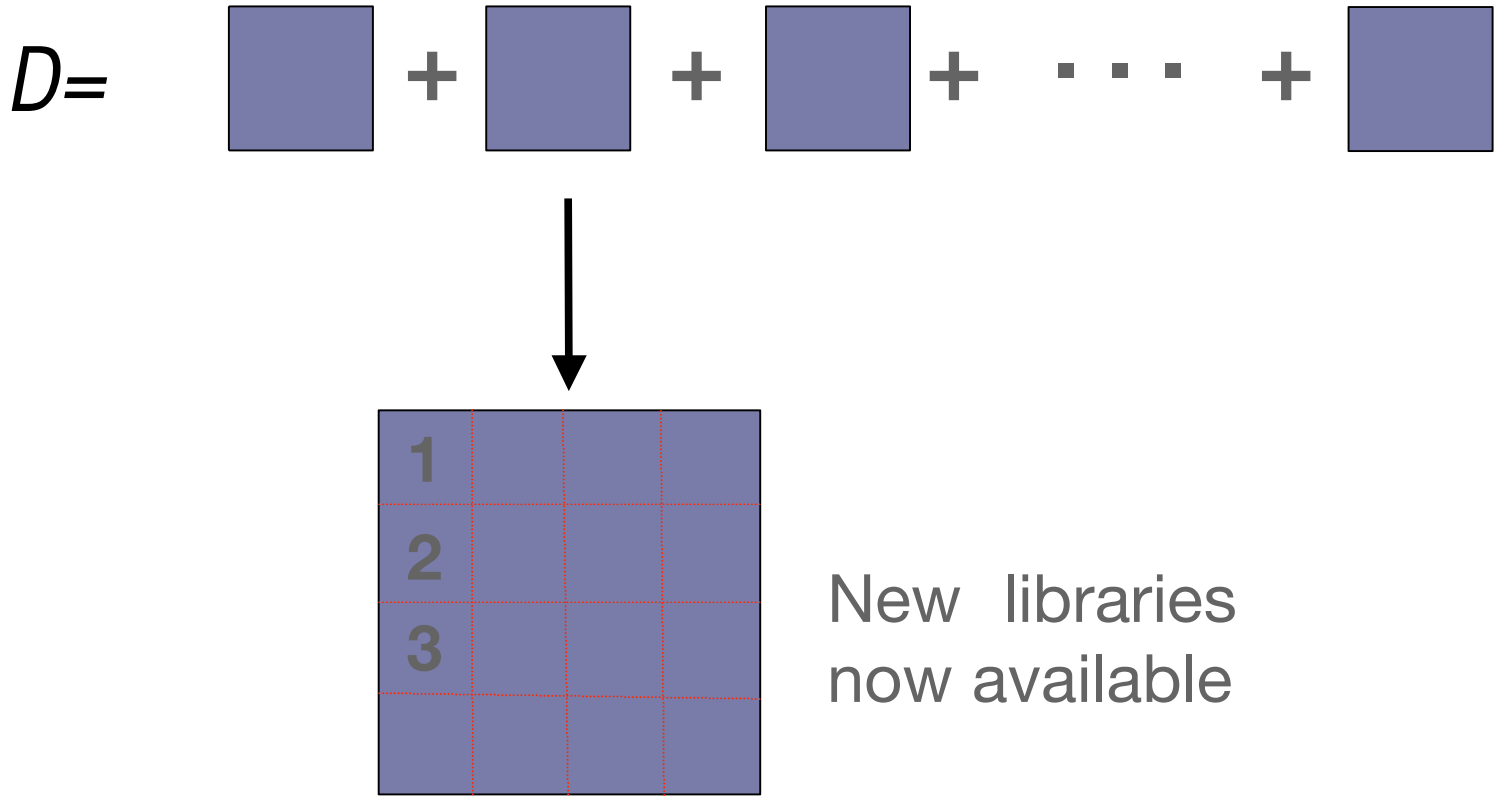


Why we can do it?

Transport across Mn_{12}

High parallelism

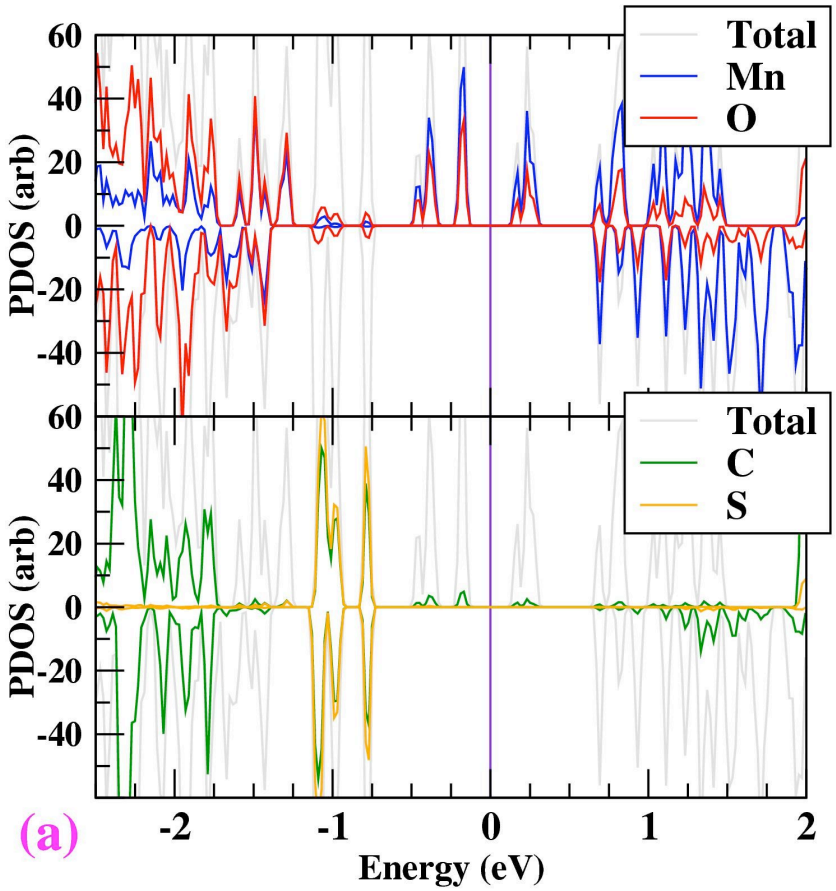
$$D = \int dE\, F(E) = \sum_i F_i$$



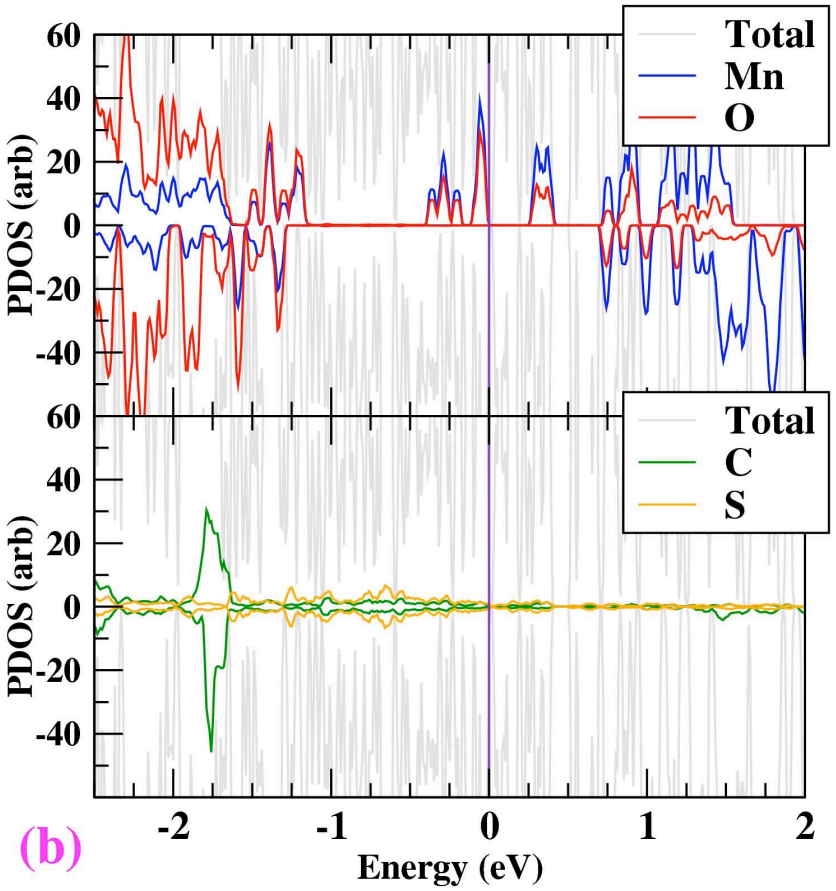
Transport across Mn_{12}

DOS: Ground State

Isolated



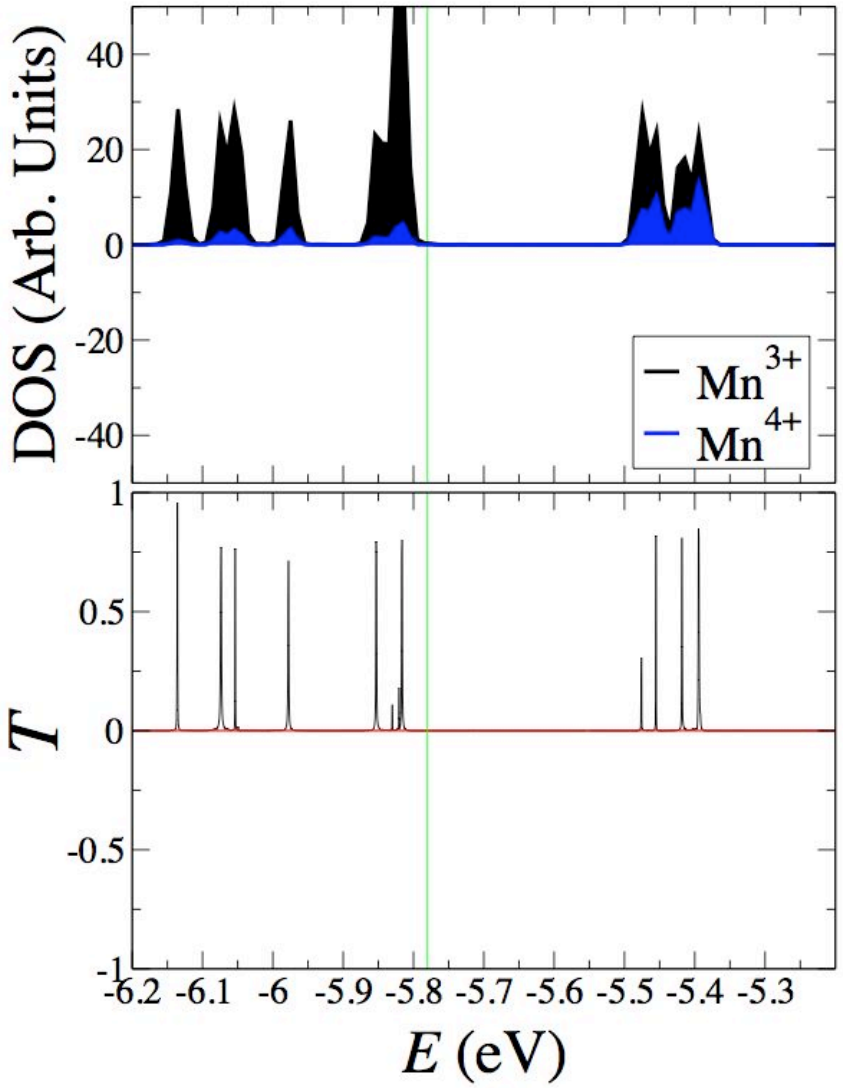
In contact



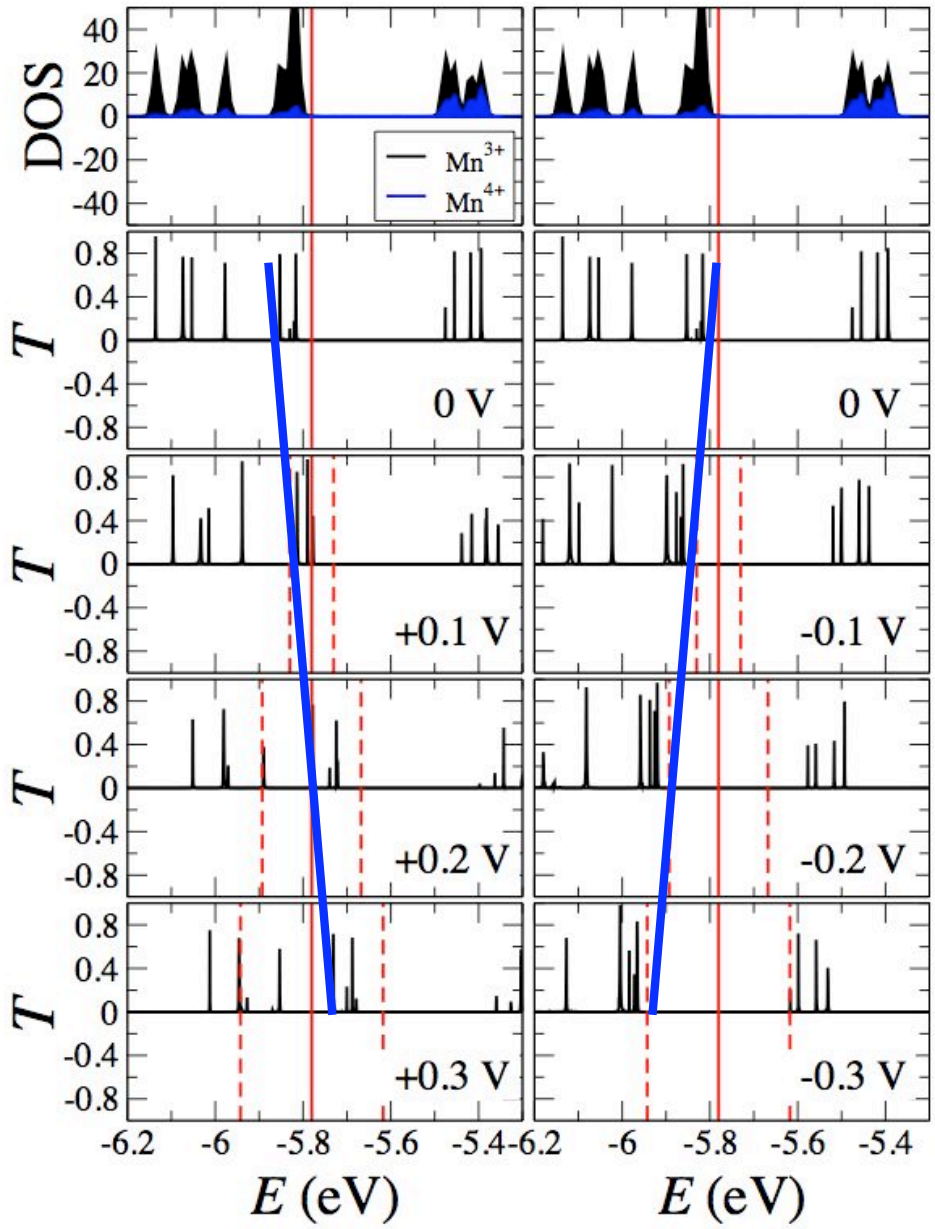
Transport across Mn_{12}

Zero bias Trasmission:

