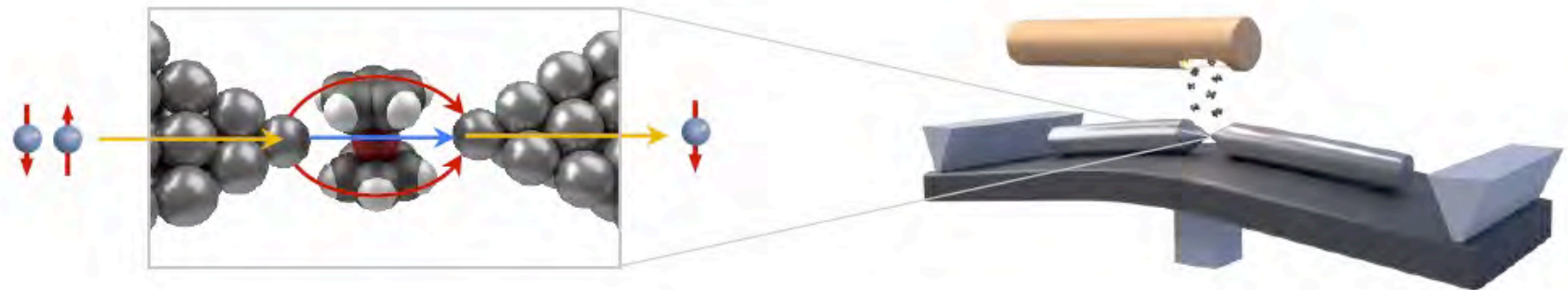


Nonmagnetic spin filter based on single molecular junction

Atindra Nath Pal

S. N. Bose National Centre for Basic Sciences, Kolkata



Nature Comm. **10**, 5565 (2019)

WEIZMANN
INSTITUTE
OF SCIENCE

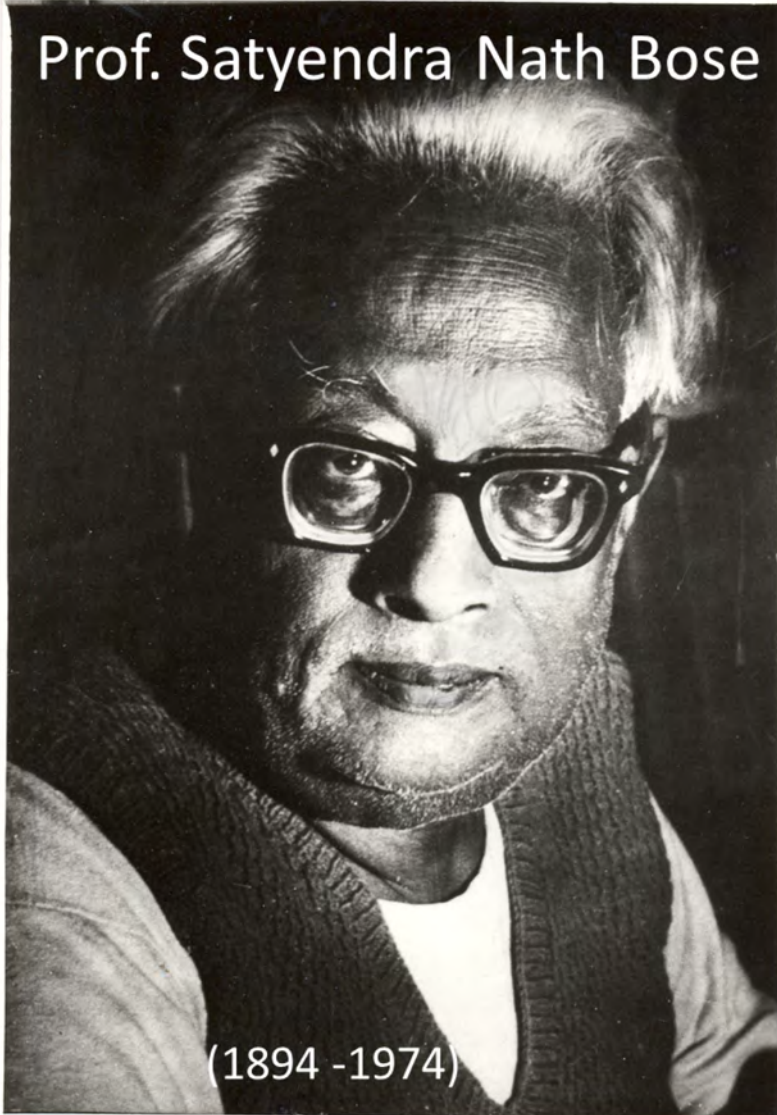


SPICE-Molecular Electro-Opto-Spintronics
Mainz, 15th – 18th October, 2019



S N Bose National Center for Basic Sciences, Kolkata

Prof. Satyendra Nath Bose

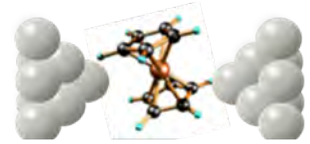


SNNCBS (32 years old)

Today's Plan

- Introduction
- Mechanically Controllable Break Junction (MCBJ)
- Shot Noise: Detecting Spin transport
- Conductance and Shot noise in single molecular junction
- Results & Discussion
- Conclusion
- Group activities

Spin transport at the limit of atomic scale



- What is the **smallest component** that can control spin transport?
- Can we **identify general concepts** that will allow efficient control over spin transport at the atomic scale?

Motivation

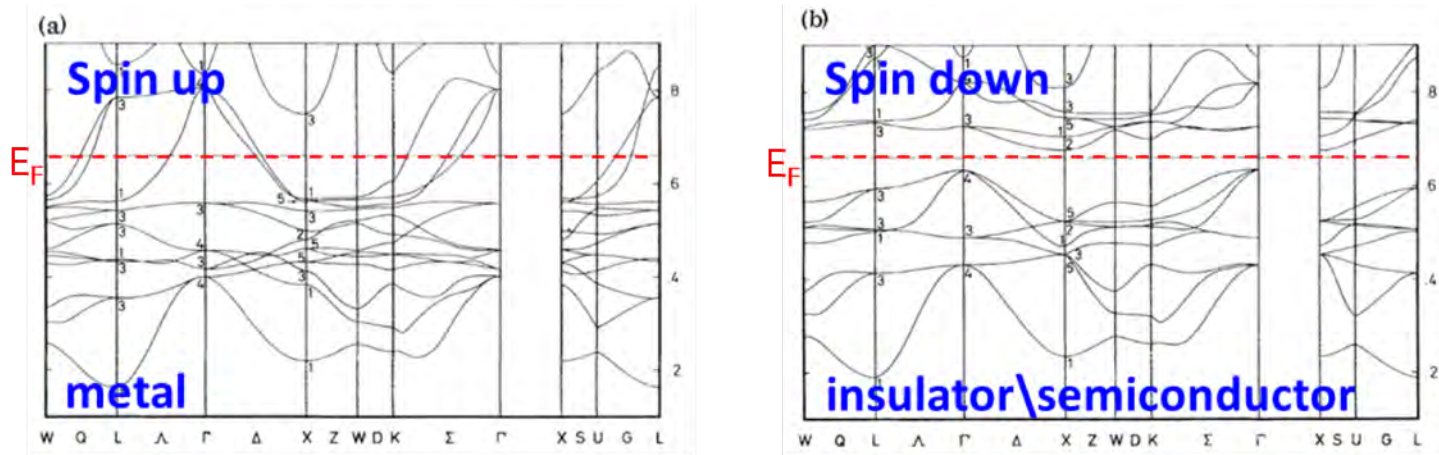
Spintronics: manipulations of electronic spin currents for electronics and spin transport physics

The most general requirement of spintronics:
high spin polarised current

Current spin polarisation:

$$P_I = \frac{I_{\uparrow} - I_{\downarrow}}{I_{\uparrow} + I_{\downarrow}}$$

Half Metals - Ideal candidate

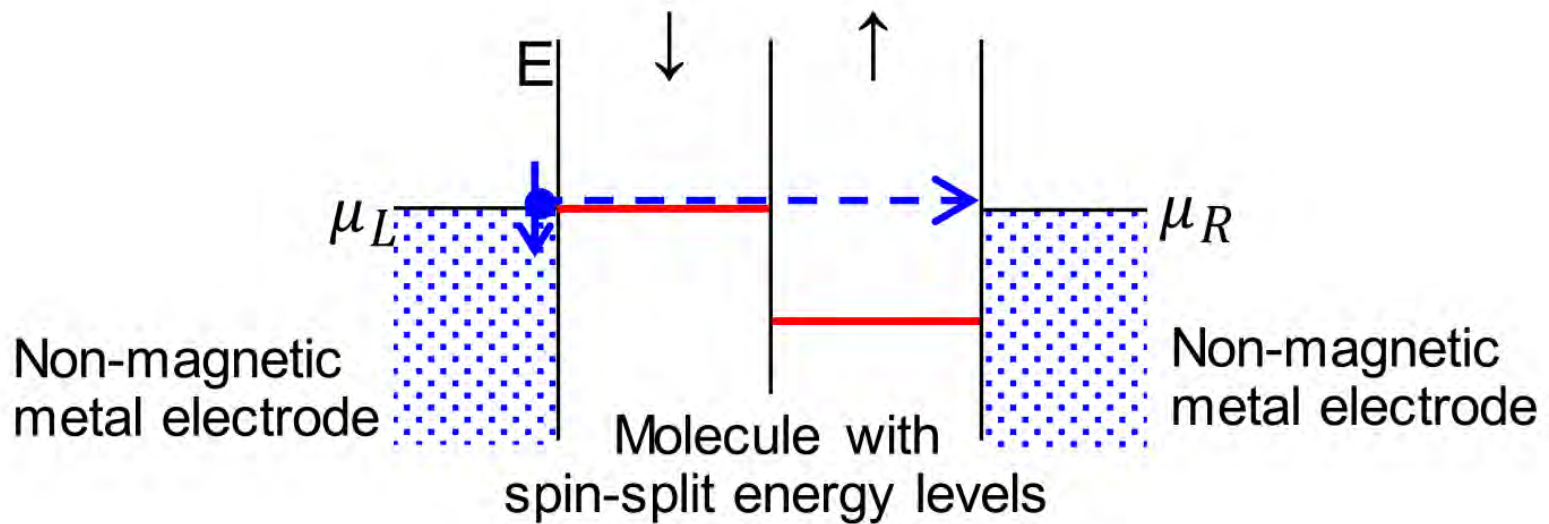


NiMnSb band structure: de Groot, R. A., Mueller, F. M., van Engen, P. G. & Buschow, K. H. J. *Phys. Rev. Lett.* 50, 2024 (1983)

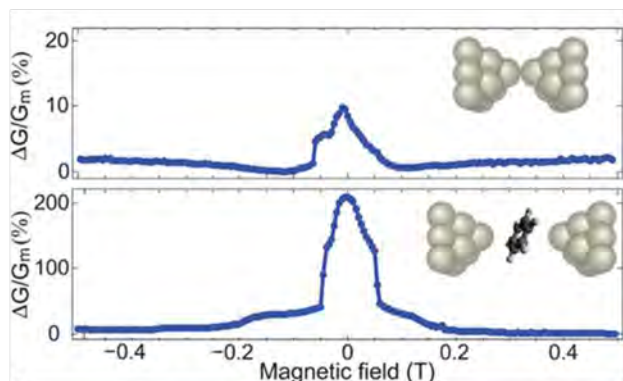
Ideal half metals are ideal materials for spintronics

