

CYBERNET SYSTEMS CO., LTD.

Emergence of a Spin Filter Effect by inserting Fe Element at CNT Nano-contact: Analysis by *Ab Initio* Calculation

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System

Transport direction →

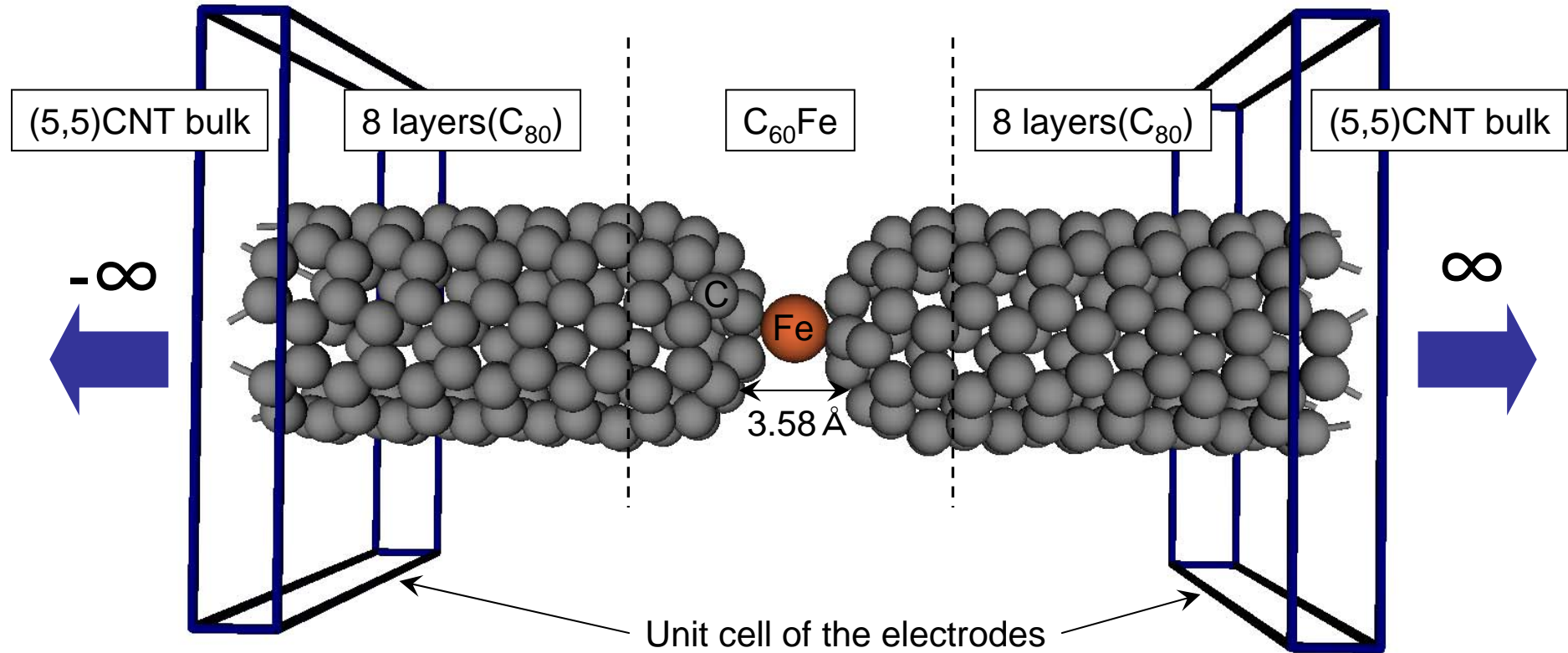


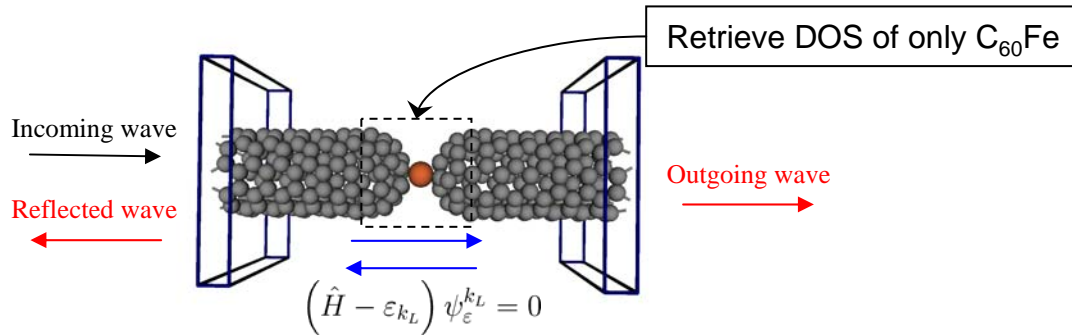
Fig. 1: Input structure used for the calculation.