Ground State

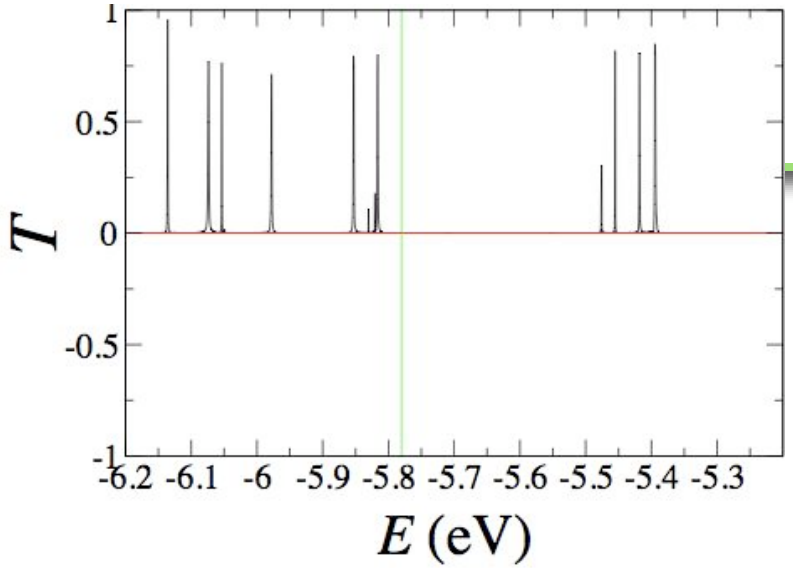


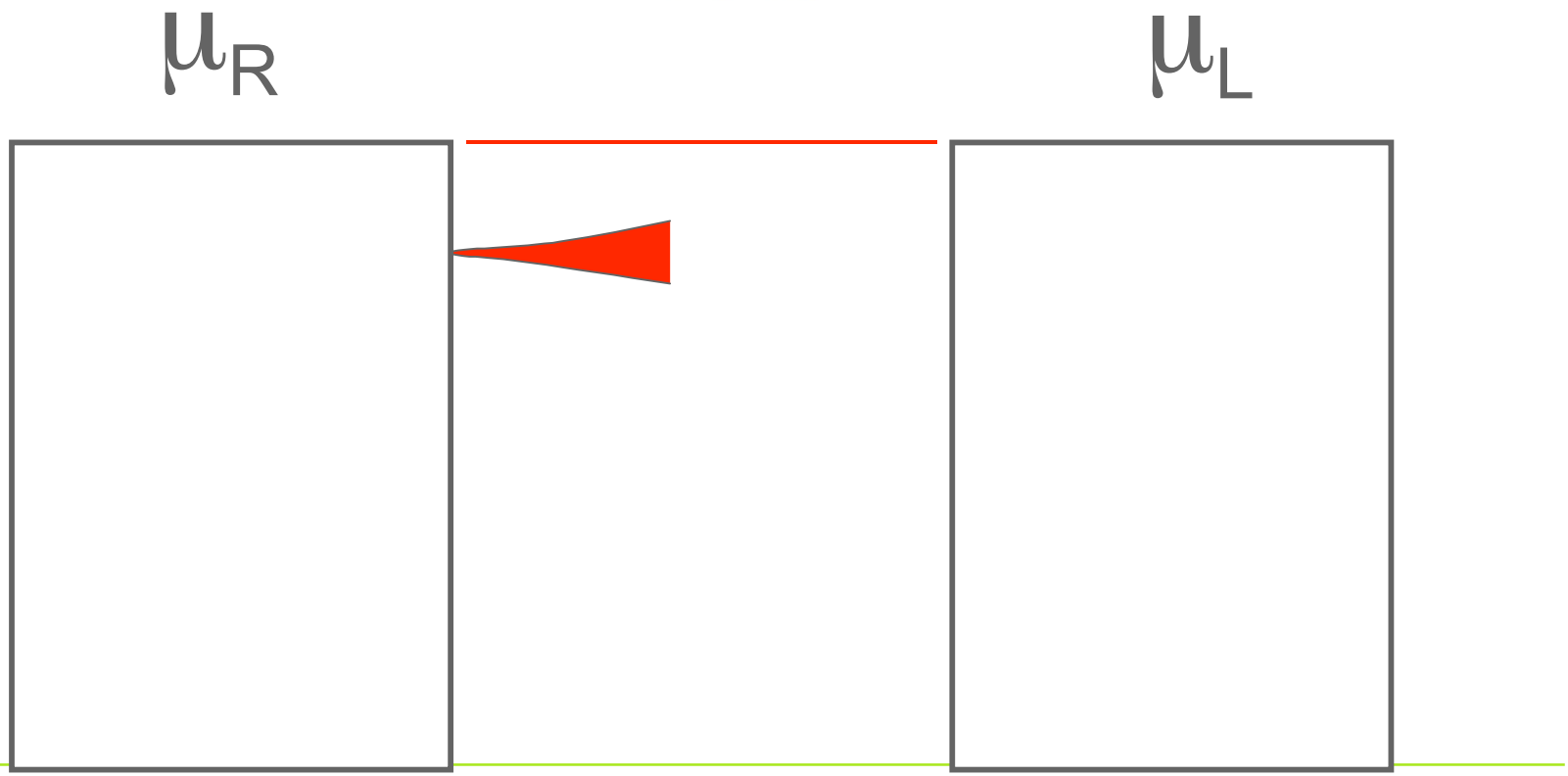
Transport across Mn_{12}



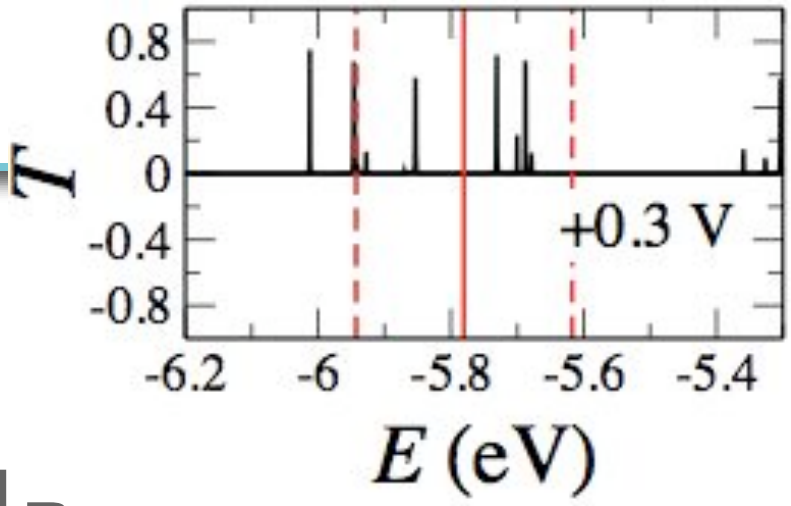
T(E) as a function of bias

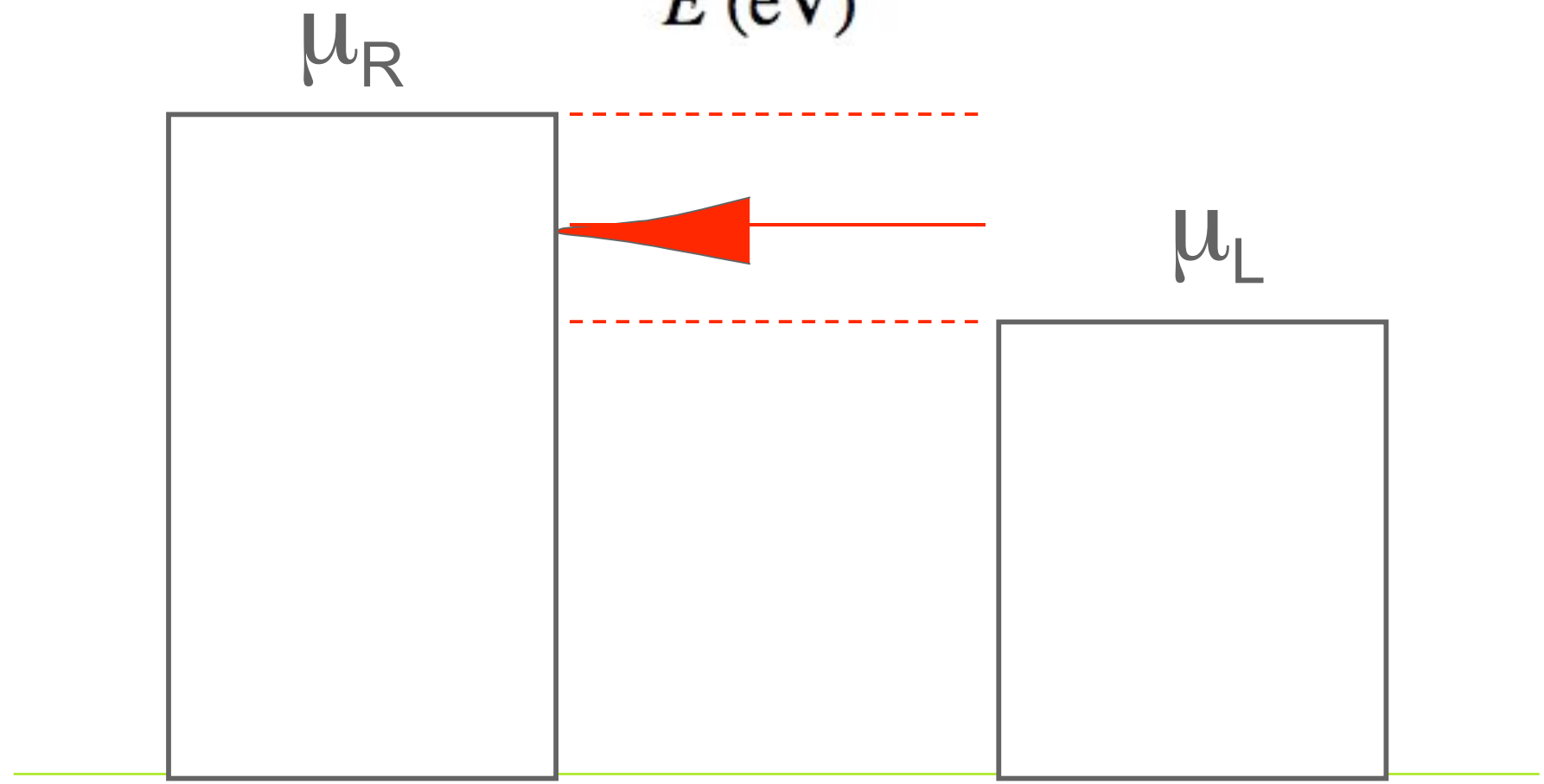
Zero Bias



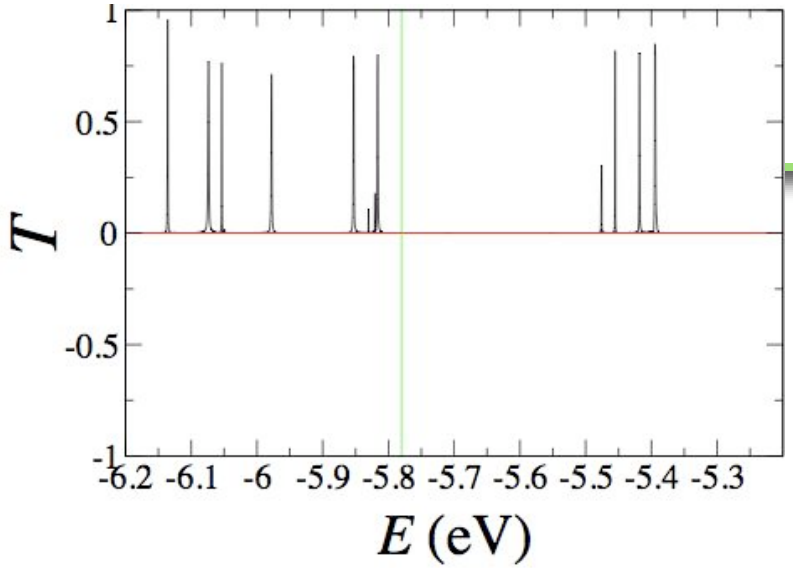


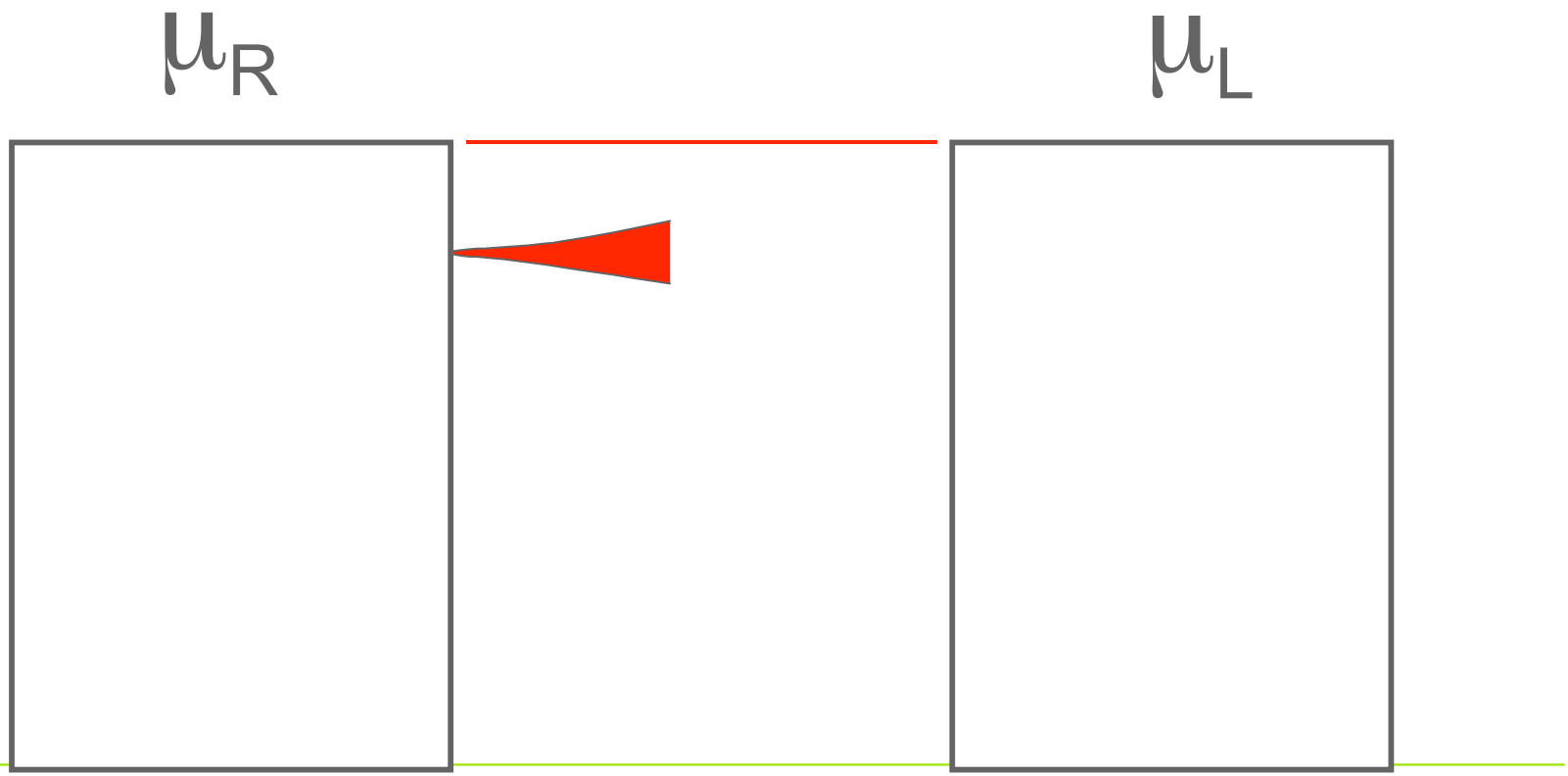
Positive Bias



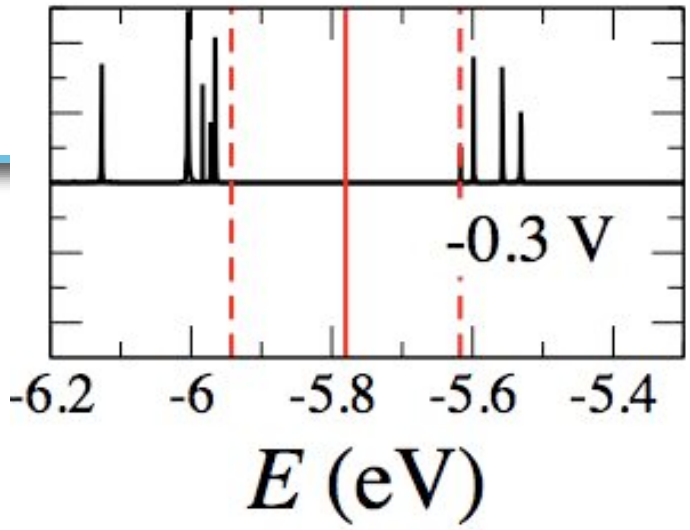


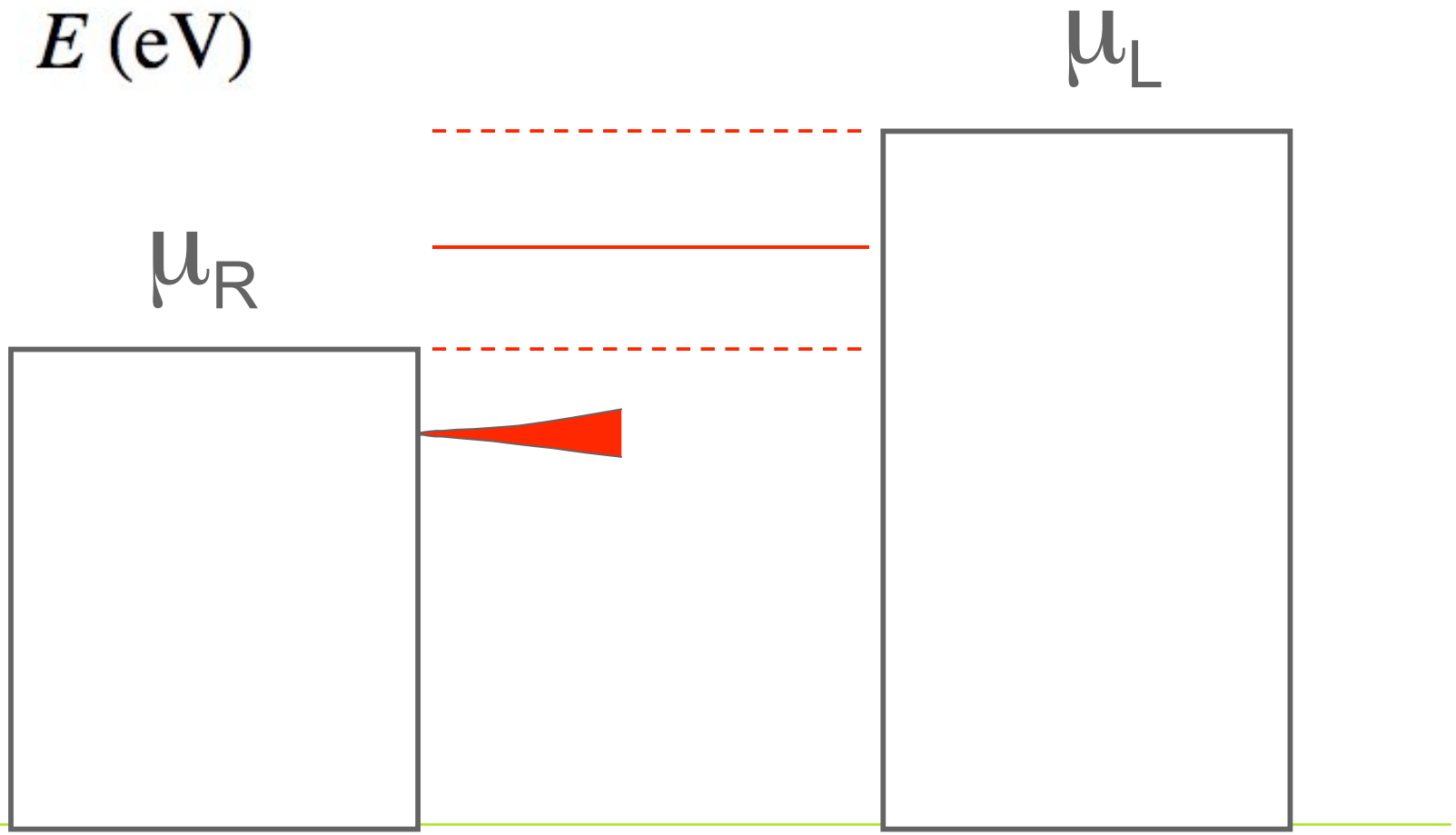
Zero Bias





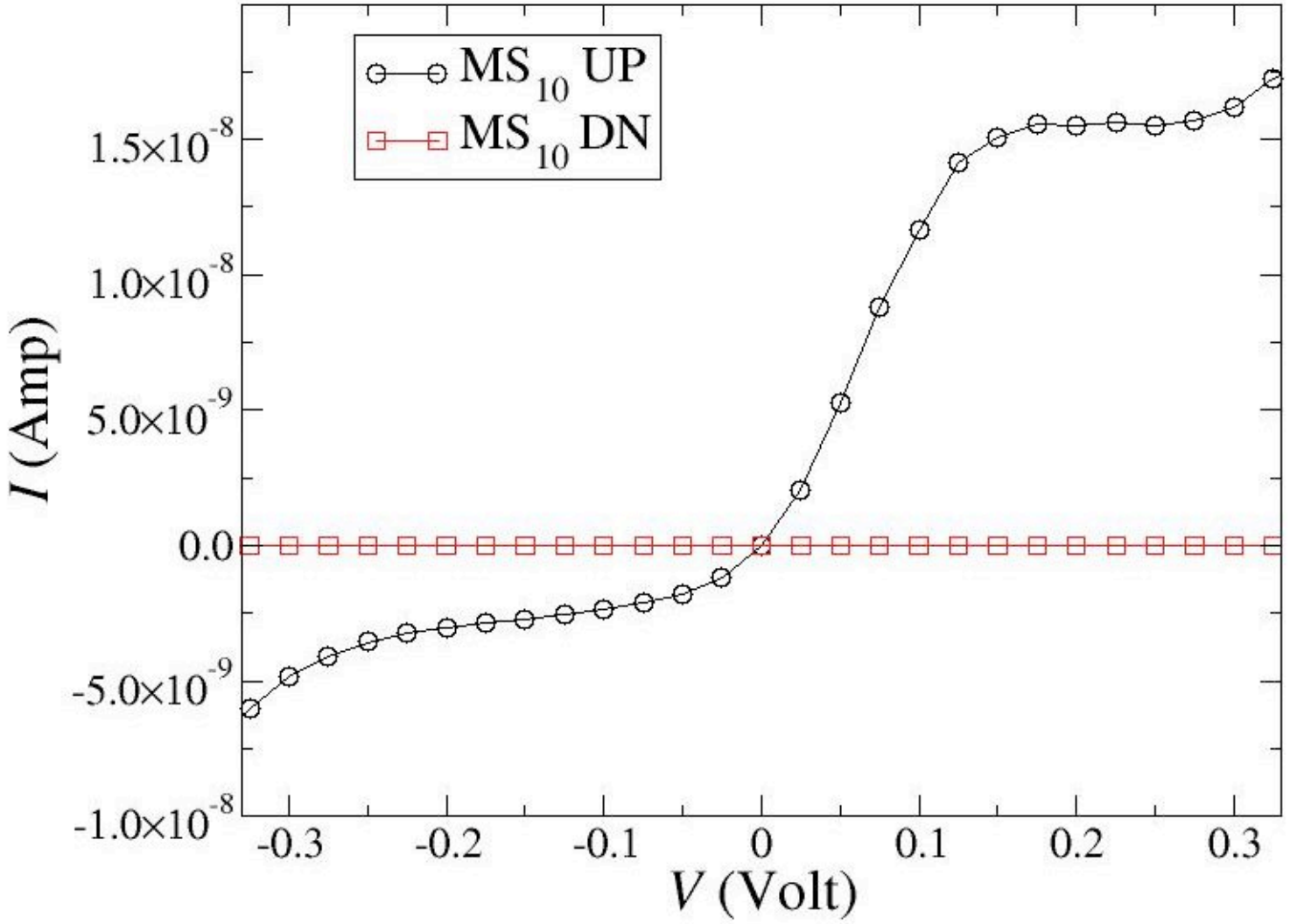
Negative Bias