Full spin polarization of the conducting electrons

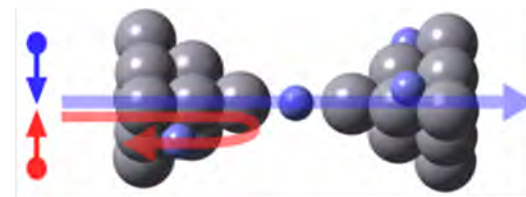
Goal: molecular scale half metallicity



Enhanced magnetoresistance



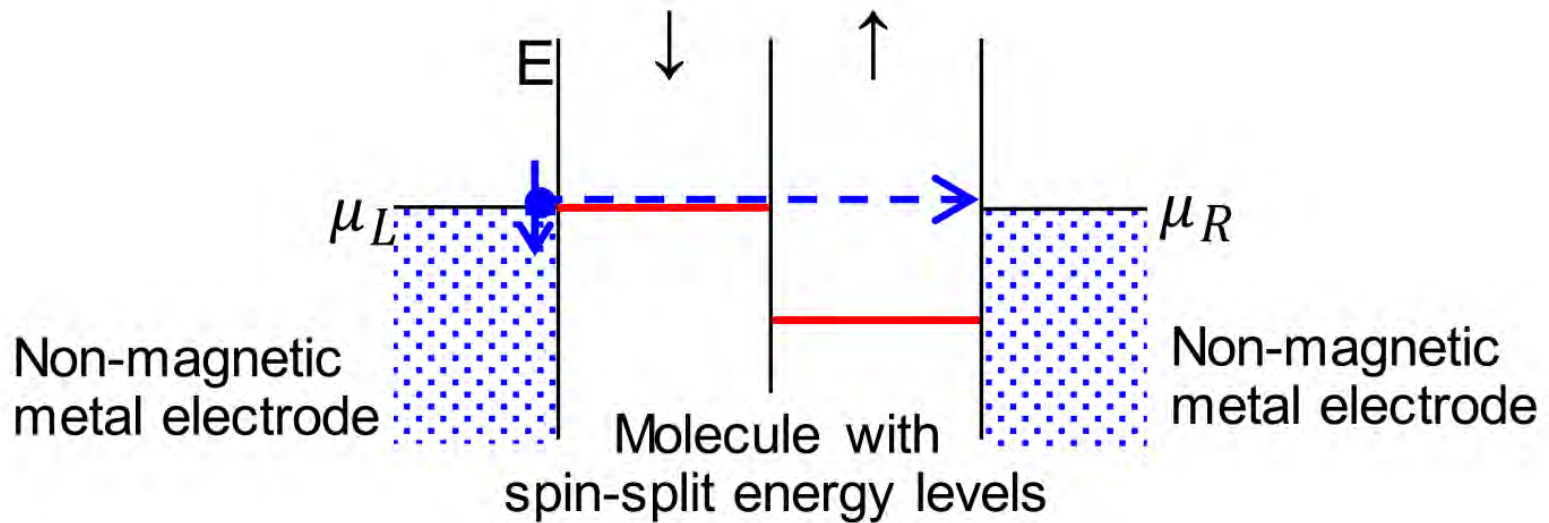
Ni – Benzene - Ni



Complete spin filtering in Ni - O - Ni junction

Vardimon, R; Klionsky, M; Tal, O; Nano Letters. **15**:3894-3898

Goal: molecular scale half metallicity

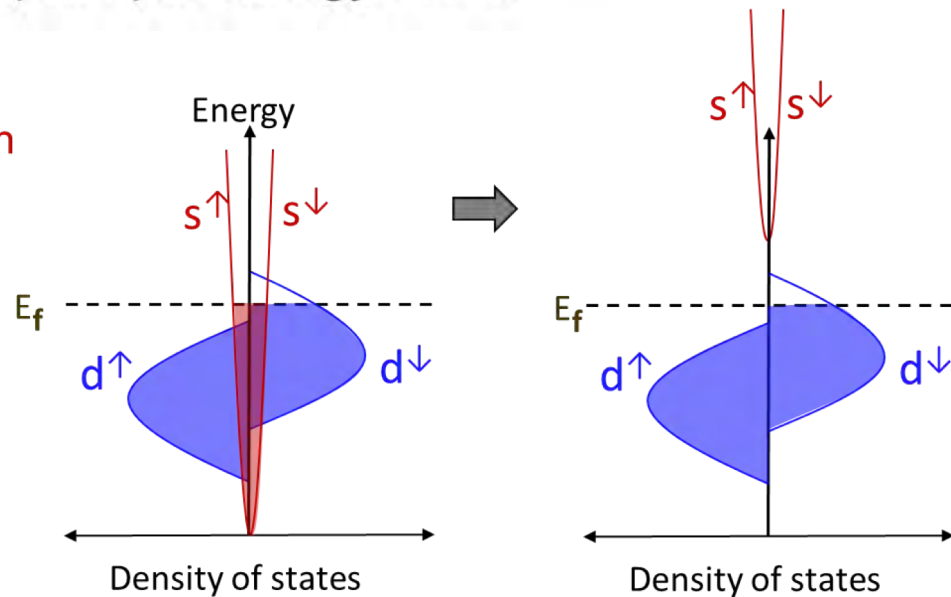


s orbitals:

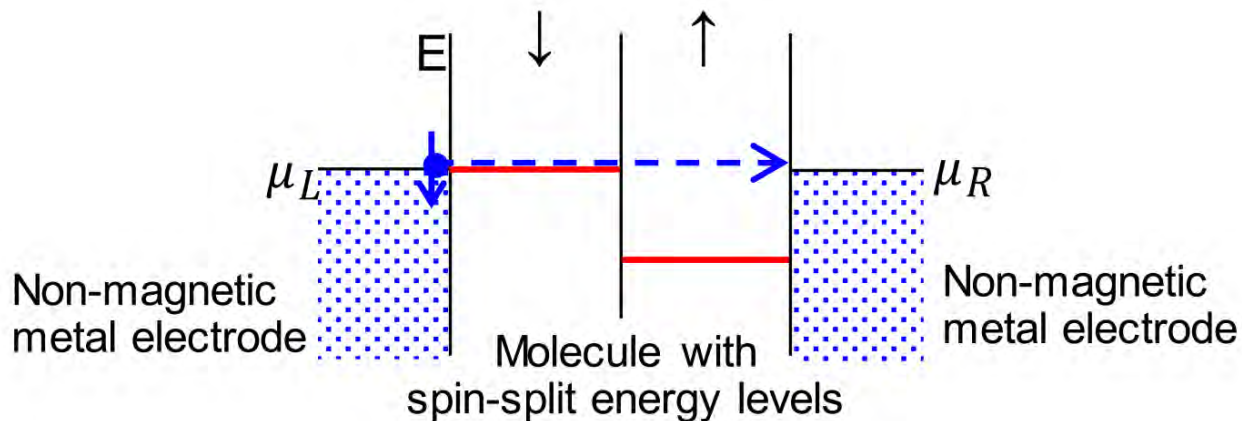
Small spin polarization
but high conductance

d orbitals:

spin polarized but
low conductance



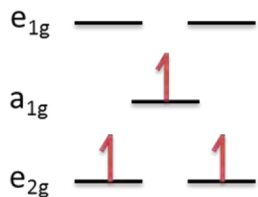
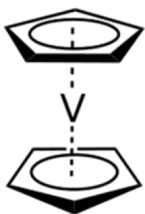
Goal: molecular scale half metallicity



paramagnetic

Vanadocene (VCp_2)

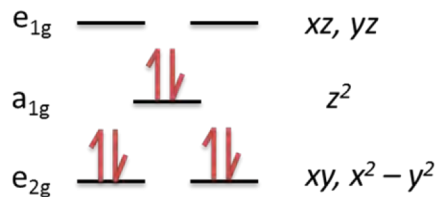
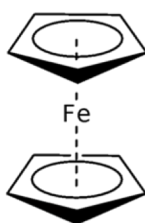
$S \neq 0$



diamagnetic

Ferrocene (FCp_2)