- (5,5)CNT electrodes are semi-infinite
- The structure of $C_{60}Fe$ in central region is obtained by the relaxed calculation

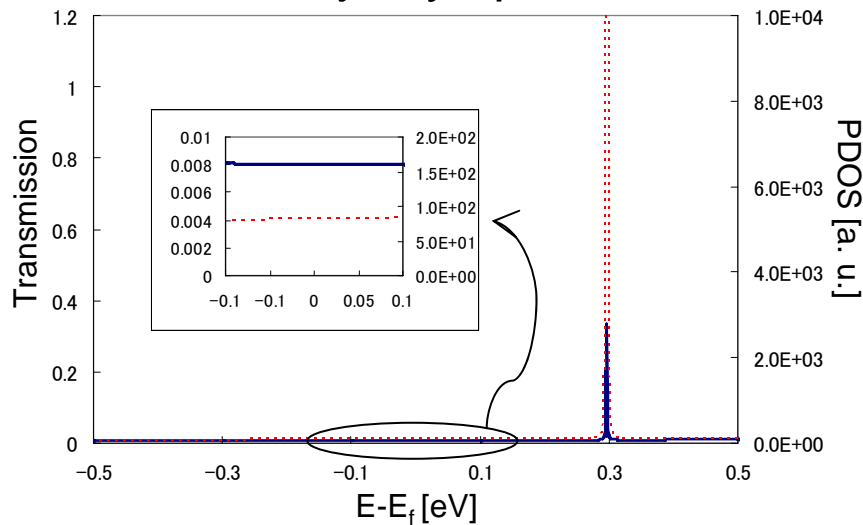
DFT parameters

- **basis set**
 - Single- ζ Polarized
- **XC functional**
 - LSDA.PZ
- **mesh-cut off**
 - 150 Ry
- **k-points sampling**
 - (1 ,1, 100)

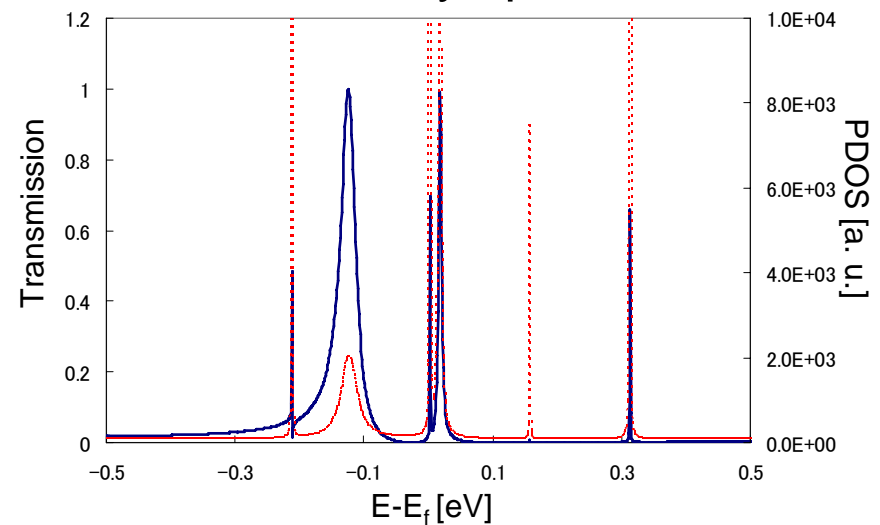
Transmission and PDOS on C₆₀Fe



majority spin



minority spin

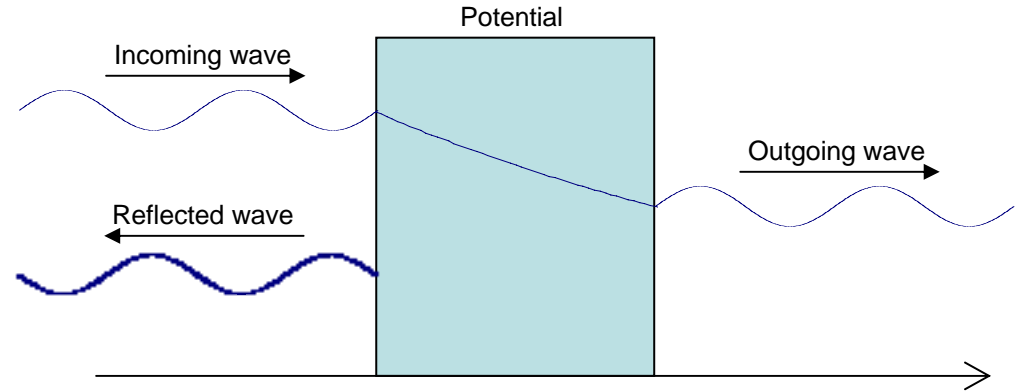


Transmission (blue solid line) and PDOS on C₆₀Fe (red dot line)