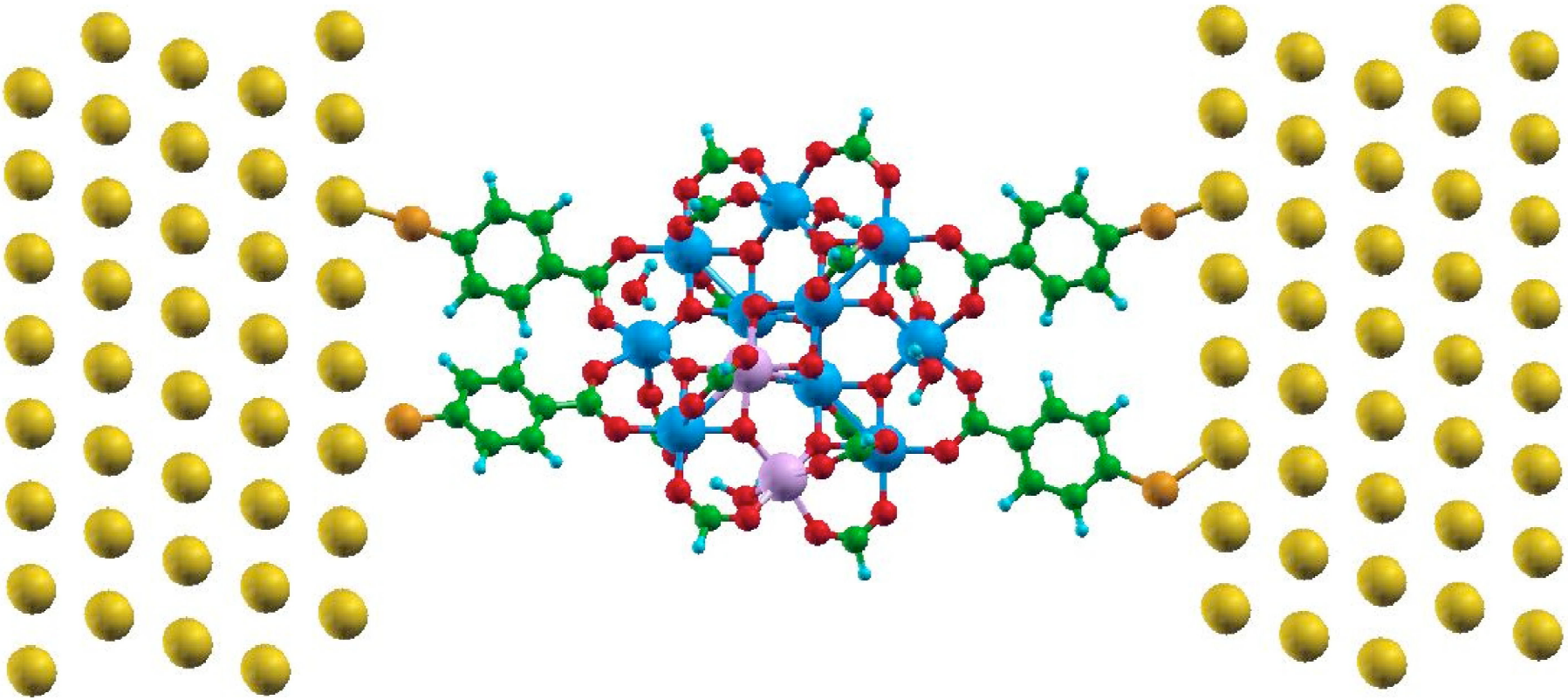
Ground State *I-V* curve

Transport across Mn_{12}



Transport across Mn_{12}

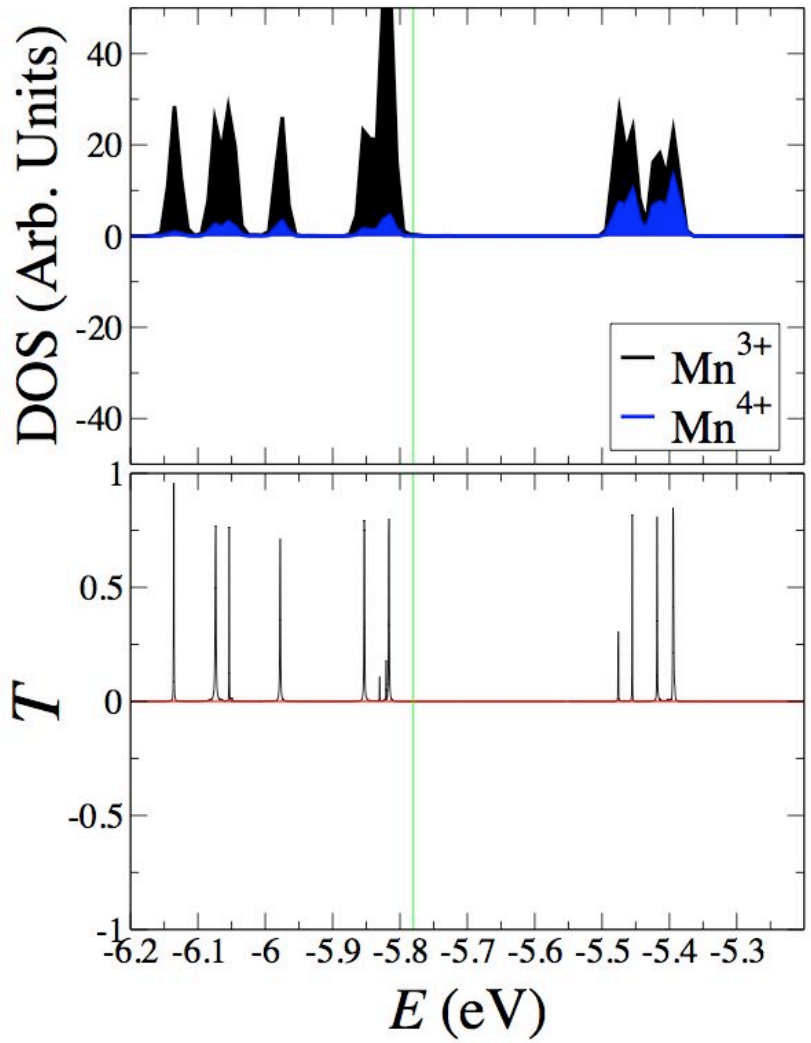
Spin-flip configuration S=9



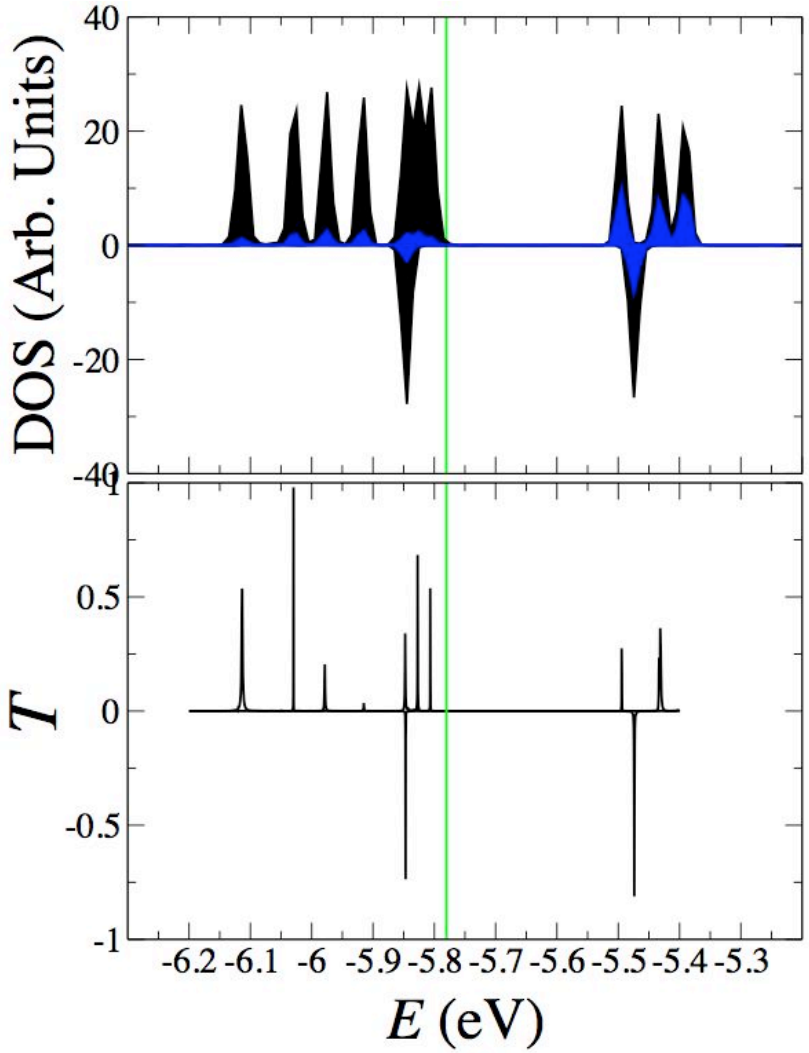
Zero bias Trasmission

Transport across Mn_{12}

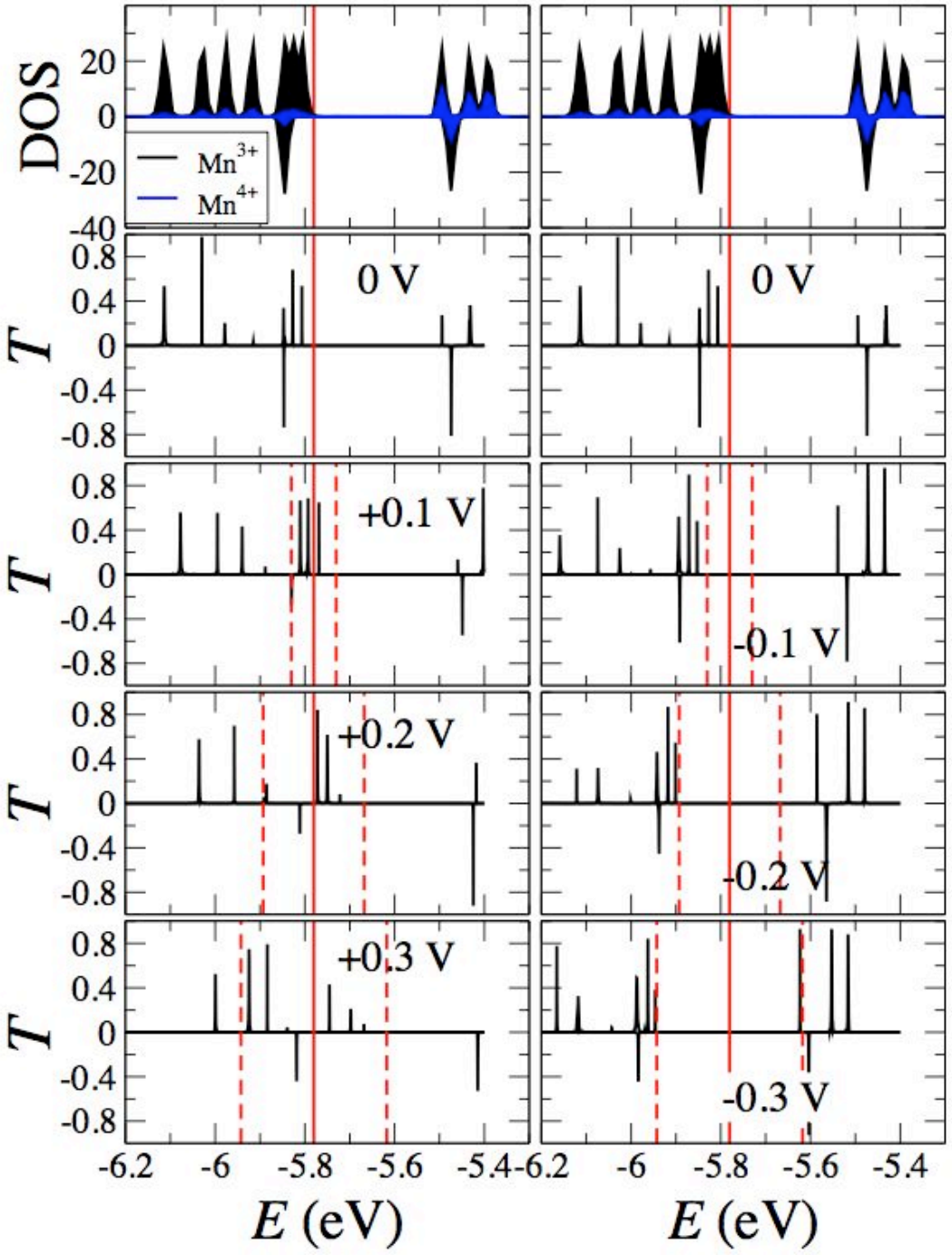
S=10

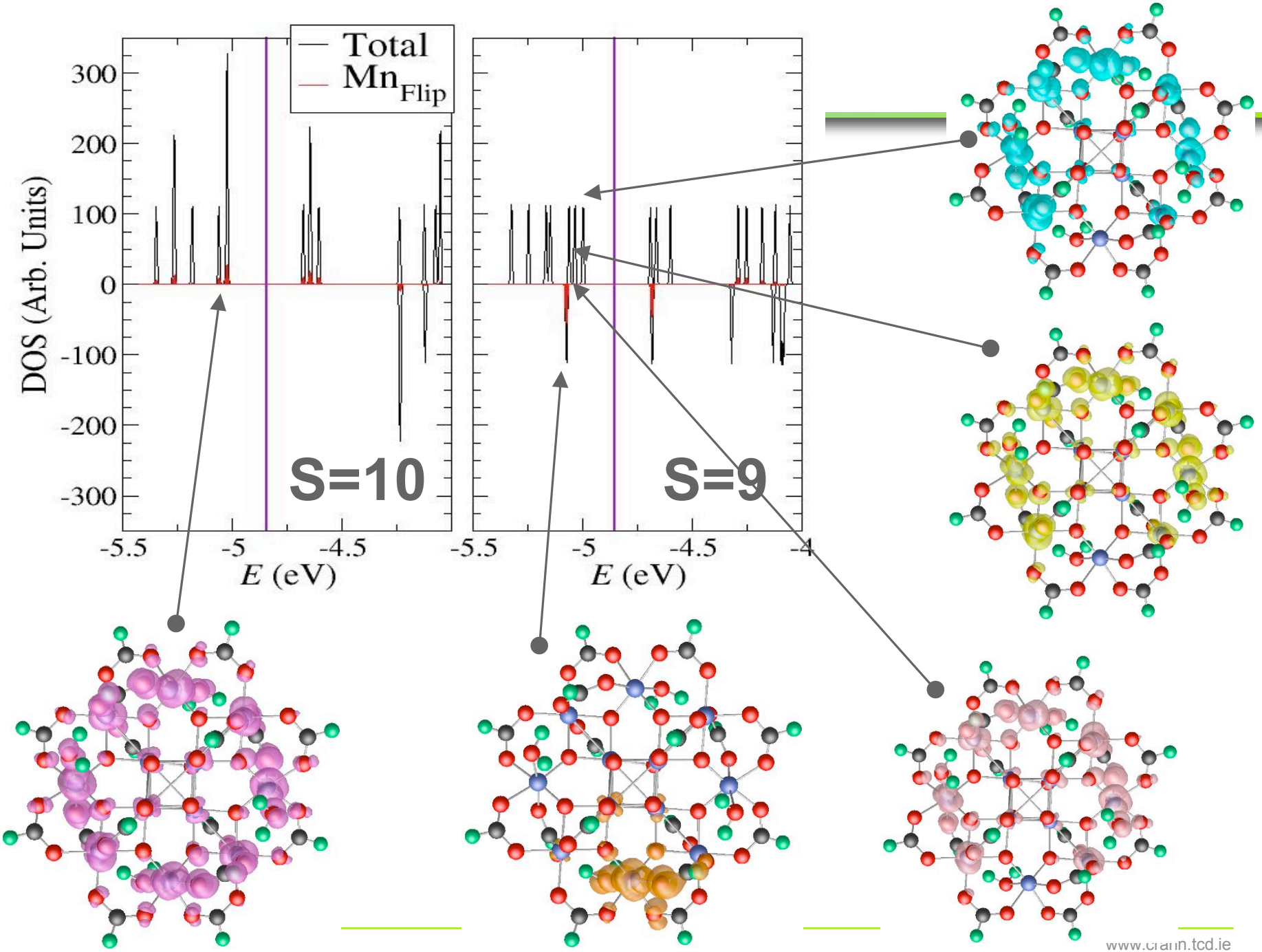


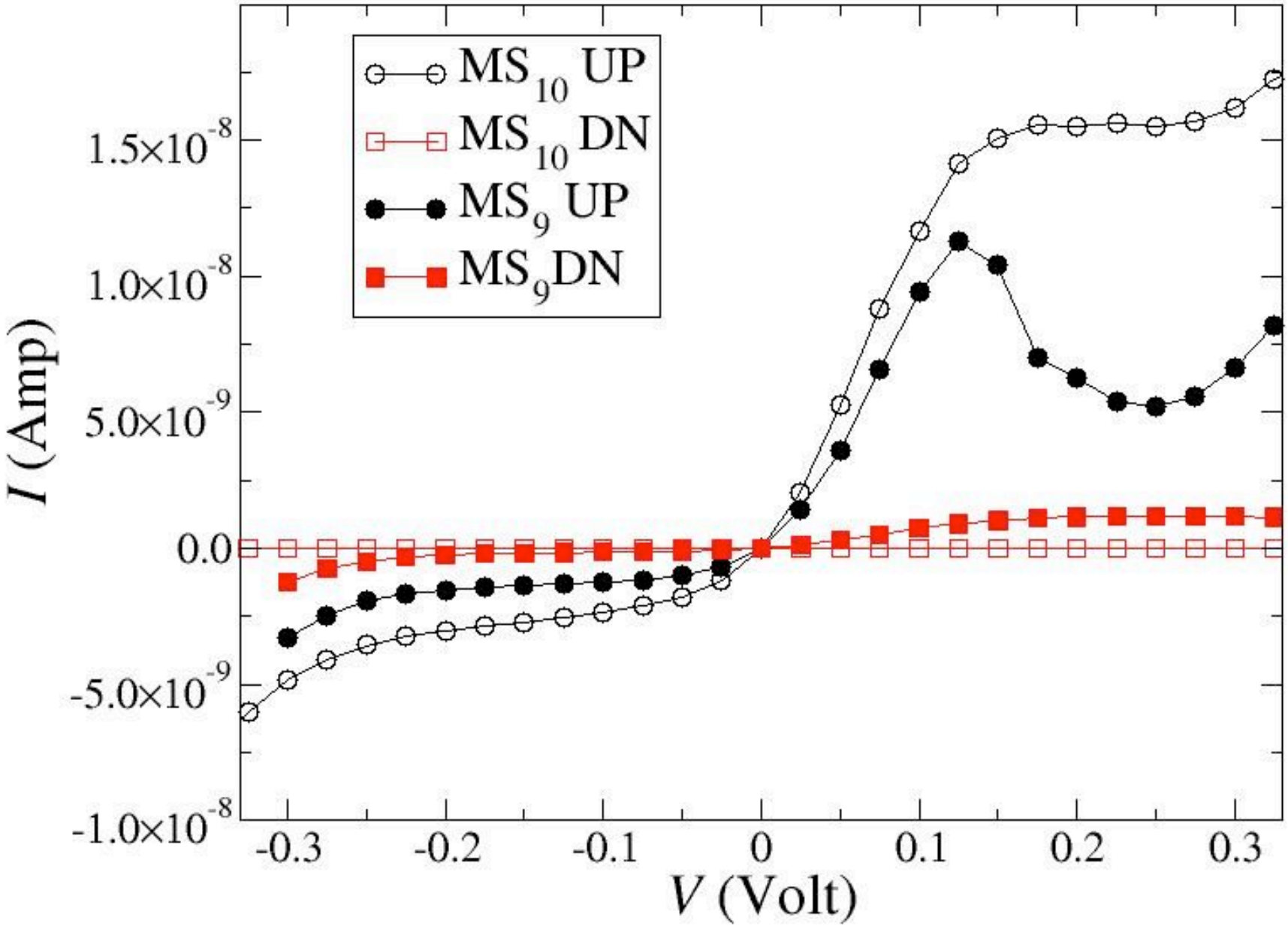
S=9



T(E) as a function of bias




Total
Mn Flip
DOS (Arb. Units)
300
200
100
0
-100
-200
-300
-5.5
-5