$S = 0$



D_{5d}

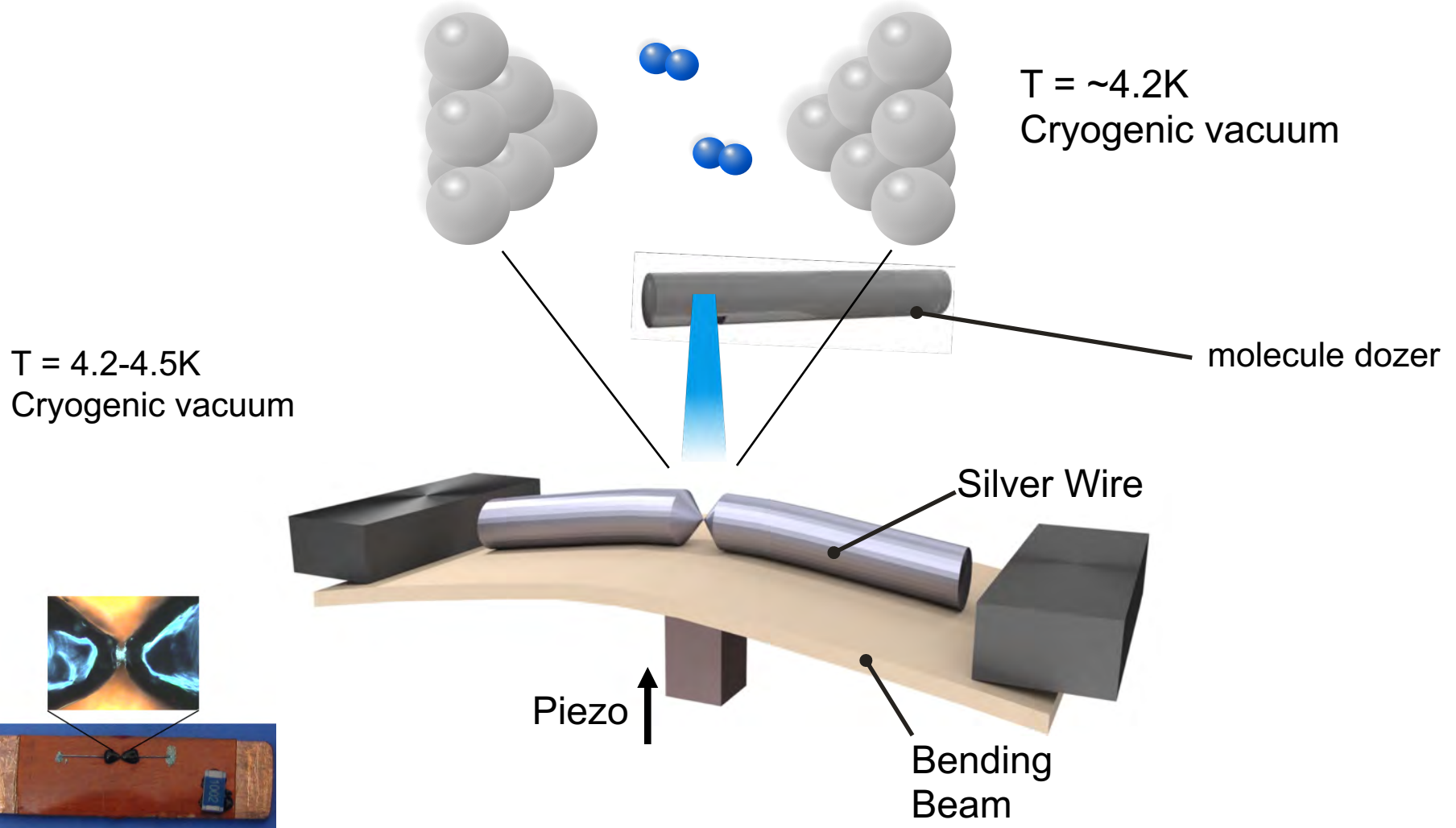
xz, yz

z^2

$xy, x^2 - y^2$

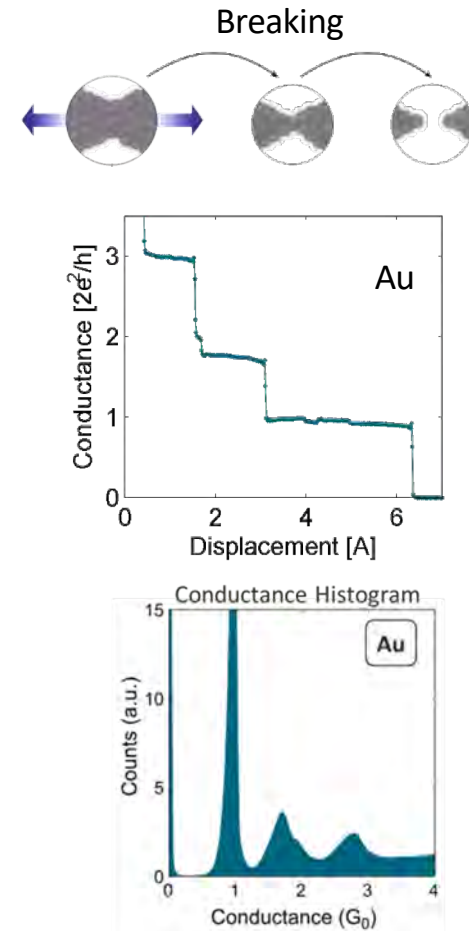
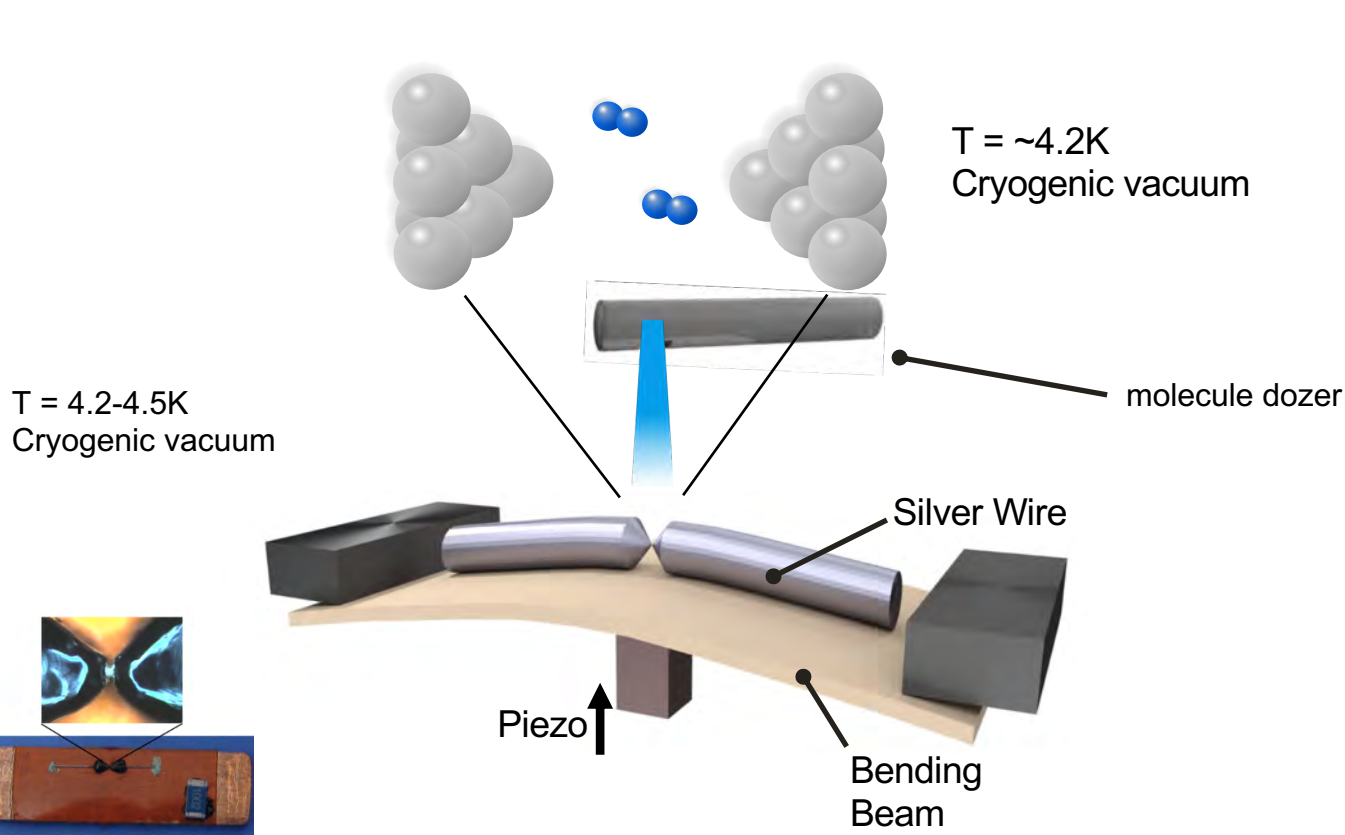
| | | | | | | | | | | | | | | | | | |
|----|----|--------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| 1 | | | | | | | | | | | | | | | | | 2 |
| 3 | 4 | | | | | | | | | | | 10 | | | | | |
| 11 | 12 | | | | | | | | | | | 18 | | | | | |
| 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 | 29 | 30 | 31 | 32 | 33 | 34 | 35 | 36 |
| 37 | 38 | 39 | 40 | 41 | 42 | 43 | 44 | 45 | 46 | 47 | 48 | 49 | 50 | 51 | 52 | 53 | 54 |
| 55 | 56 | 57-71 | 72 | 73 | 74 | 75 | 76 | 77 | 78 | 79 | 80 | 81 | 82 | 83 | 84 | 85 | 86 |
| 87 | 88 | 89-103 | 104 | 105 | 106 | 107 | 108 | 109 | 110 | 111 | 112 | 113 | 114 | 115 | 116 | 117 | 118 |
| 57 | 58 | 59 | 60 | 61 | 62 | 63 | 64 | 65 | 66 | 67 | 68 | 69 | 70 | 71 | | | |
| 89 | 90 | 91 | 92 | 93 | 94 | 95 | 96 | 97 | 98 | 99 | 100 | 101 | 102 | 103 | | | |

Formation of atomic and molecular junctions by mechanically controllable break junction

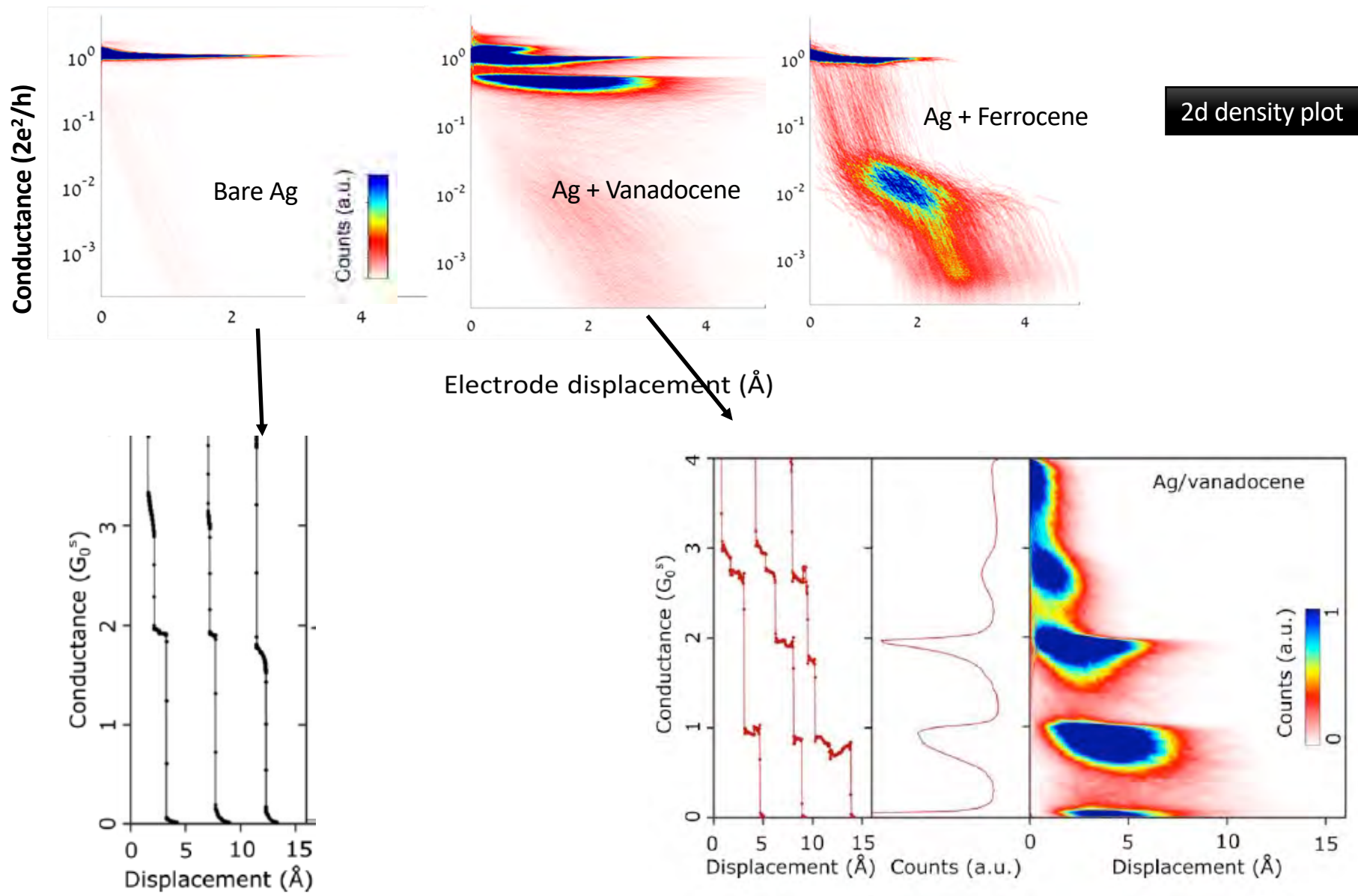


e.g.: T. Yelin, R. Vardimon, N. Kuritz, R. Korytar, A. Bagrets, F. Evers, L. Kronik and O. Tal Nano Letters **13**, 1956 (2013)