Spin-dependent Transport properties

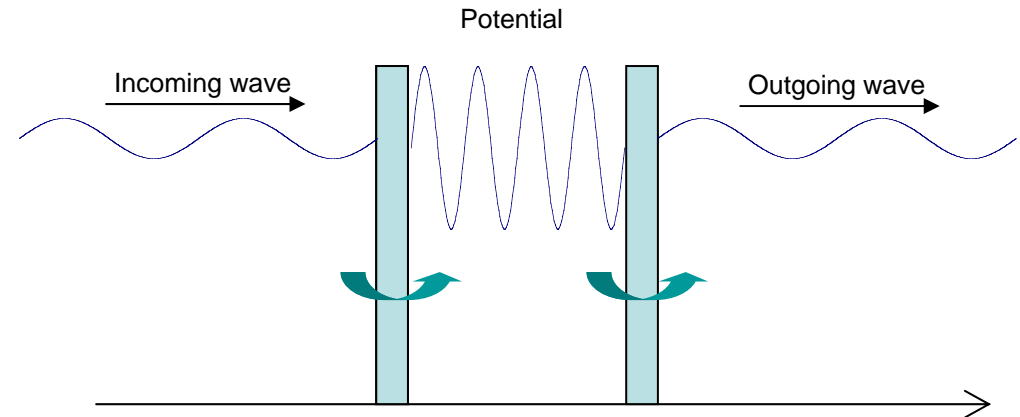
majority spin: Tunneling

There are no interface states around fermi energy

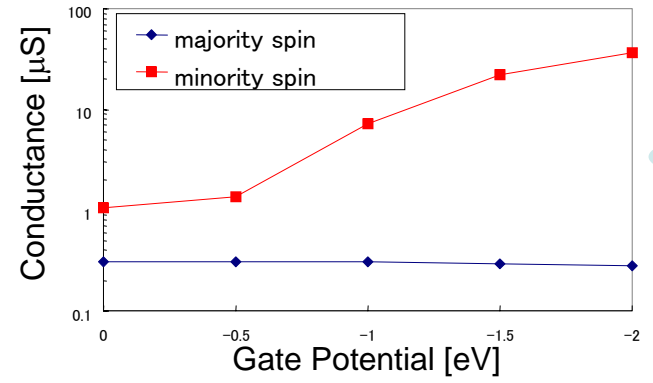
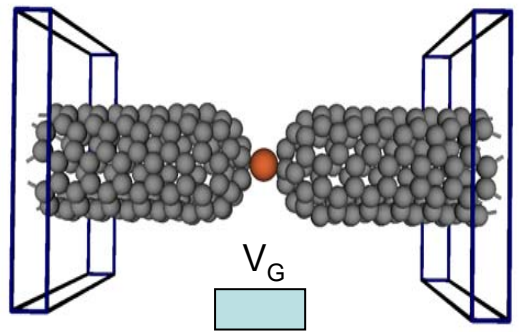


minority spin: Resonant

Resonant scatterings though interface states dominate transmission



Gate-dependence of transmission

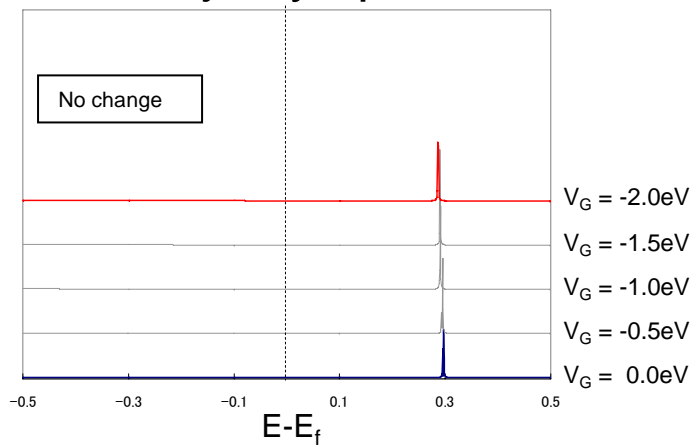


Only minority can be changed

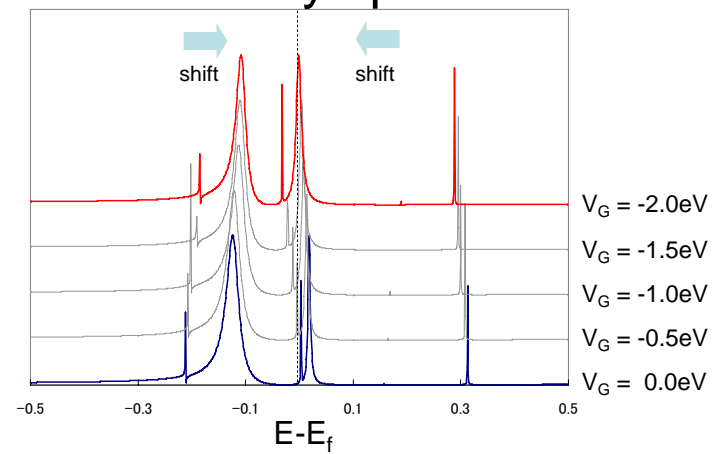
⇒ control of spin-filter

0-bias conductance vs. gate potential

majority spin



minority spin



Transmission under each gate potential

Conclusion & future work

- Conclusion
 - Spin-dependent transport properties
 - majority spin: Tunneling
 - minority spin: Resonant scattering
(minority spin dominates conductance at low bias)
 - Spin-filter property is controllable by gate voltage
- Future work
 - Finite bias calculation
 - Distance between electrodes
 - etc