-4.5
E (eV)
S=10
S=9


MS10 UP
MS10 DN
MS9 UP
MS9DN
1.5×10-8
1.0×10-8
5.0×10-9
0.0
-5.0×10-9
-1.0×10-8
I (Amp)
-0.3
-0.2
-0.1
0
0.1
0.2
0.3
V (Volt)

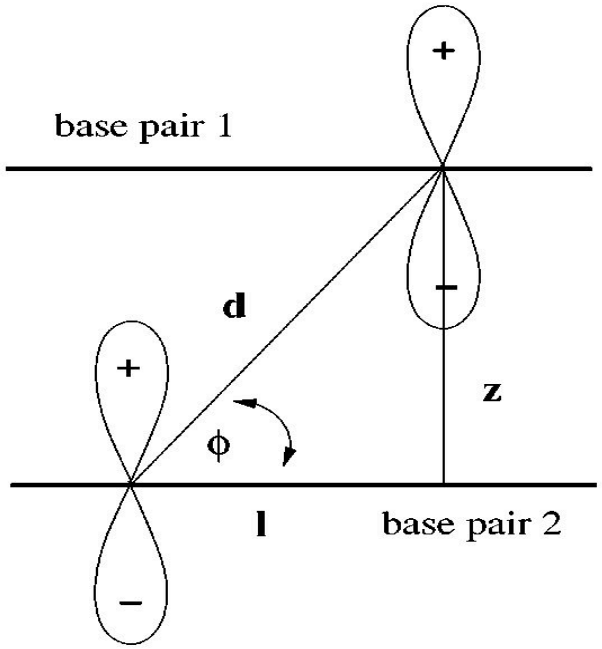
Conclusion MM

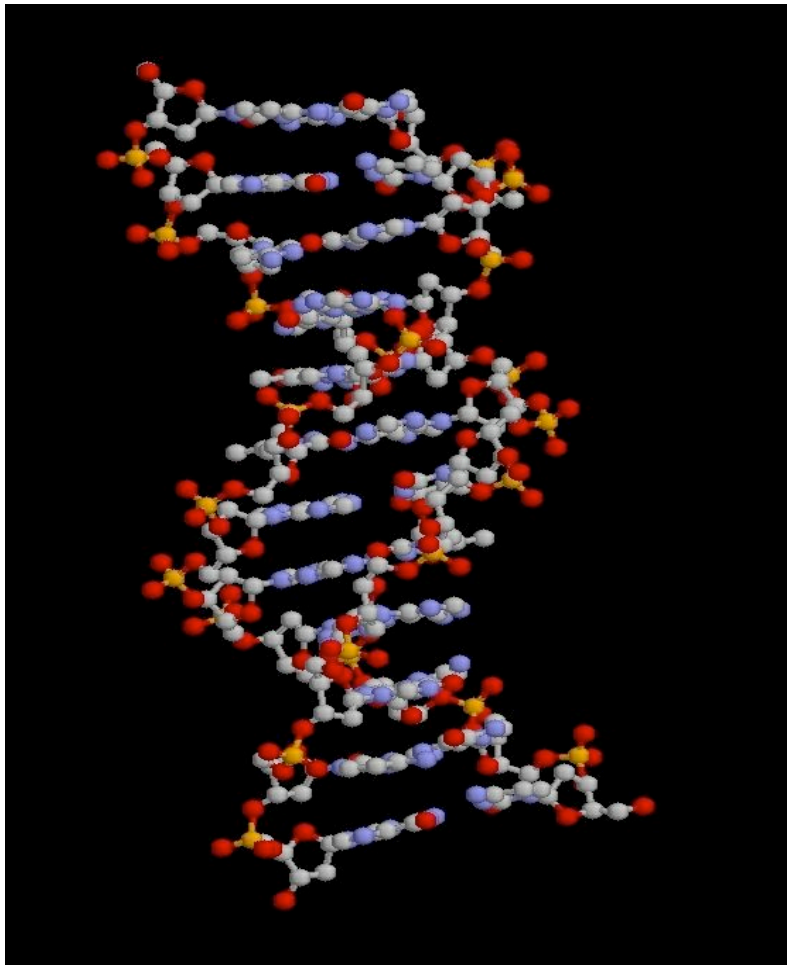
- Change in static potential due to spin-flip is electrically readable
- It seems that the magnetic state of Mn_{12} can be read electronically
- Most of the information are in the full *I-V* curve: zero-bias misleading

DNA Transport

DNA Transport

Is DNA a metal?