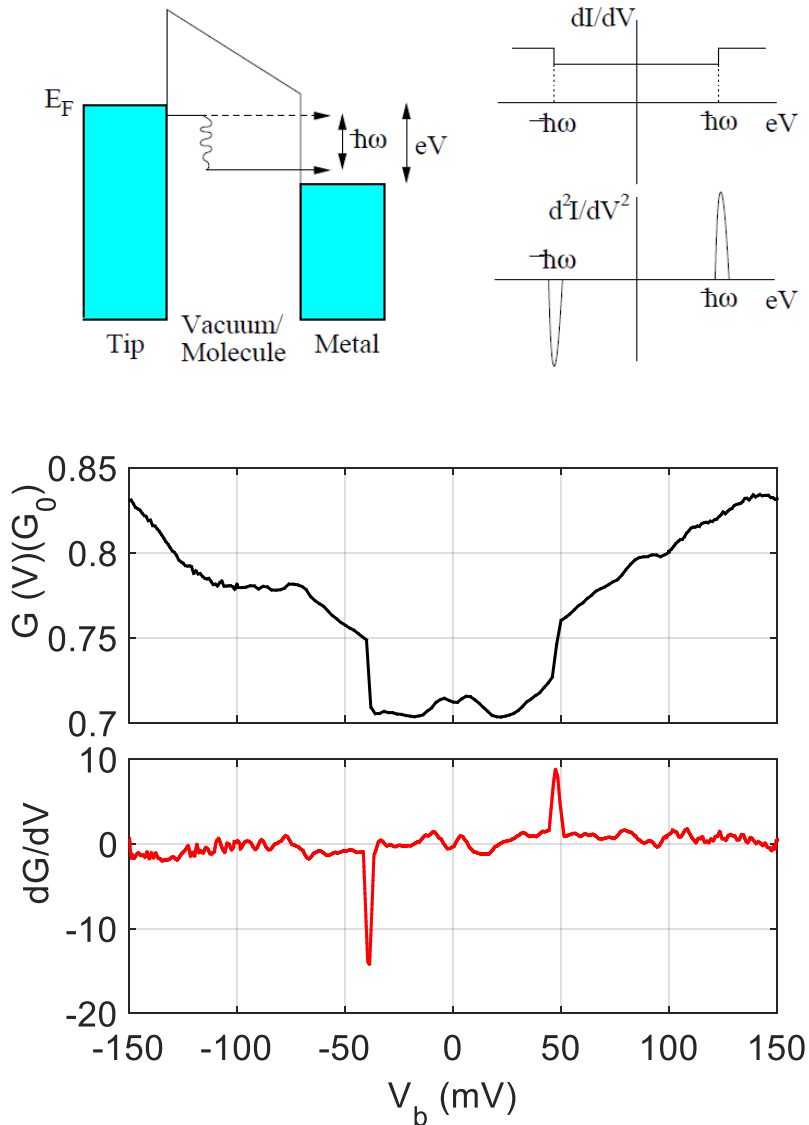
Formation of atomic and molecular junctions by mechanically controllable break junction



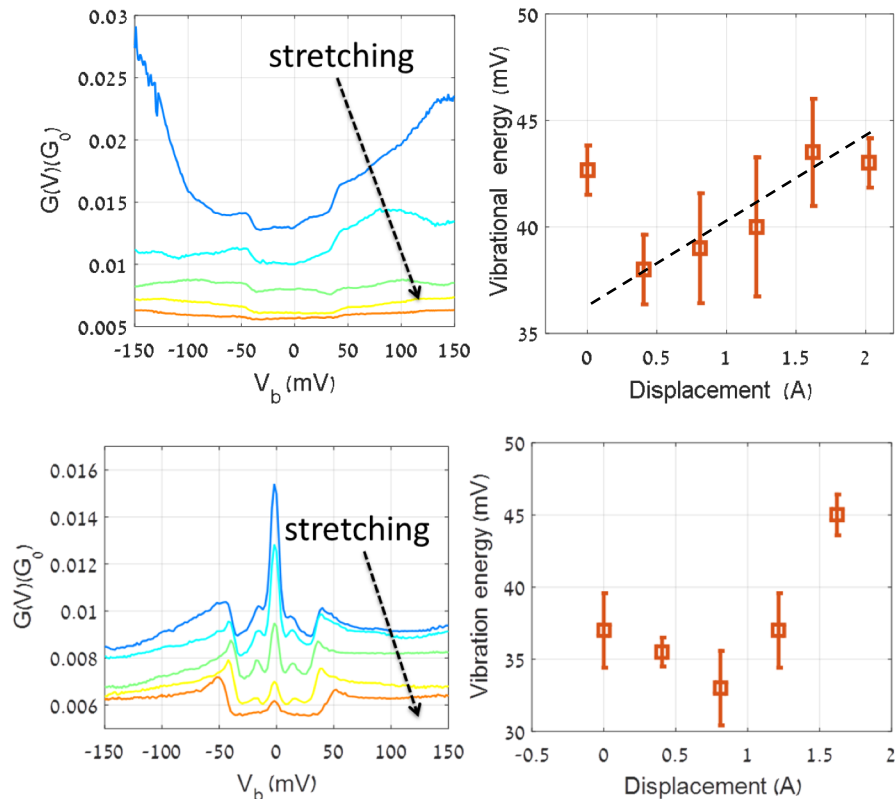
Characterization of metal – molecule – metal junction



Inelastic spectroscopy: vibrational modes

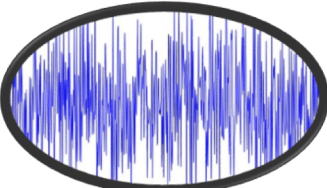


Ag – Vanadocene – Ag junction

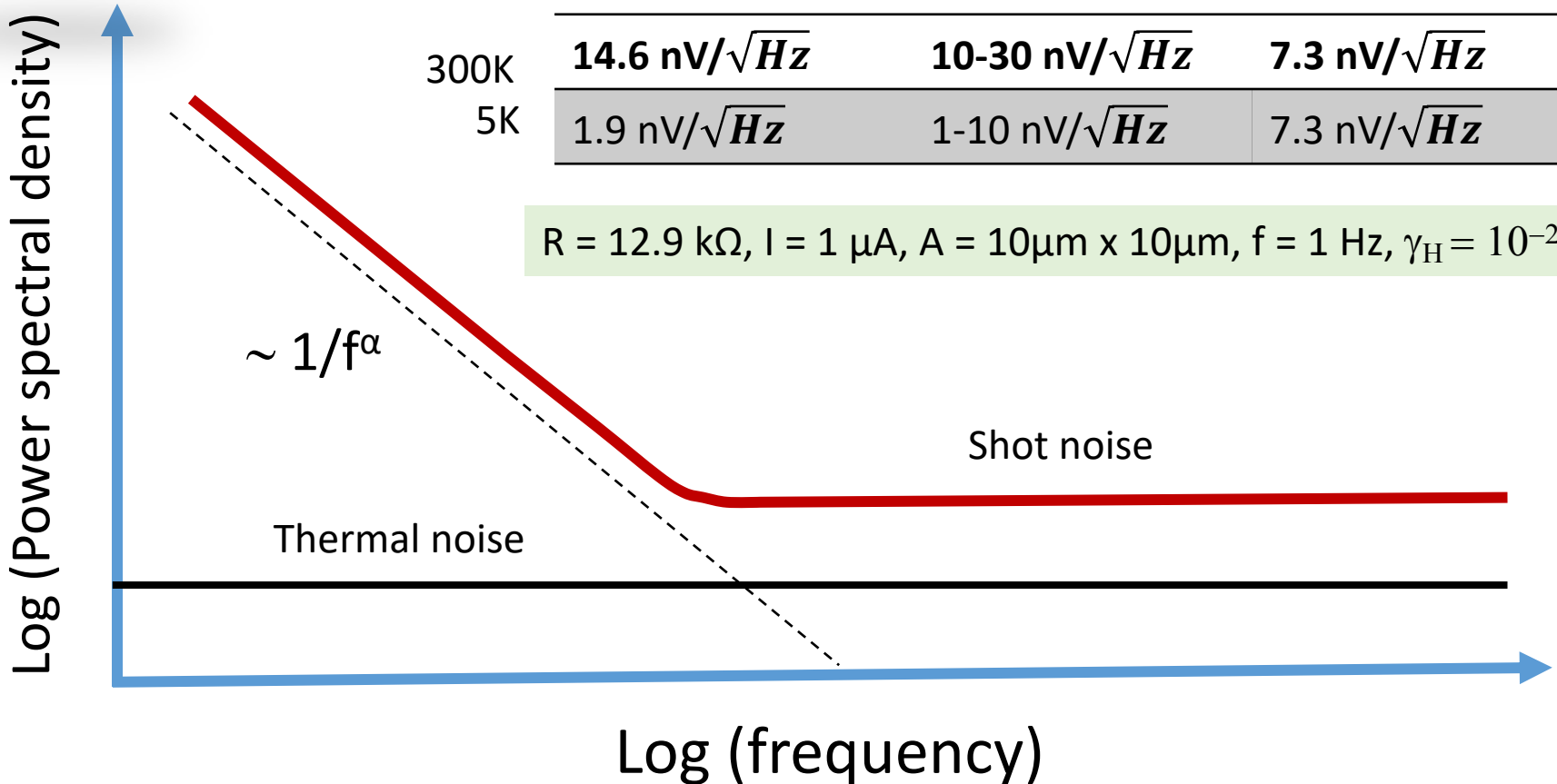


Types of noise

Noise = Thermal noise + 1/f noise + shot noise

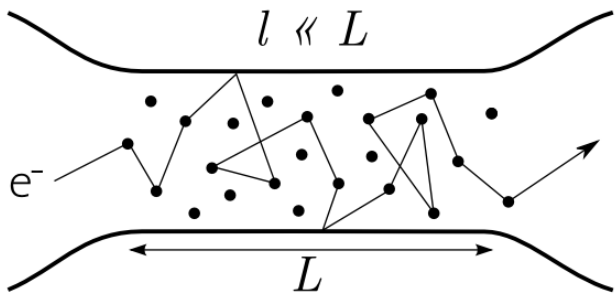


$(4k_BTR)$ Hooe parameter $\gamma_H AV^2/f^\alpha$ Fano factor $2e\langle I \rangle F$



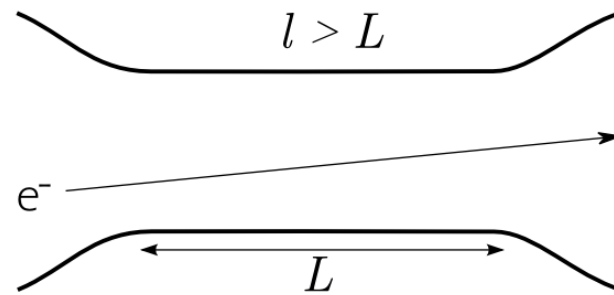
Ballistic Transport

Diffusive



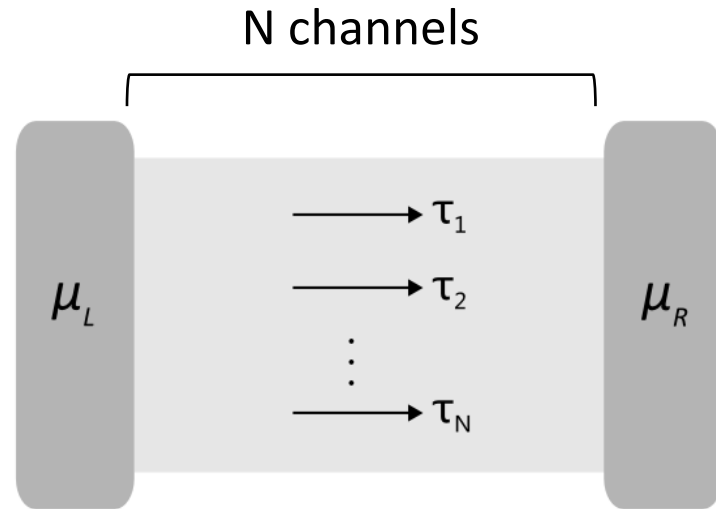
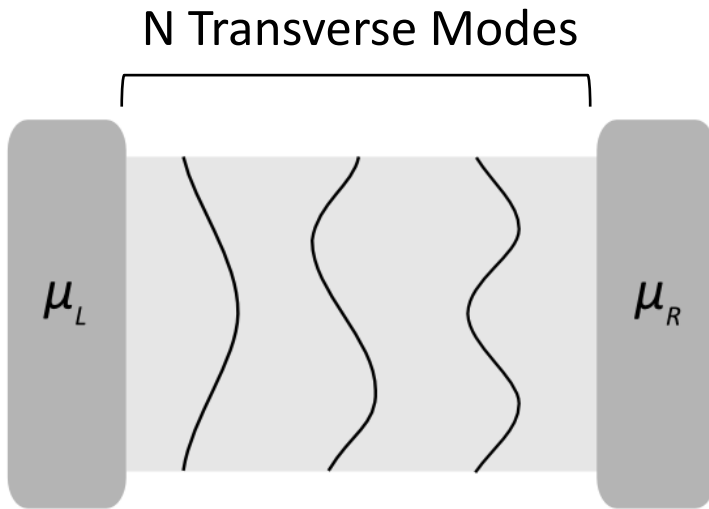
l
| \longleftrightarrow | Mean Free Path