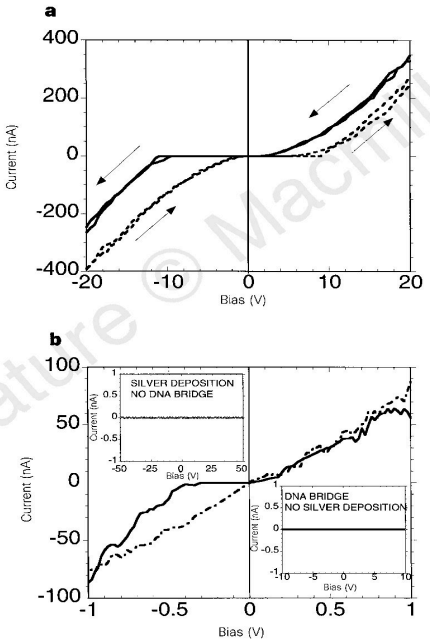




Eley and Spivey, *Trans. Faraday Soc.* **58**, 411 (1962)

DNA Transport

Gap = 10 – 12 Volts

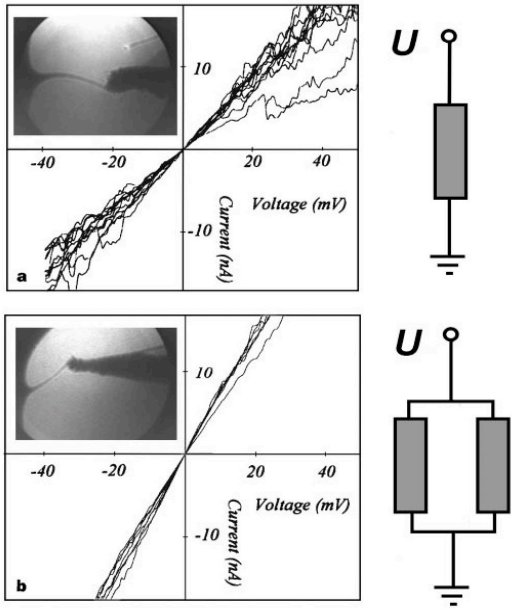


Braun et. al., Nature **391**, 775 (1998)

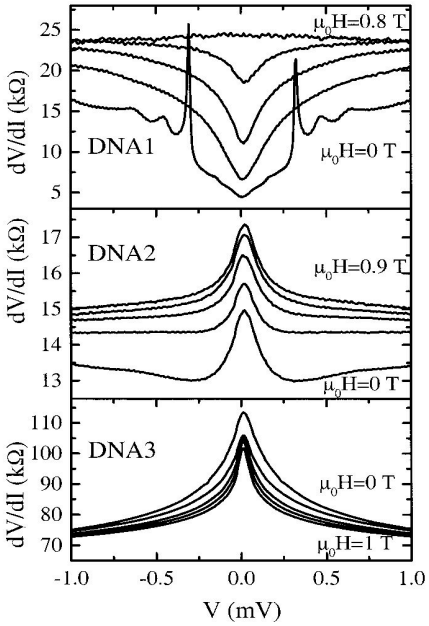
de Pablo et. al., PRL **85**, 4992 (2000)

Metal

Fink et. al., Nature **398**, 407 (1999)



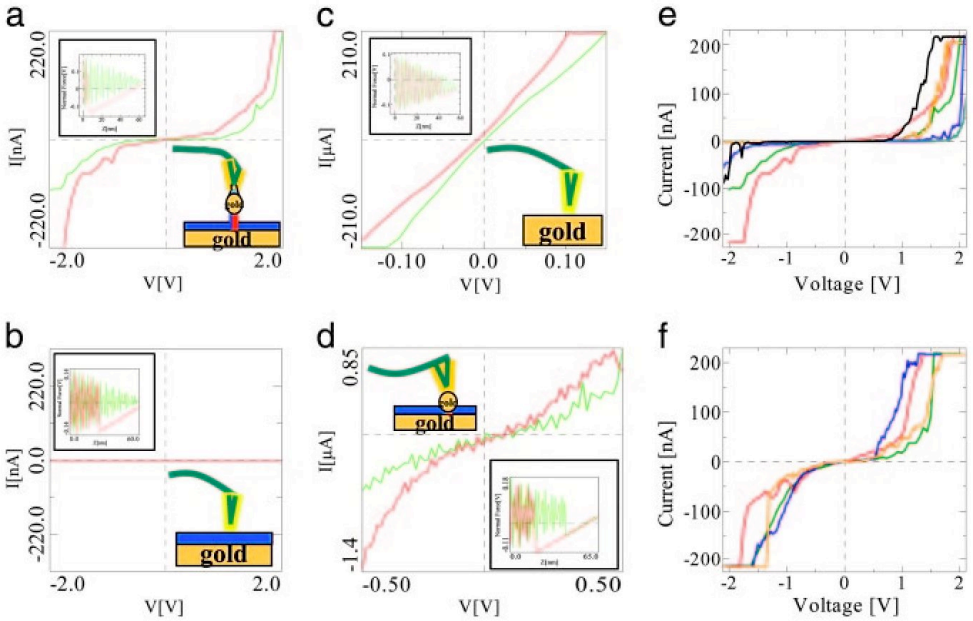
Superconductor



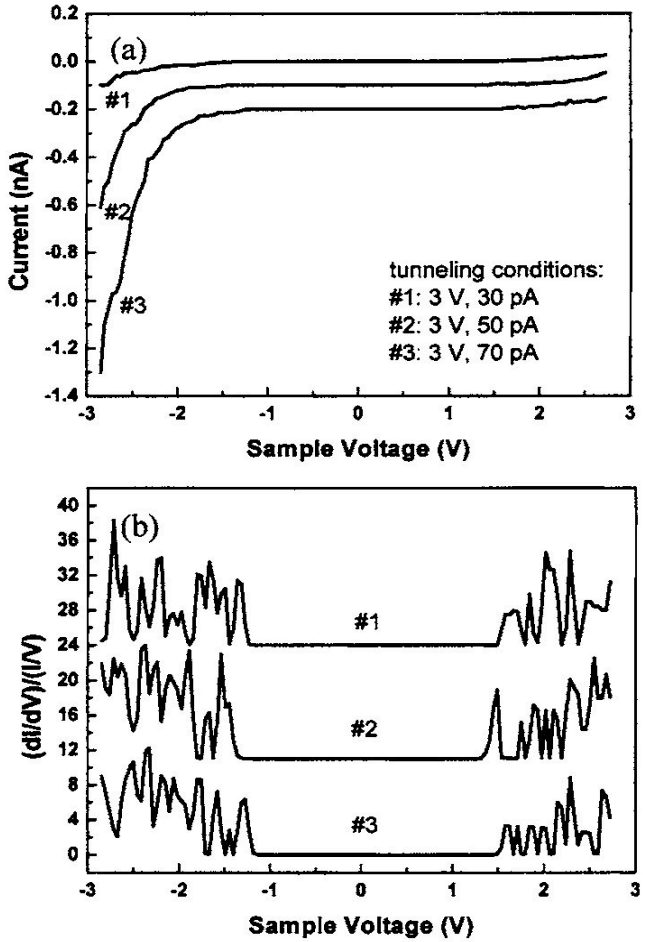
Kasumov et. al.,
Science **291**, 280 (2001)

DNA Transport

Small DNA strands



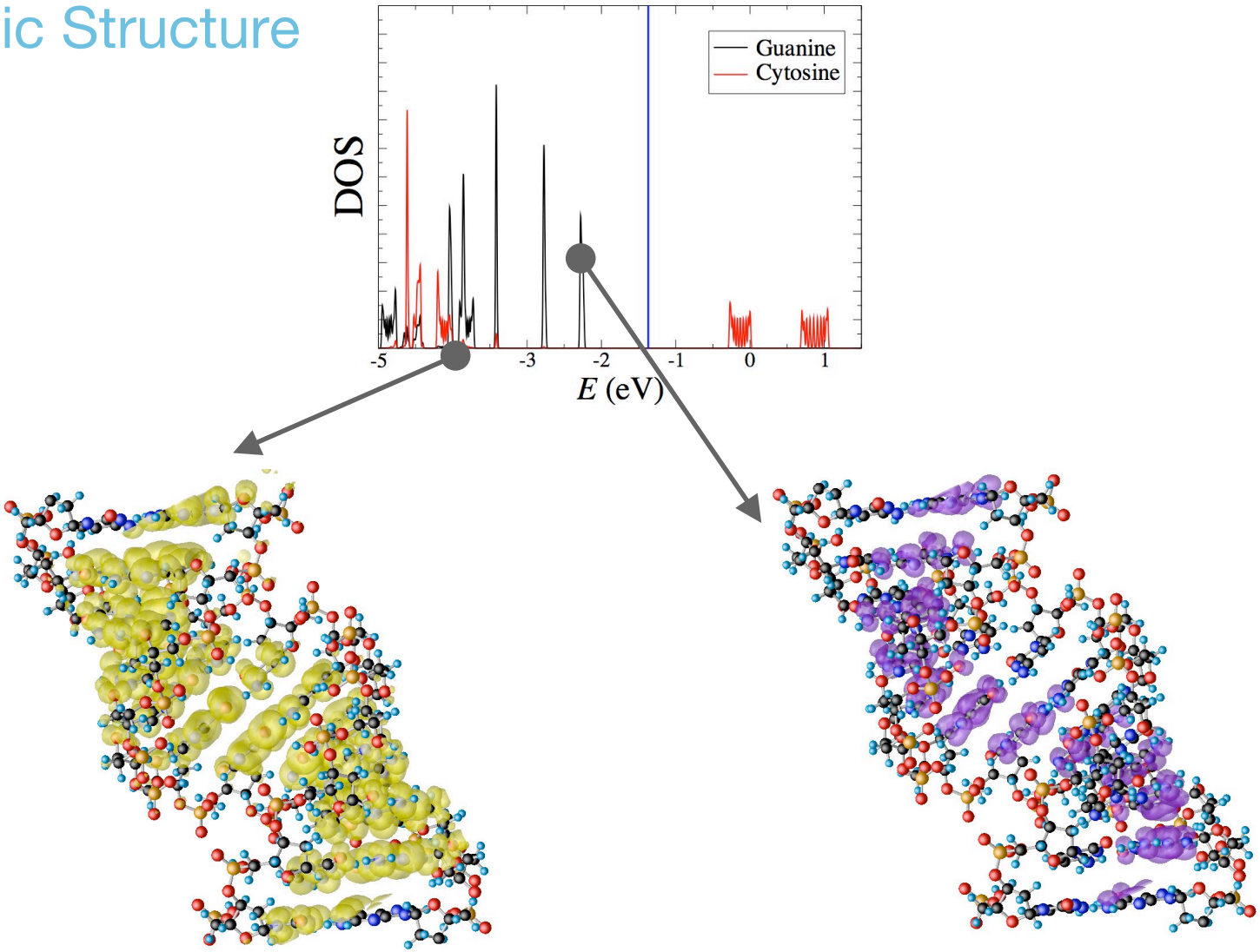
Cohen *et al,* PNAS **33**, 11589 (2005)



Xu *et al,* APL **87**, 083902 (2005)

DNA Transport

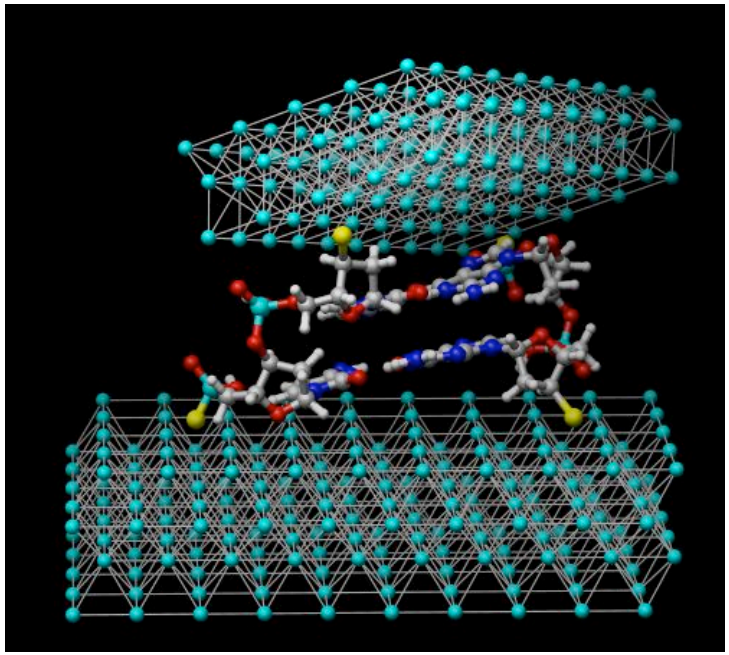
Electronic Structure



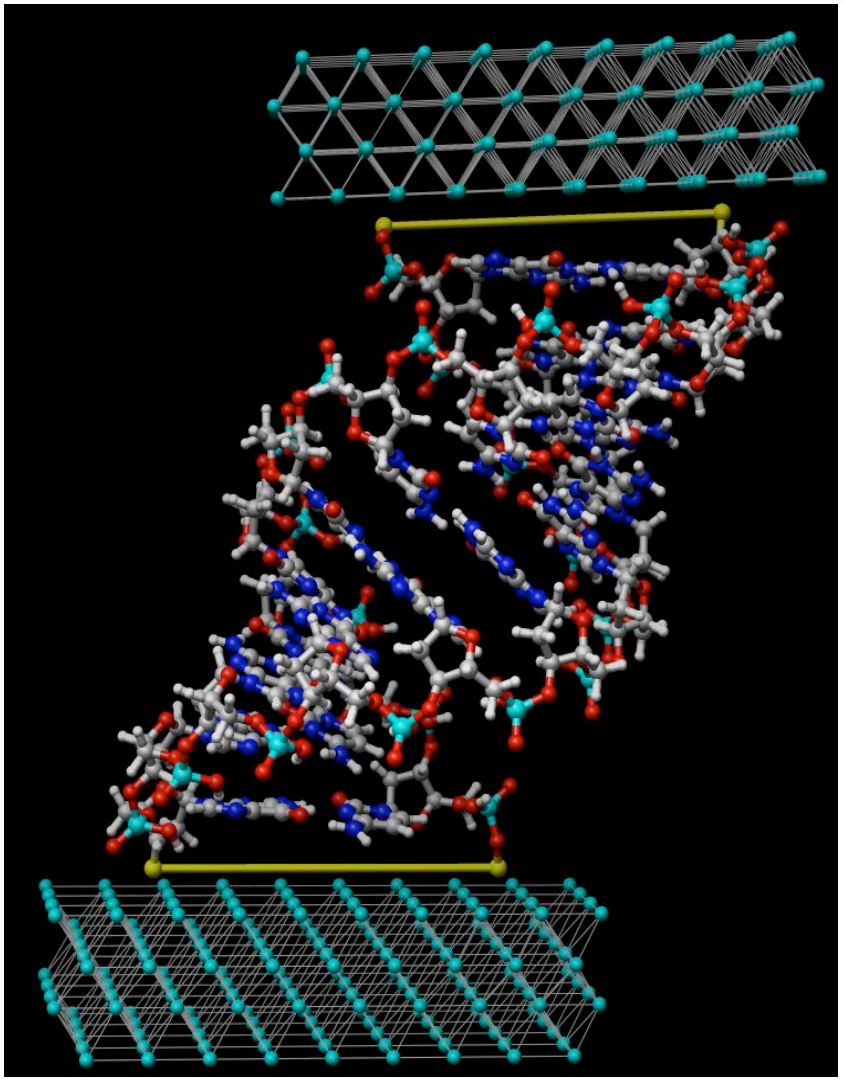
DNA Transport

Our *Smeagol* attempt

Poly(C)-Poly(G)

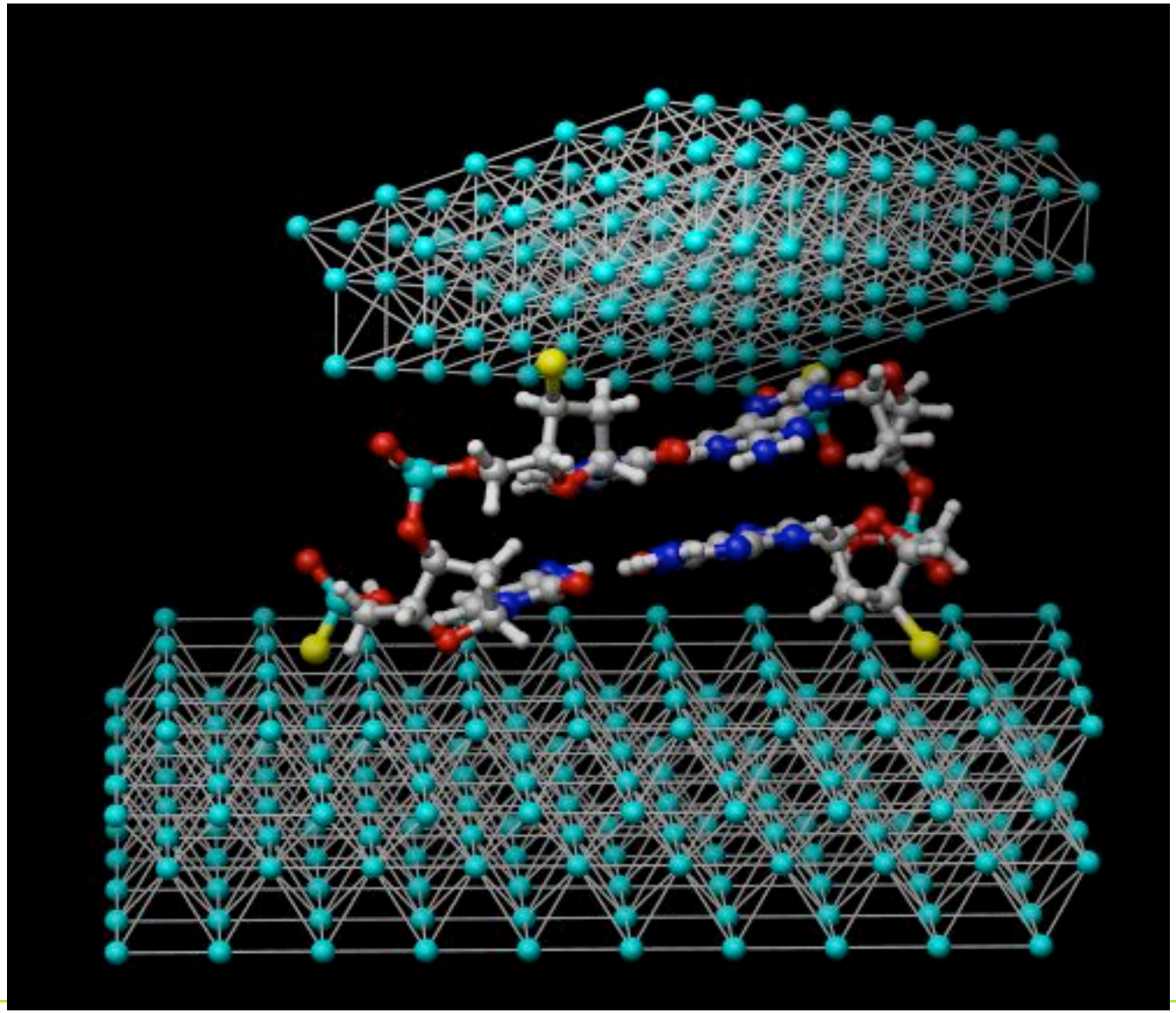


2 base pairs



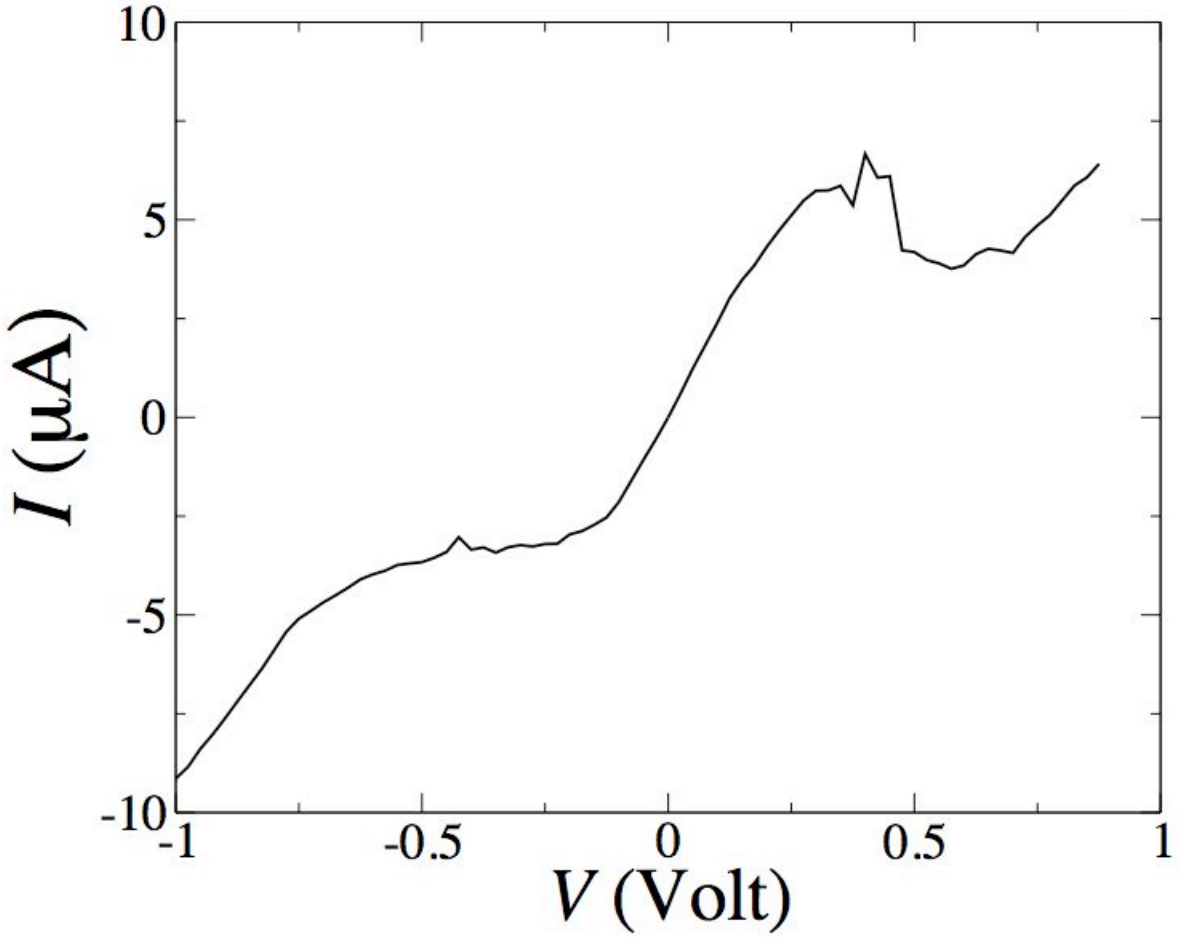
11 base pairs

DNA Transport



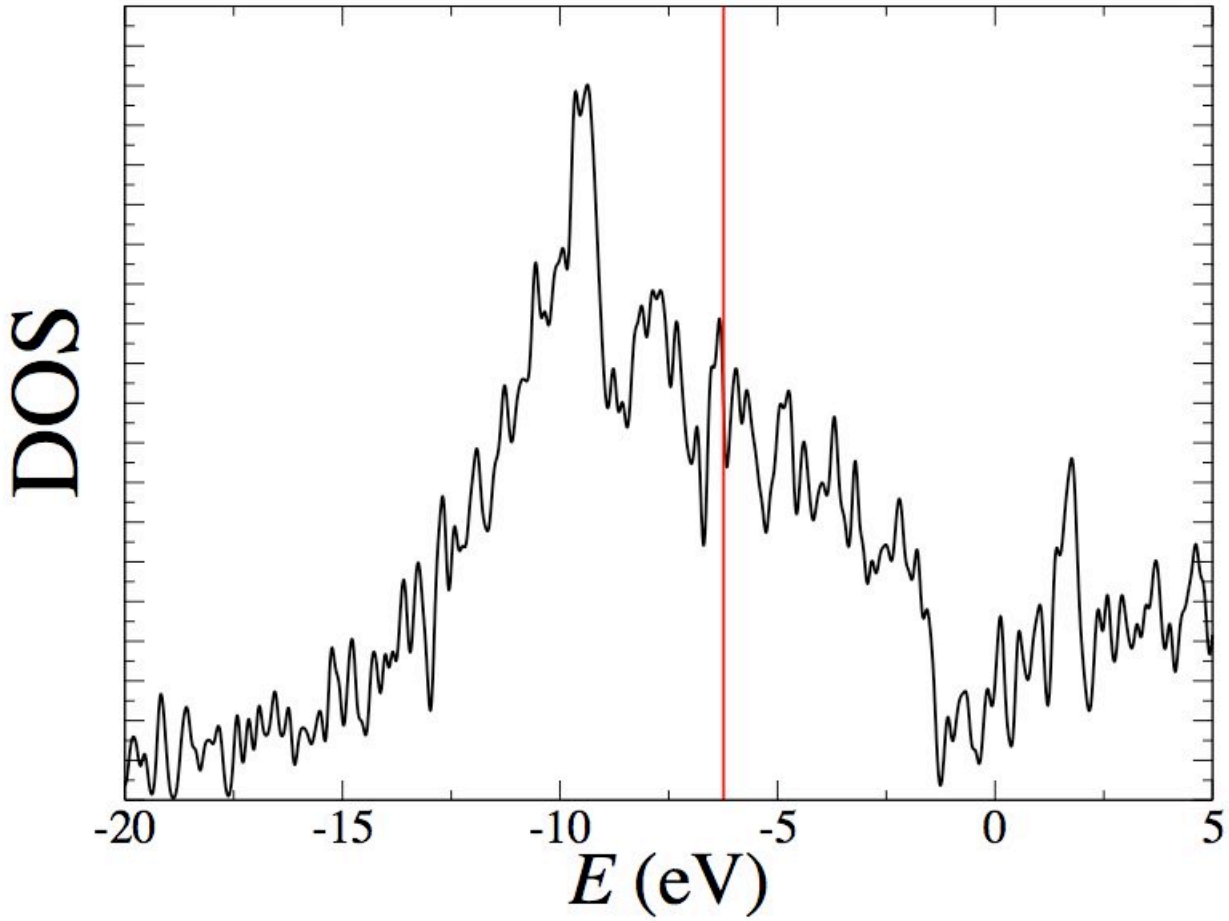
DNA Transport

I-V curve



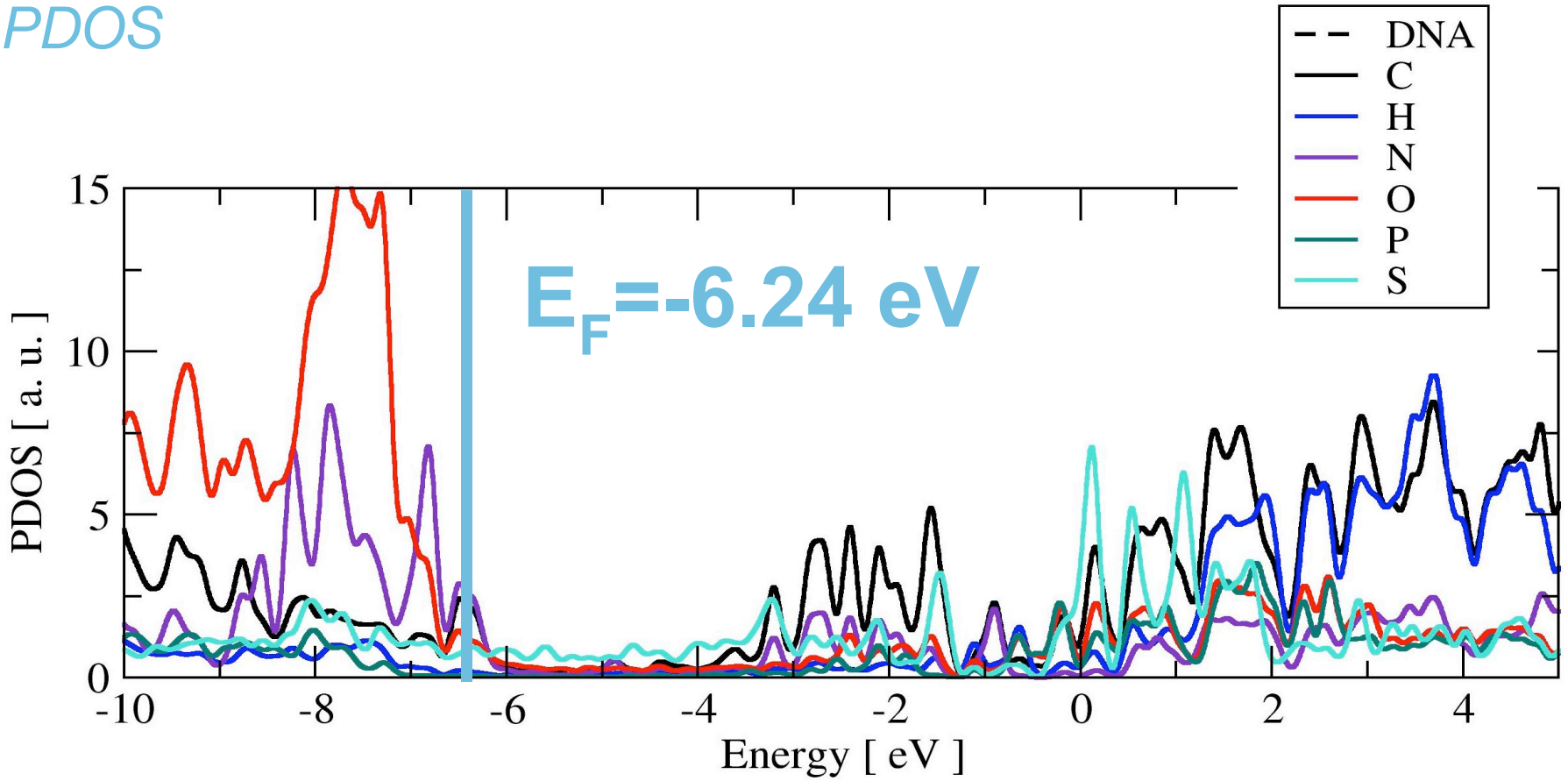
DNA Transport

DOS



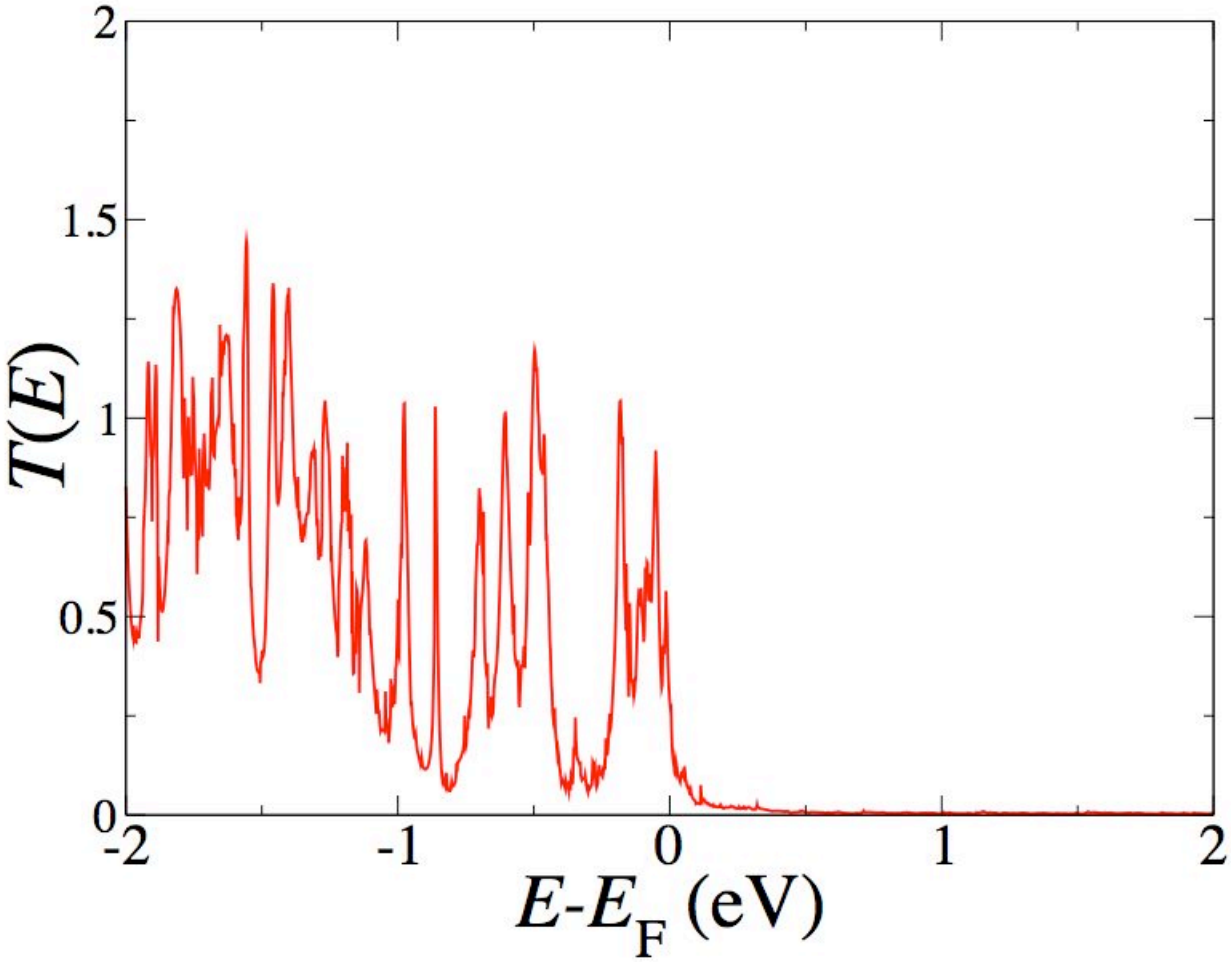
DNA Transport

PDOS



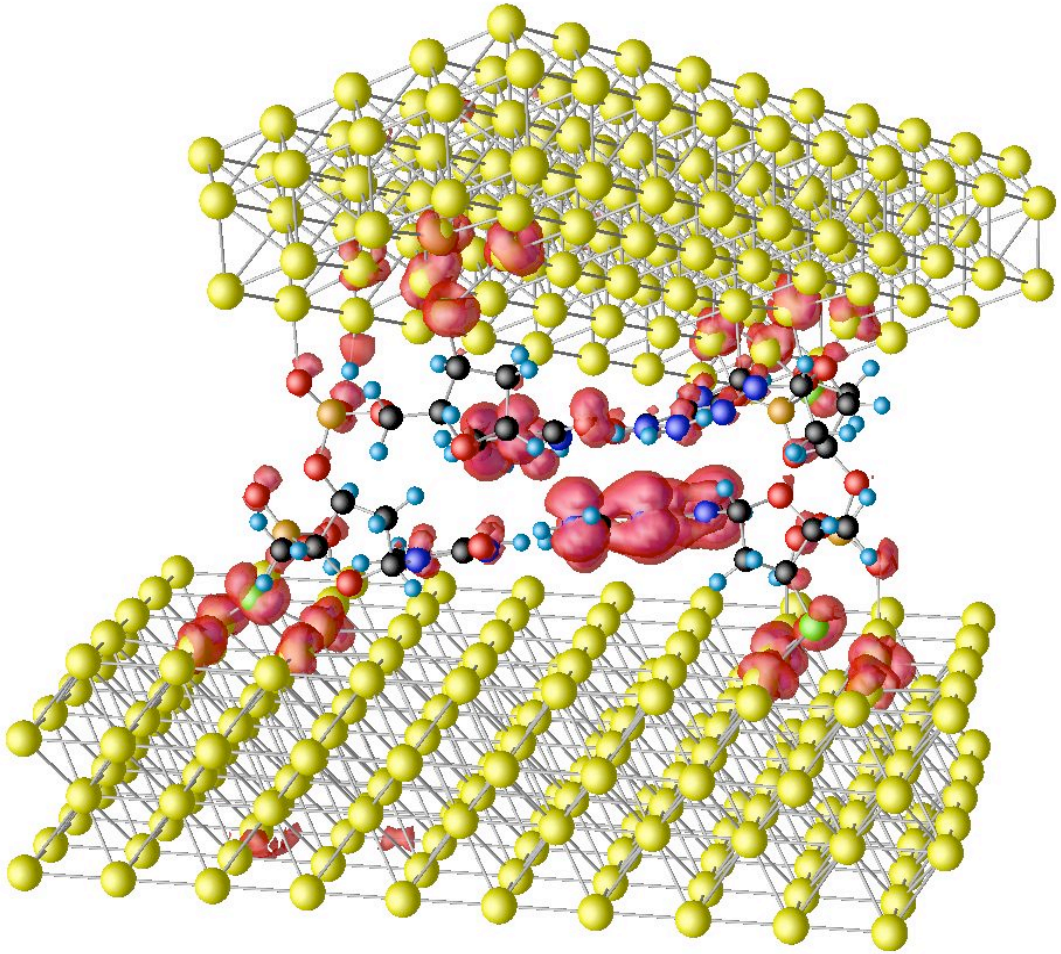
DNA Transport

T(E)