Ballistic



l
| \longleftrightarrow |

Conduction Channels



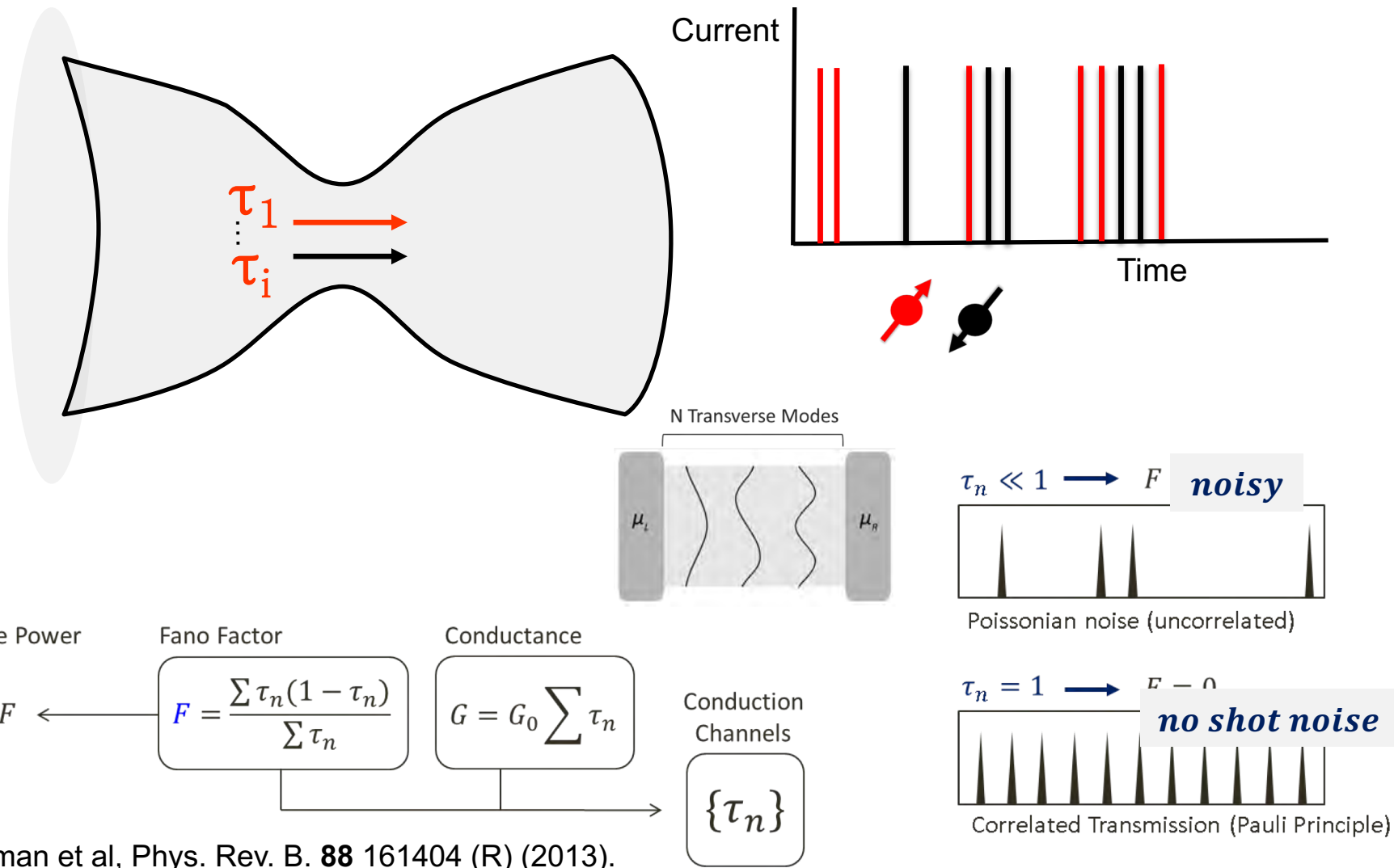
Landauer Formula

$$G = G_0 \sum_{n=1}^N \tau_n$$

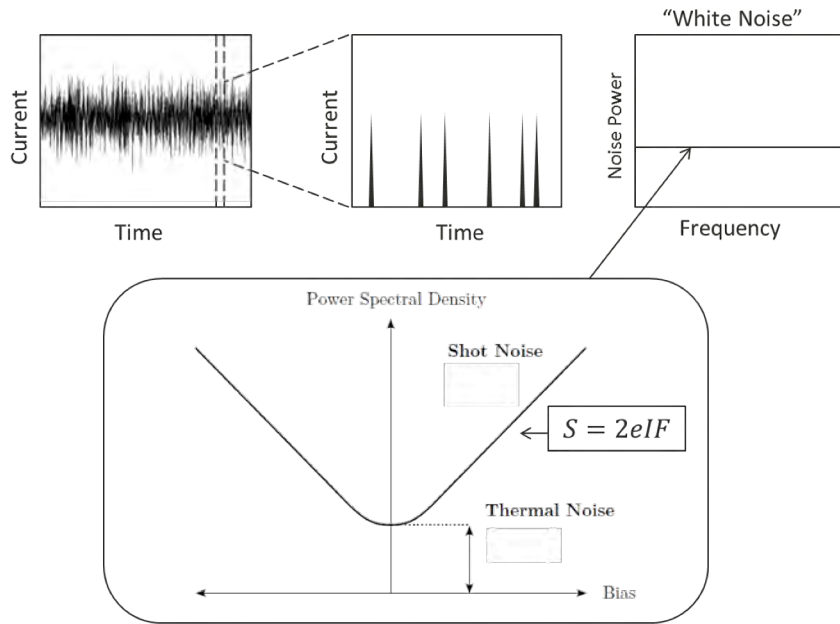
Quantum of conductance

$$G_0 = \frac{2e^2}{h} = (12.9k\Omega)^{-1}$$

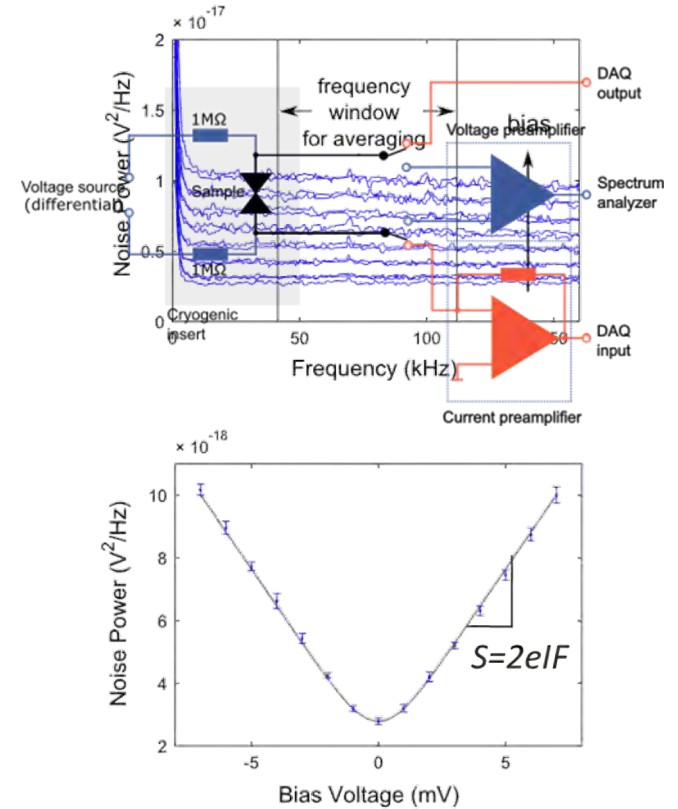
Electronic shot noise in point contact



Shot noise measurement and extraction of Fano factor



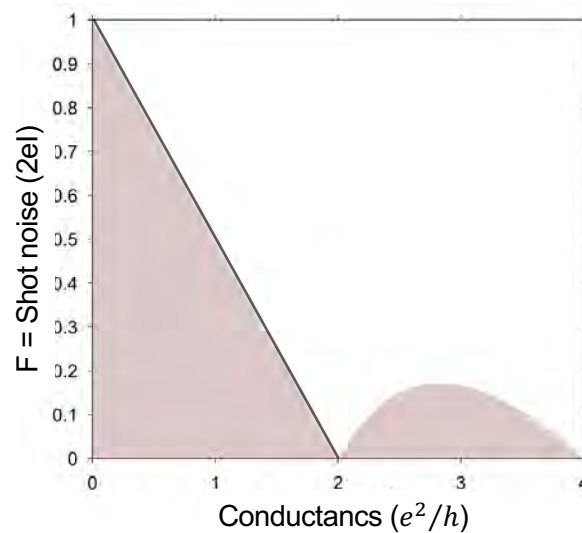
Shot noise Power $S = 2eIF$ ← Fano Factor $F = \frac{\sum \tau_n (1 - \tau_n)}{\sum \tau_n}$ Conductance $G = G_0 \sum \tau_n$ Conduction Channels $\{\tau_n\}$



R. Vardiman et al, Phys. Rev. B. **88** 161404 (R) (2013).

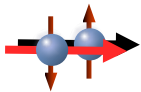
M. Kumar et al., Phys. Rev. Lett. **108**, 146602 (2012).