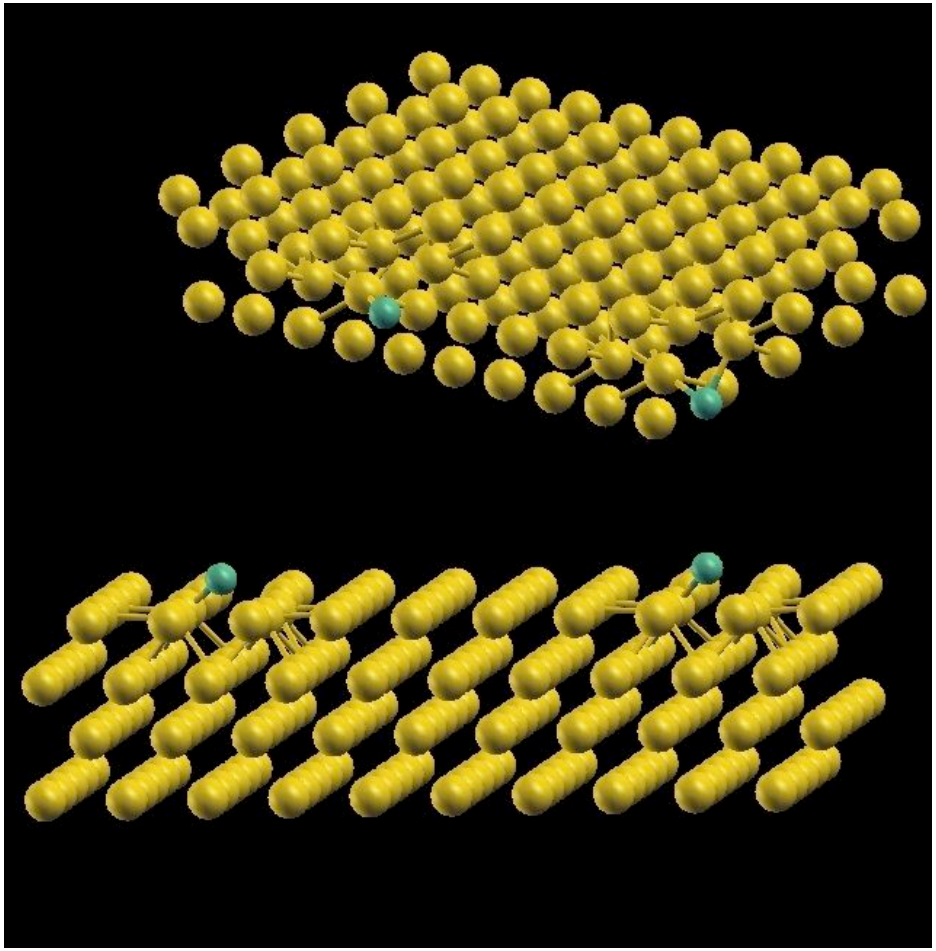
DNA Transport

LDOS

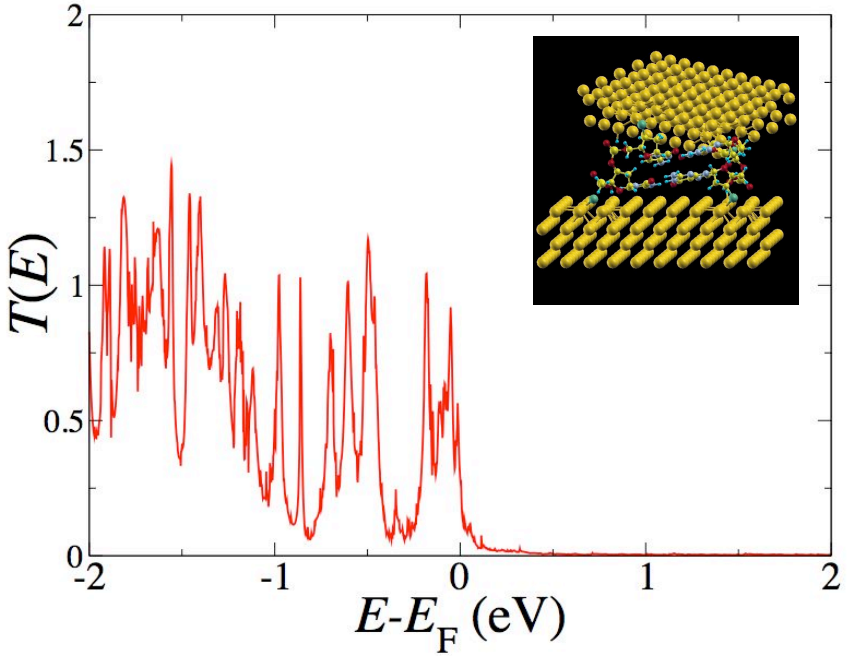


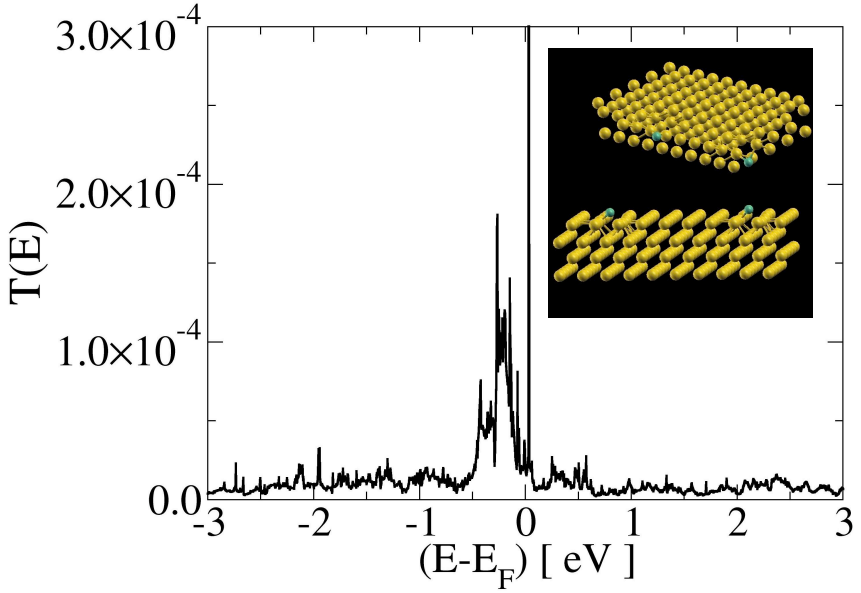
DNA Transport

Remove the DNA



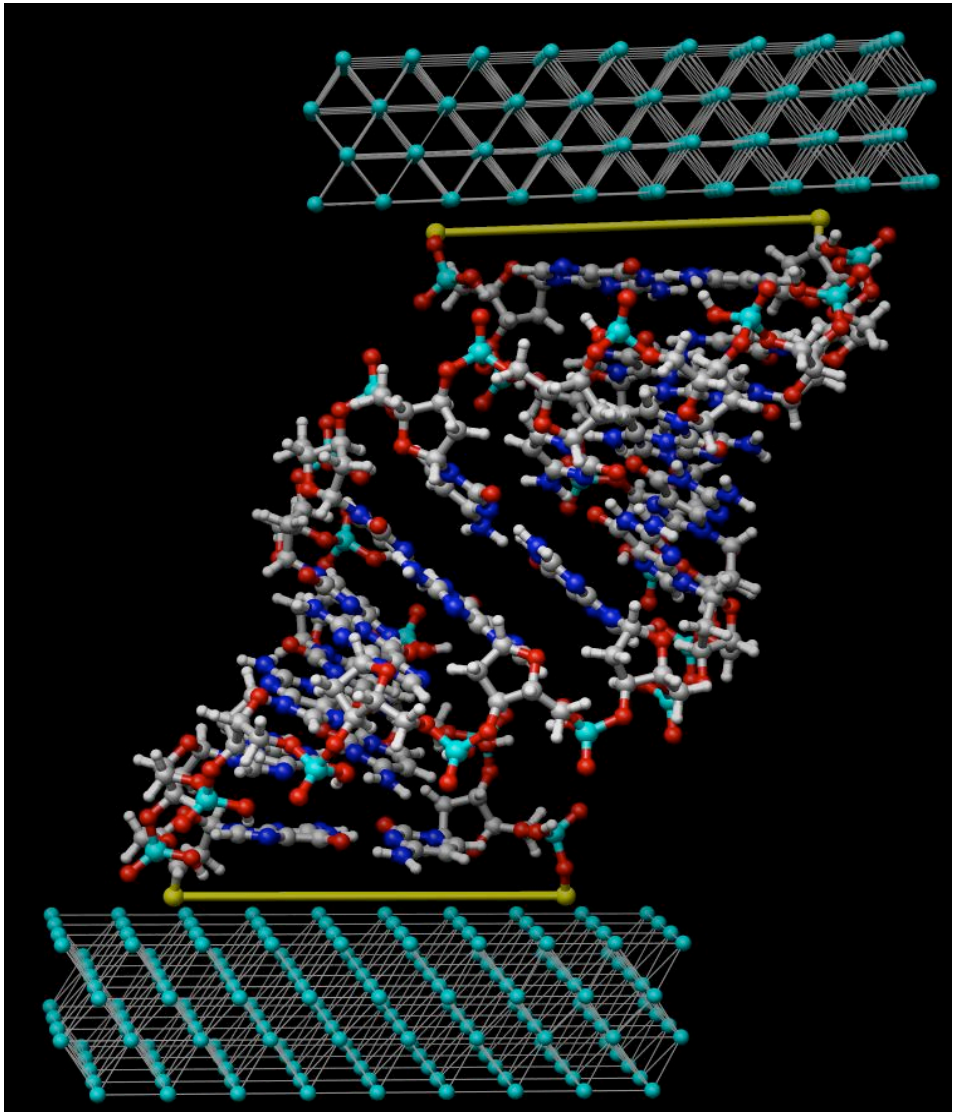
DNA Transport





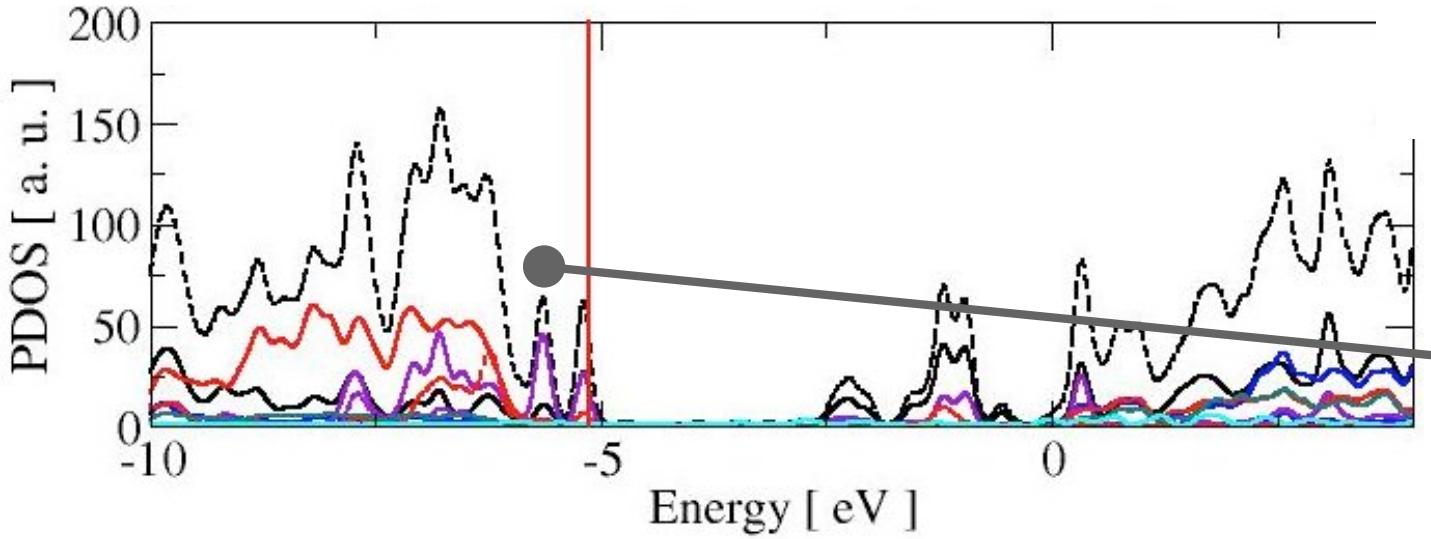
DNA Transport

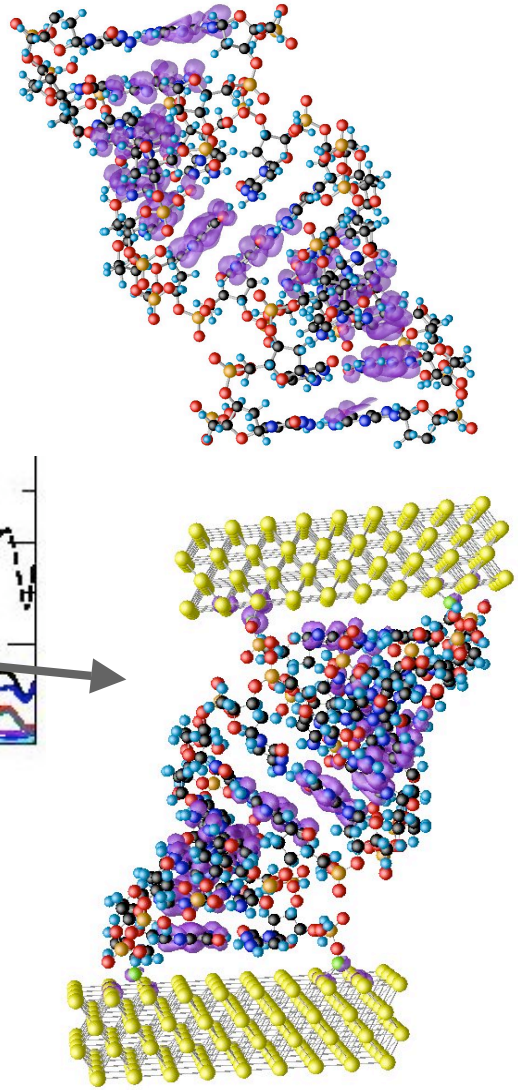
- *About 1,800 atoms in the simulation*
- *Fully RELAXED structure*



DNA Transport

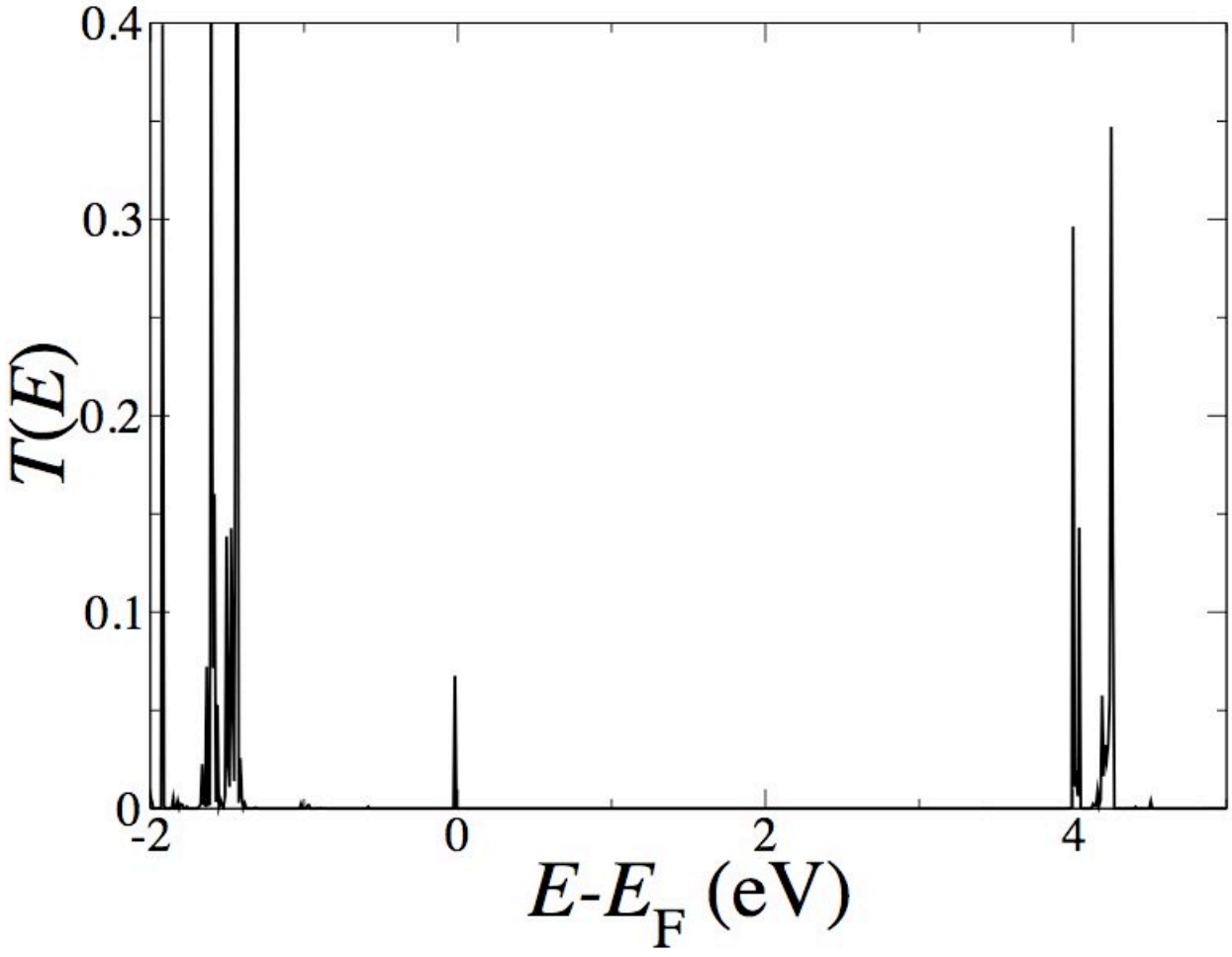
PDOS & LDOS





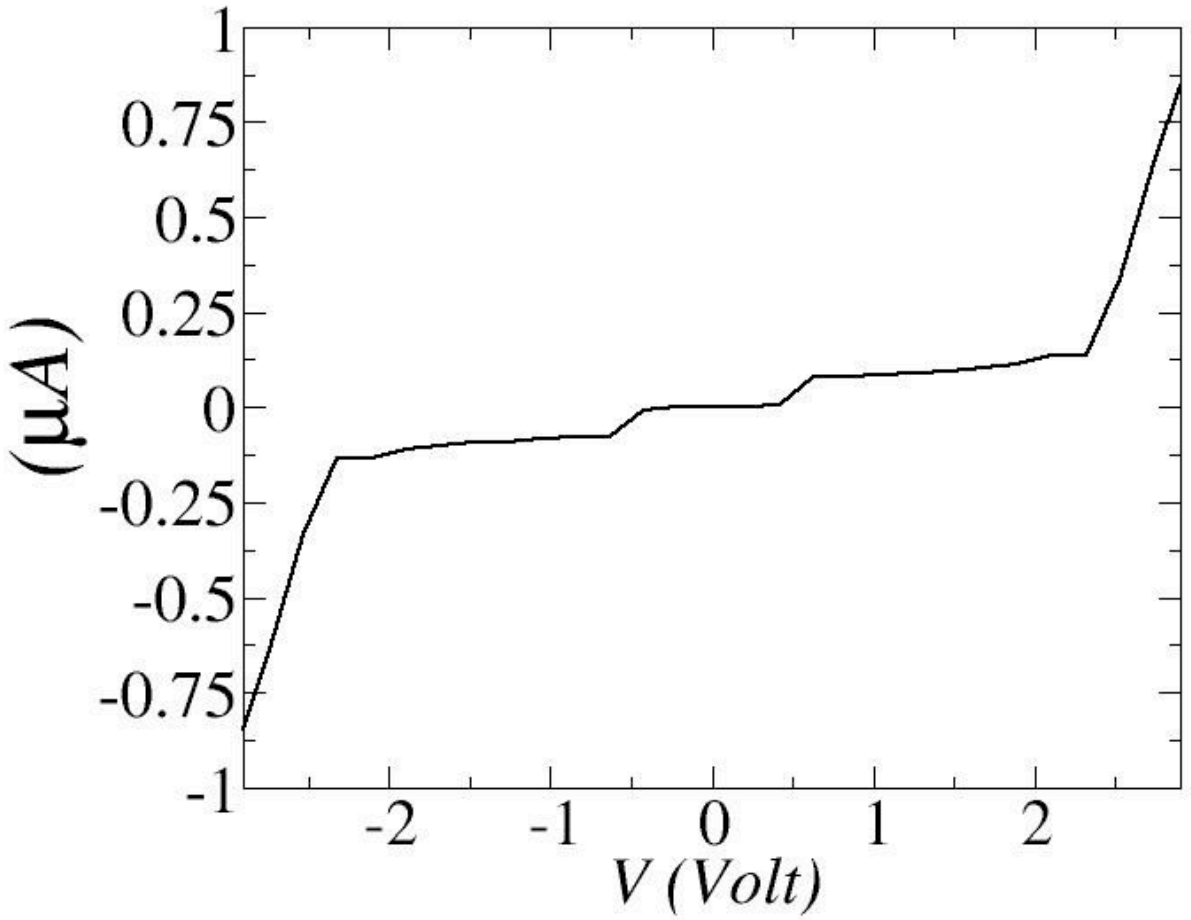
DNA Transport

T(E)



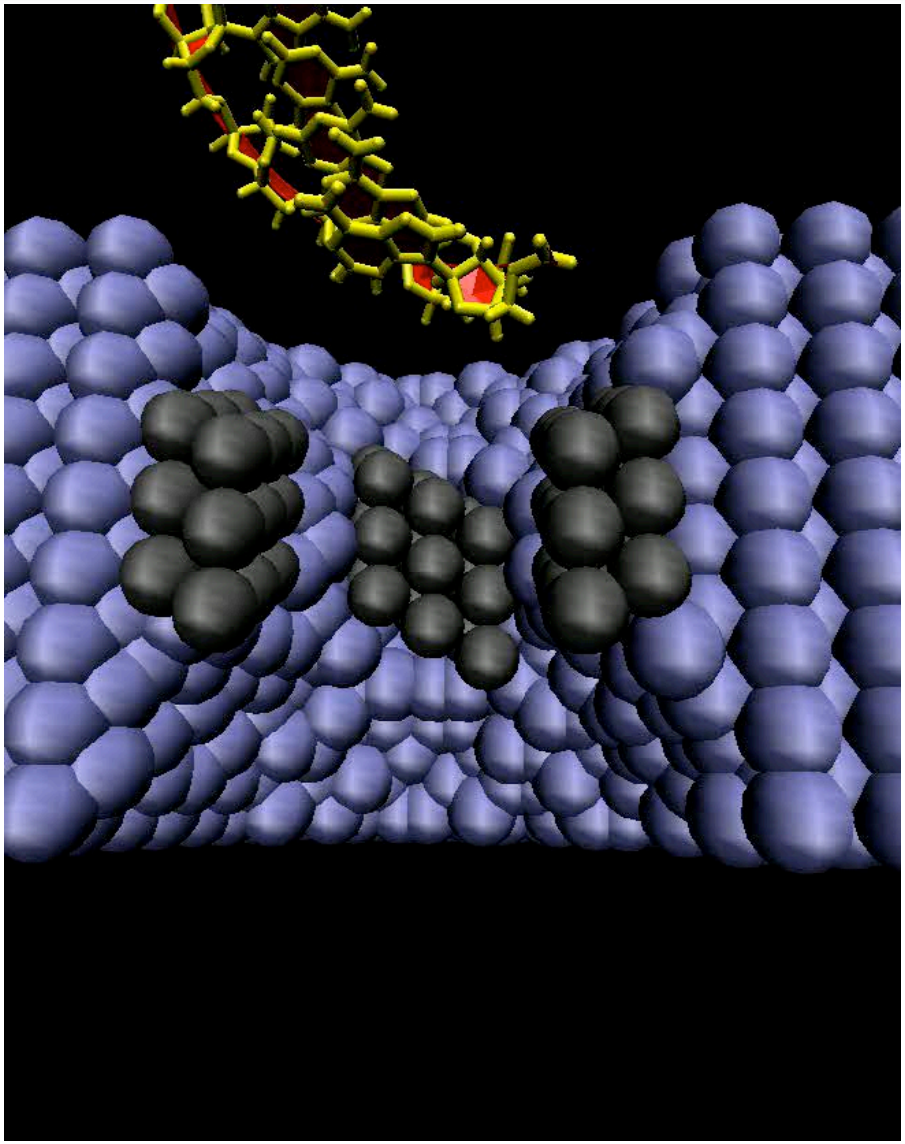
DNA Transport

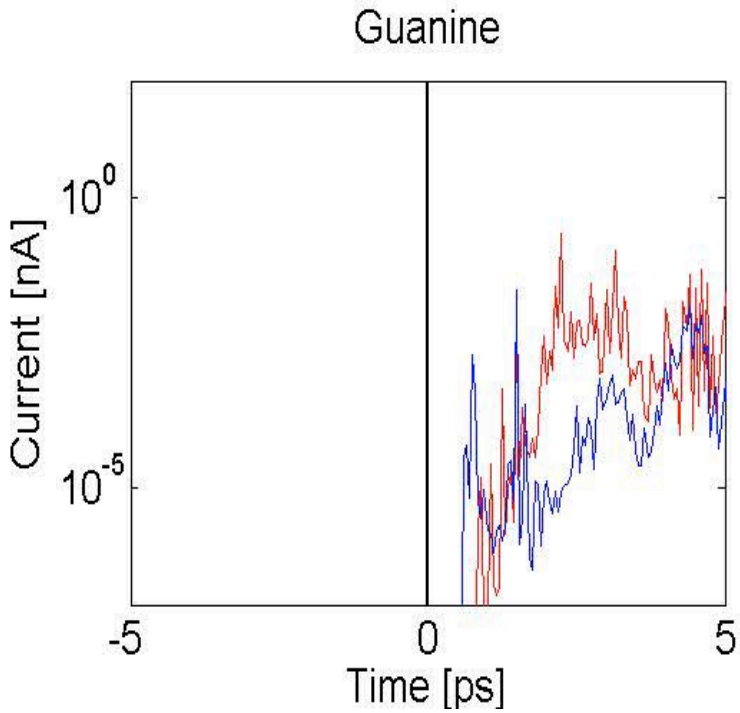
I-V Curve



DNA Sequencing

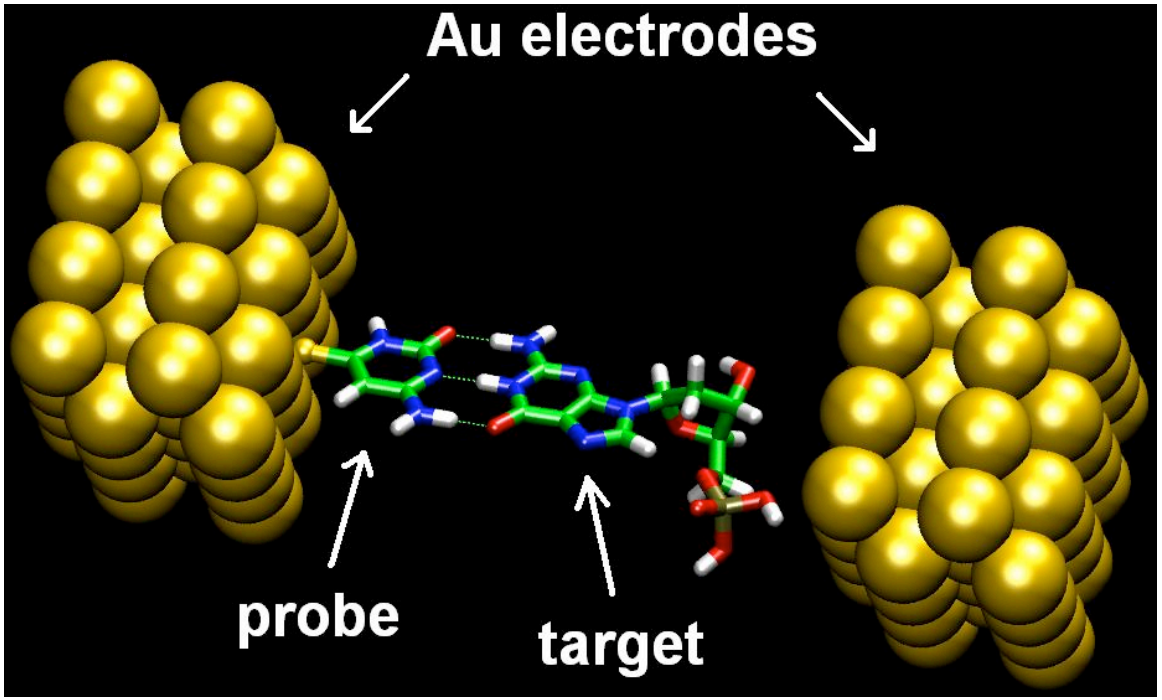
DNA Sequencing



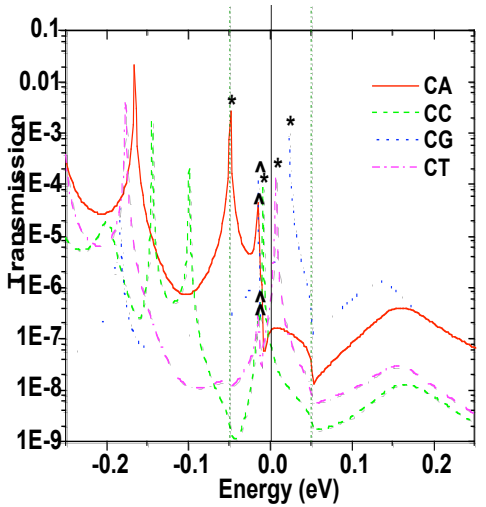


J. Langerqvist et at., Nano Lett. **6**, 779 (2006)

DNA Sequencing



Protocol for DNA sequencing



Probe\Bias	100 mV	250 mV	E_b
A	(A, C, G) from T	A from (C, G) from T	(A, C) from (G, T)
C	(A, G) from (C, T)	A from G, C from T	(A, C) from T from G
G	(A, C, G) from T	(A, C, G) from T	G from (A, T) from C
T	(A, C, G) from T	C from (A, G) from T	-

with Ravindra Pandey (MTU, USA), J. Phys. Chem. (in press)

Outlook: the challenges

More Accurate

Orbital-dependent functionals

- Full derivative discontinuity
- NEGF using orbital densities
- Practical ways: OEP

Scalable

Smeagol10K & *Smeagol100K*

- Downfolding low and high spectrum
- Embedding methods
- Self-consistent minimal basis sets
- Sparse matrix technology