Probing spin polarized conduction by shot noise



Shot noise Power $S = 2eIF$ ← Fano Factor $F = \frac{\sum \tau_n(1 - \tau_n)}{\sum \tau_n}$

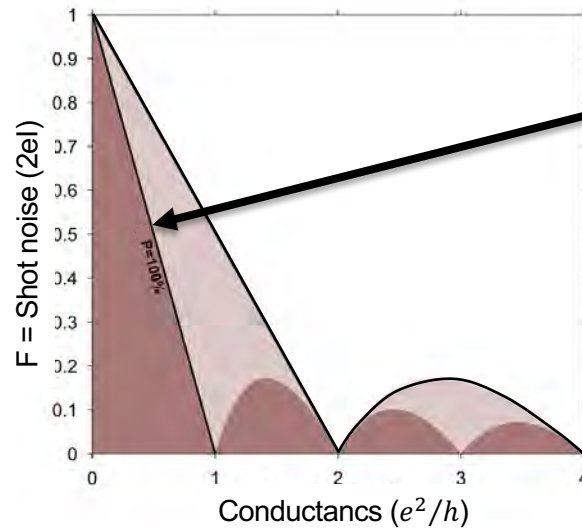
No spin polarized current (**light brown** area is forbidden)



$$S_I = 2eV \coth\left(\frac{eV}{2kT}\right) \frac{2e^2}{h} \sum_i \tau_i(1 - \tau_i) + 4kT \frac{2e^2}{h} \sum_i \tau_i^2$$

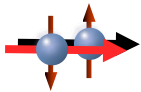
$$G = \frac{2e^2}{h} \sum_i \tau_i$$

Probing spin polarized conduction by shot noise



For one single spin channel
 $F = 1 - \tau_1$
 Linear

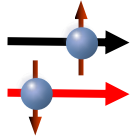
No spin polarized current (**light brown** area is forbidden)



$$S_I = 2eV \coth\left(\frac{eV}{2kT}\right) \frac{2e^2}{h} \sum_i \tau_i (1 - \tau_i) + 4kT \frac{2e^2}{h} \sum_i \tau_i^2$$

$$G = \frac{2e^2}{h} \sum_i \tau_i$$

Spin polarized current (**dark brown** area is forbidden)

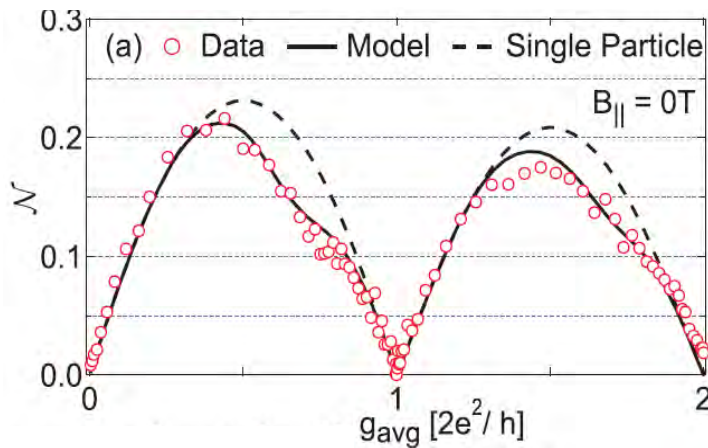
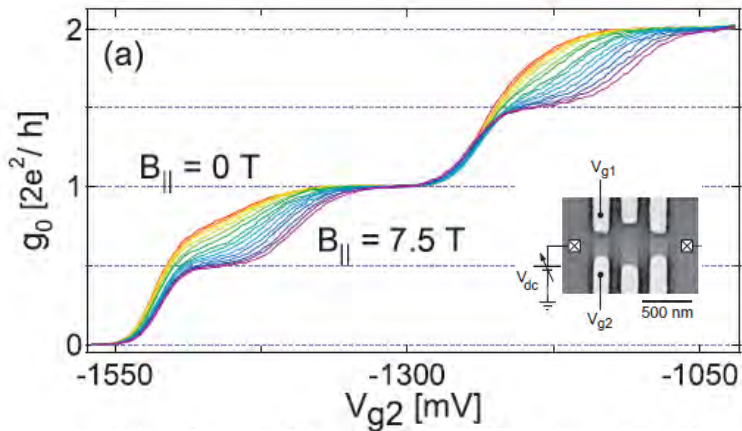


$$S_I = 2eV \coth\left(\frac{eV}{2kT}\right) \frac{e^2}{h} \sum_i \tau_i (1 - \tau_i) + 4kT \frac{e^2}{h} \sum_i \tau_i^2$$

$$G = \frac{e^2}{h} \sum_i \tau_i$$

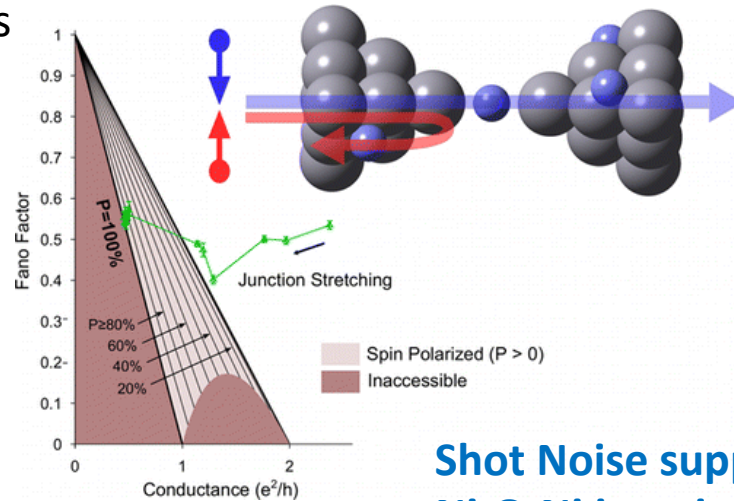
Spin polarization through Shot noise

Quantum point contact – Mesoscopic Physics



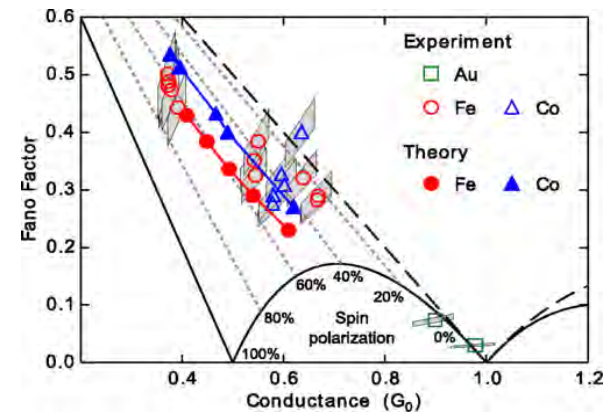
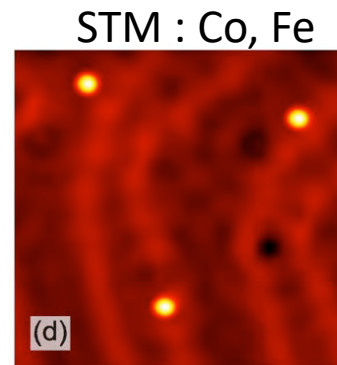
Suppression of Shot Noise near 0.7 anomaly – Spin origin

L. DiCarlo et al., PRL 97, 036810 (2006)



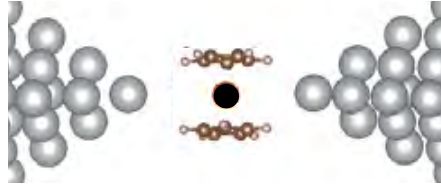
Shot Noise suppression in Ni-O-Ni junction

Vardimon, R et al., Nano Lett. 15, 3894-3898 (2015)

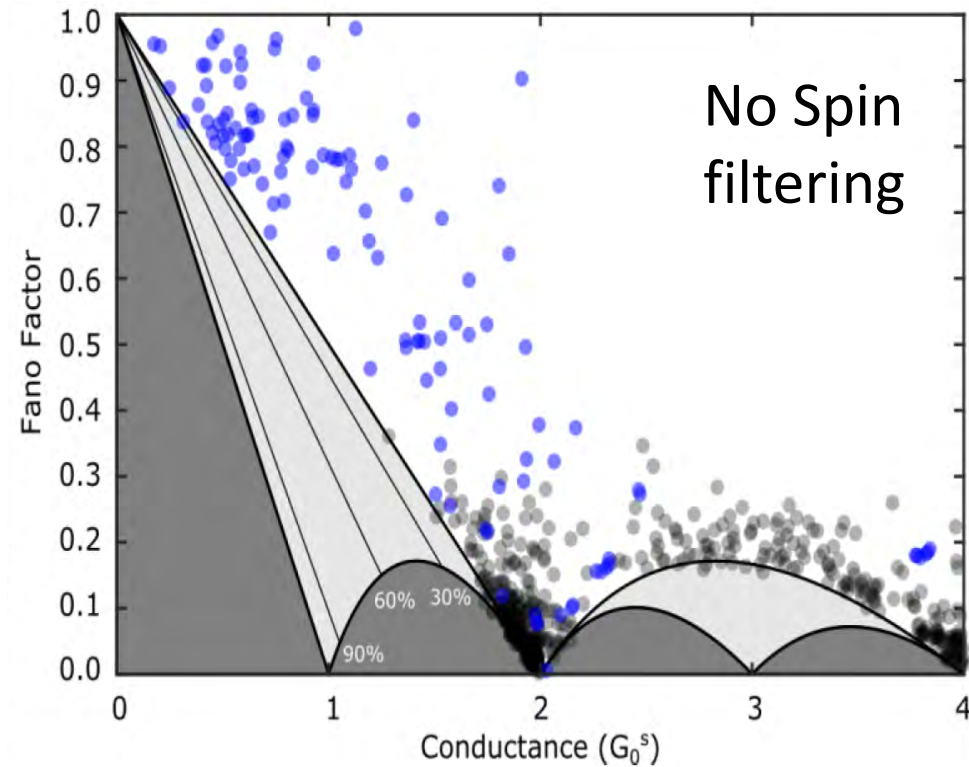


A. Burtzloff et al., Phys. Rev. Lett. 114, 016602 (2015)

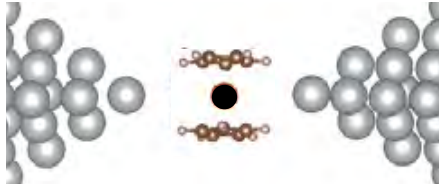
Diamagnetic electrodes and a magnetic molecule ($S=3/2$)



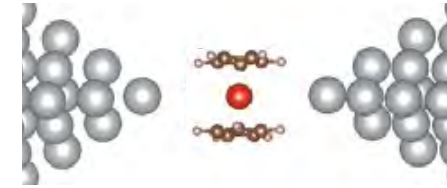
Silver-Ferrocene-Silver
($S=0$)



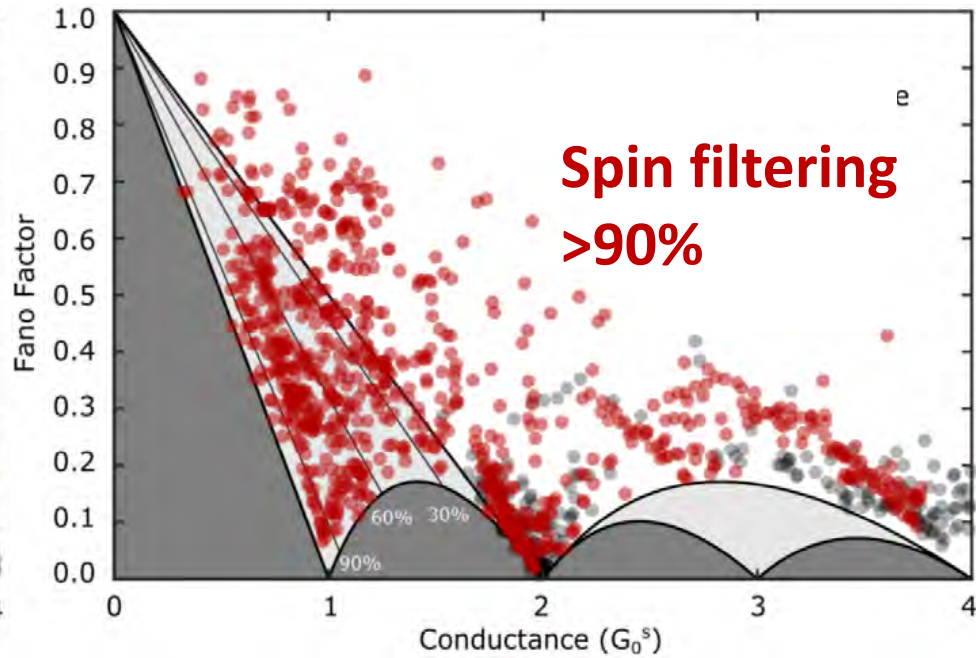
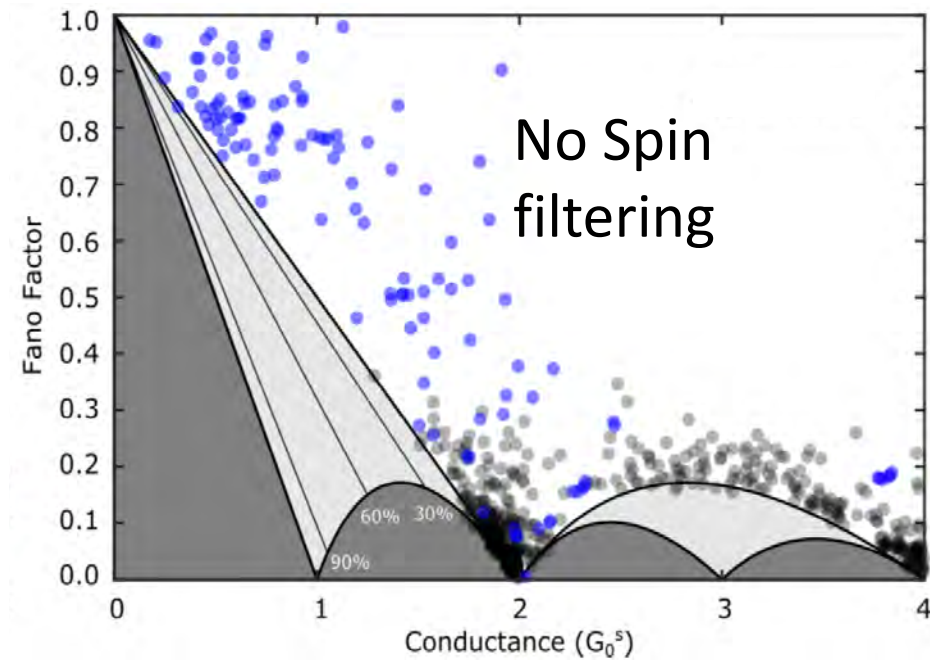
Diamagnetic electrodes and a magnetic molecule ($S=3/2$)



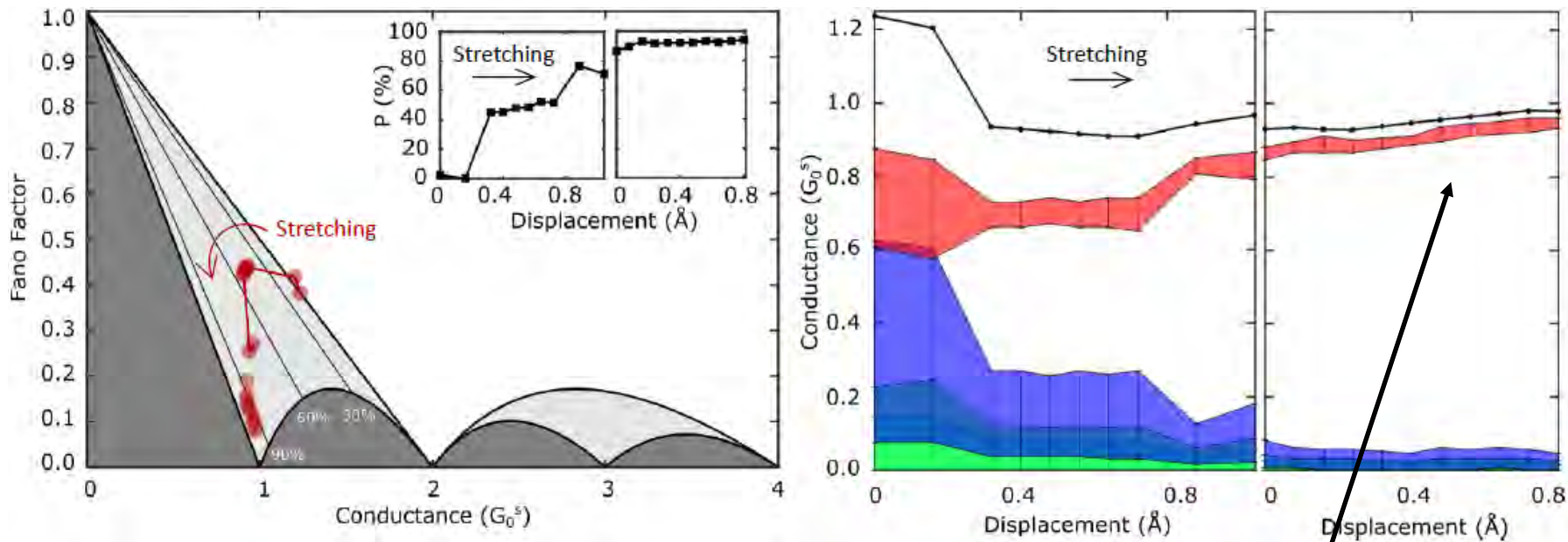
Silver-Ferrocene-Silver
($S=0$)



Silver-Vanadocene-Silver
($S=3/2$)



Stretching dependence of spin polarization Ag-vanadocene-Ag molecular junctions



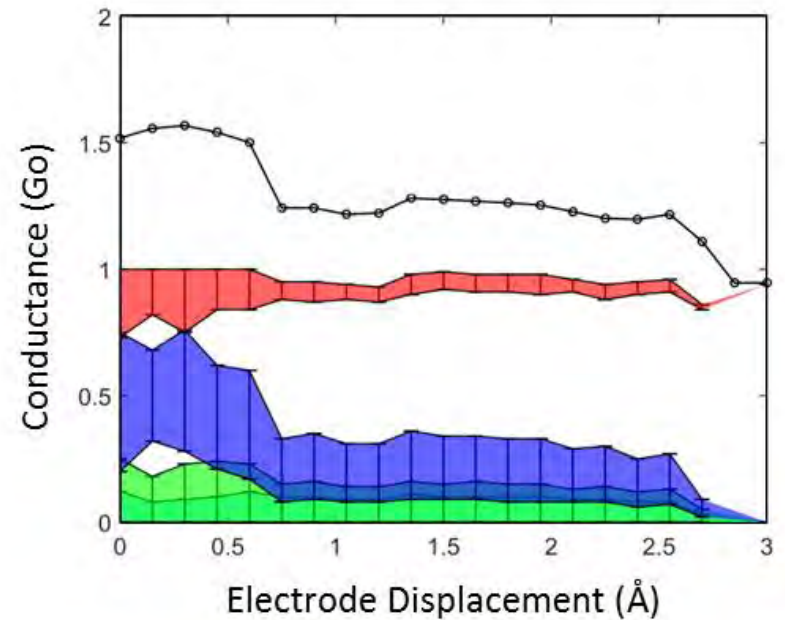
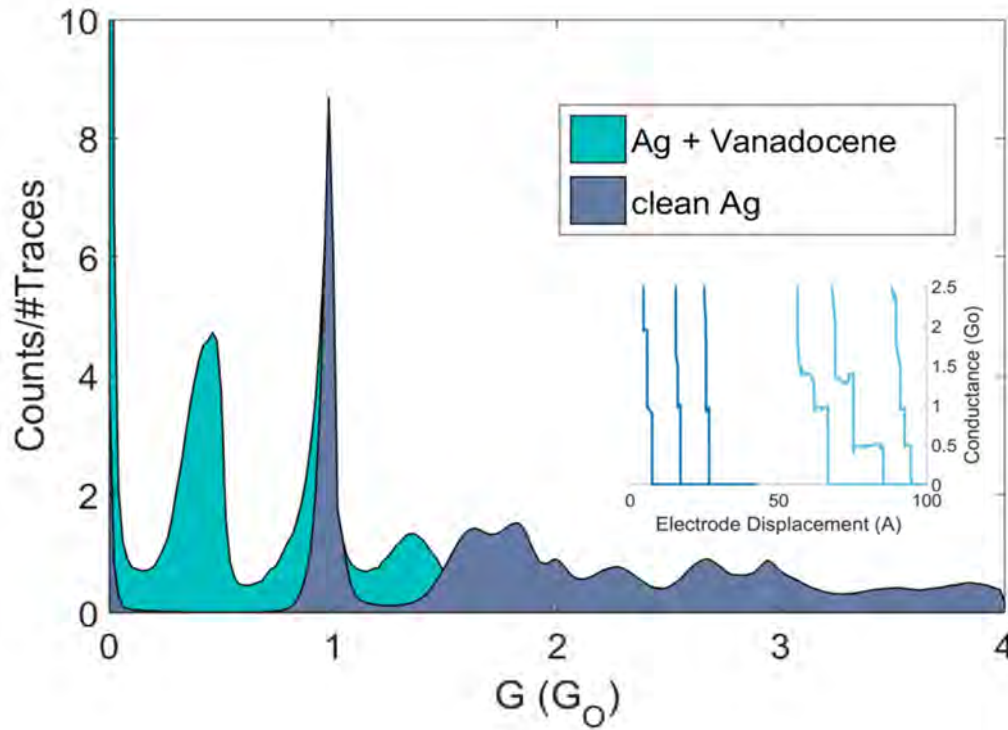
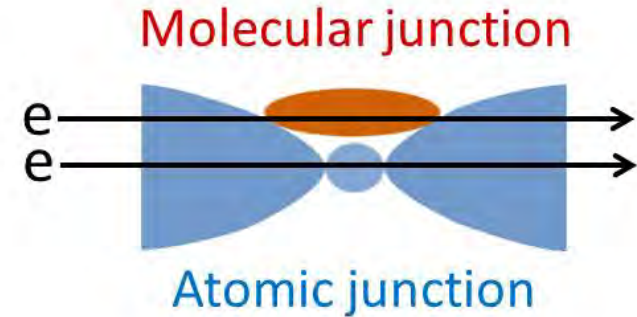
- >90% spin polarized current

- One dominant spin conduction channel

- Spin transmission probability close to 1

~ballistic spin conductance

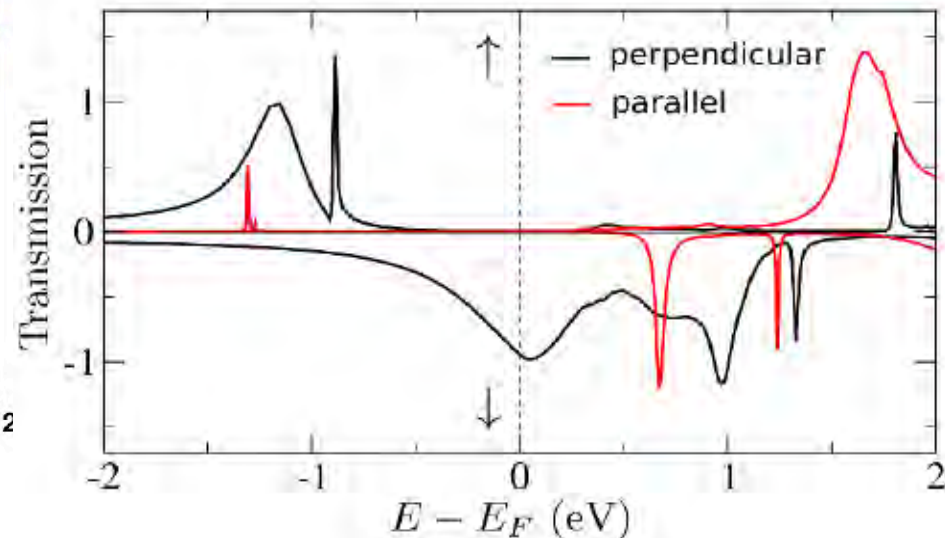
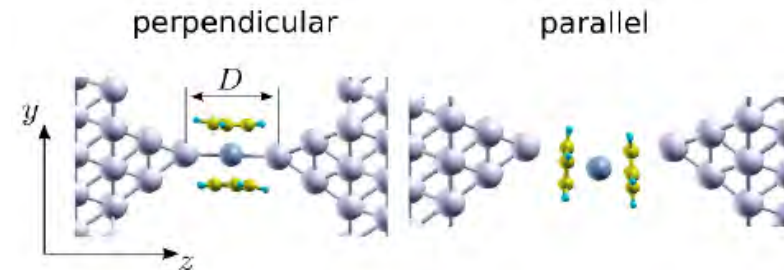
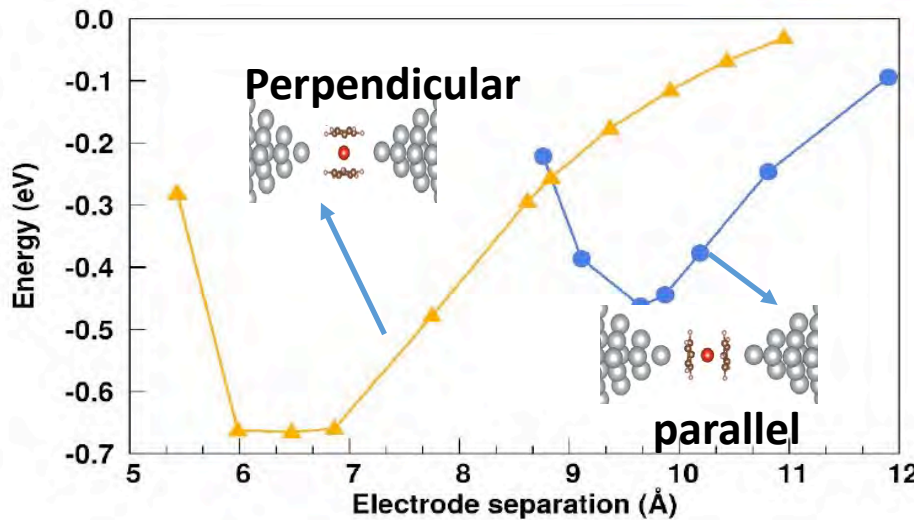
Early stage of Formation of molecular junction



A.N. Pal et al., BJ Nano 9 (1), 1471-1477 (2018)

Orientation of molecule inside the junction

Silver-Vanadocene-Silver

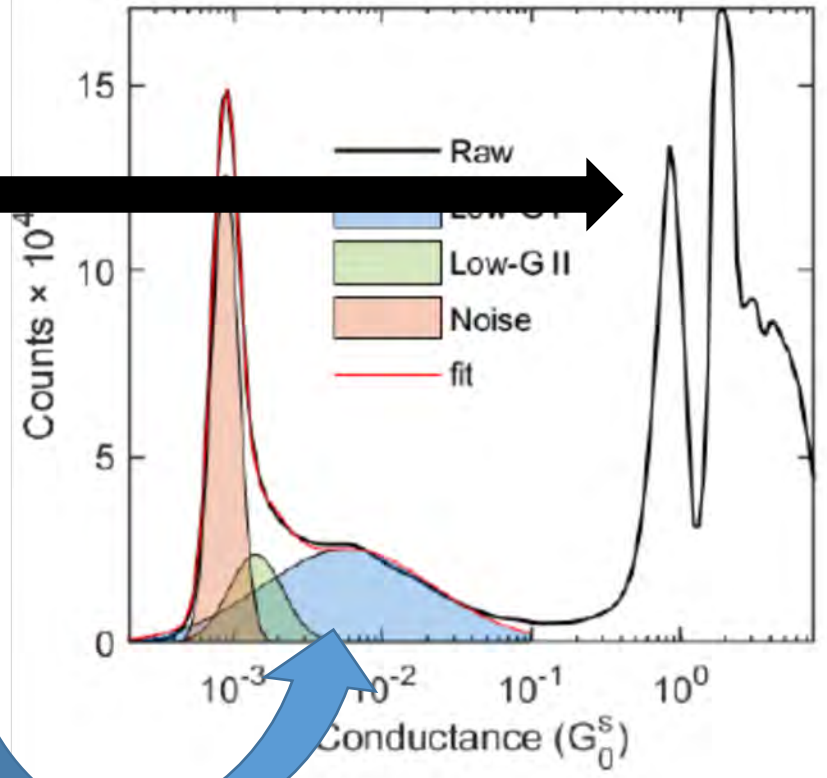
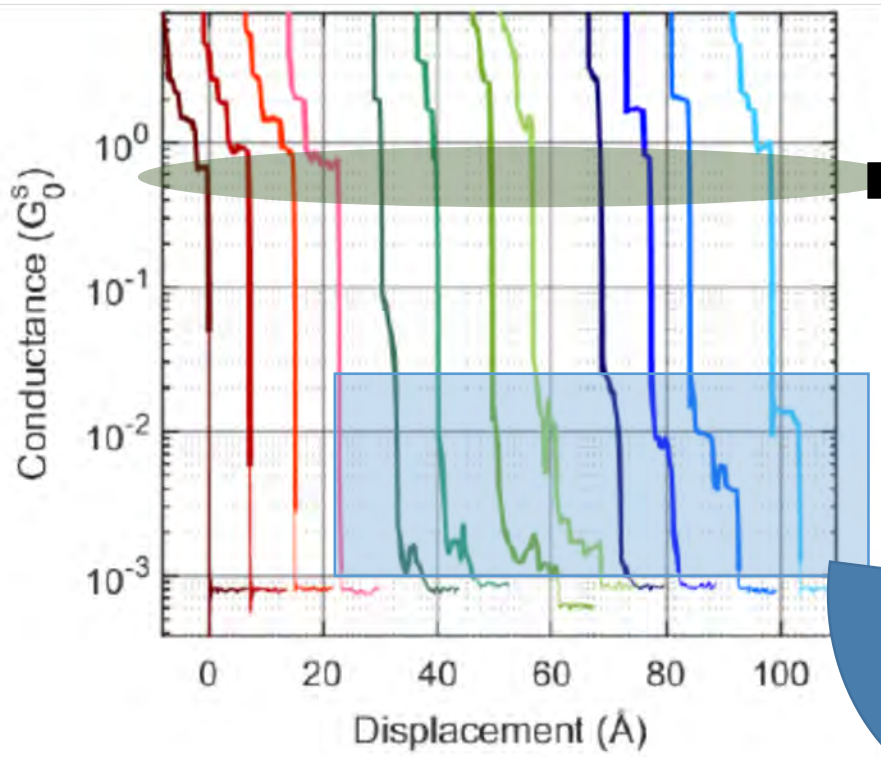


Calculations:

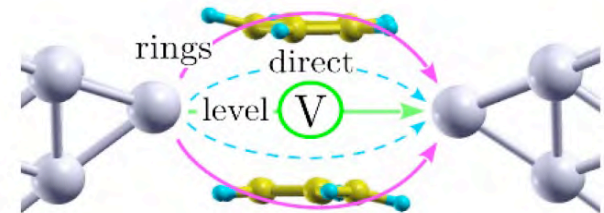
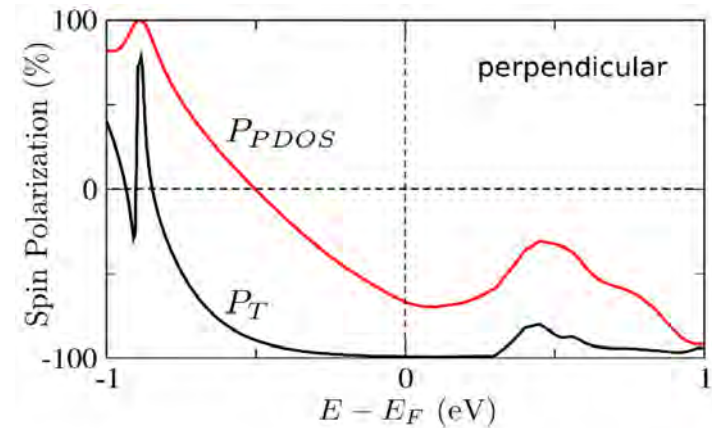
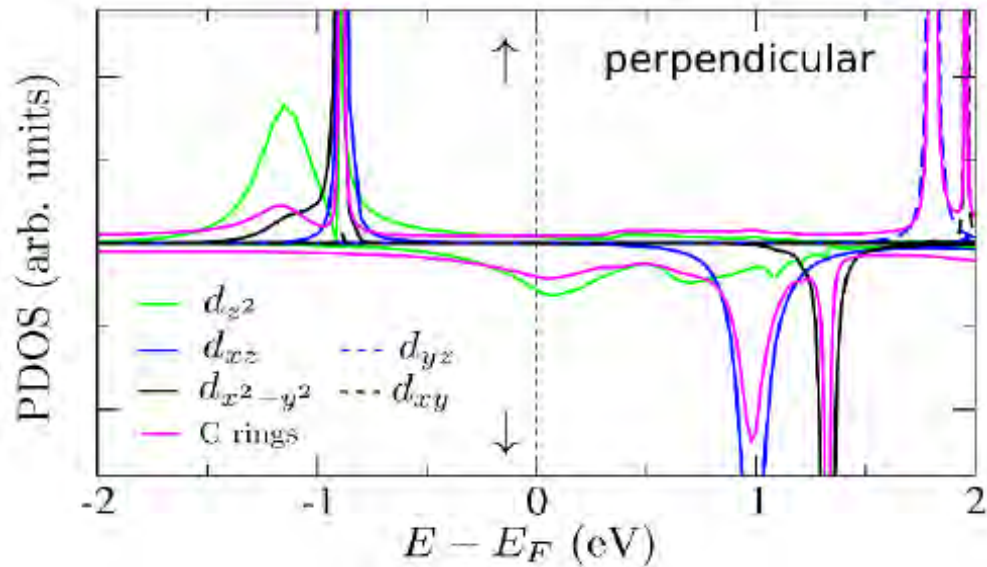
A. Smogunov and D. Li, Université Paris-Saclay, France

L. Kronik and S. Sarkar, Weizmann Institute

Low and High Conducting states

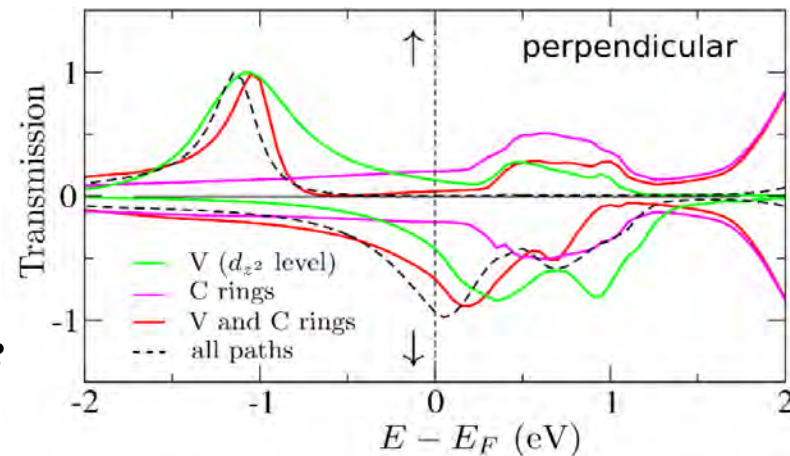


Origin of close to 100% Spin filtering: Spin Polarized DFT



**Quantum Interference
through Spin Polarized
Channels**

Calculations:
A. Smogunov and D. Li, *Université Paris-Saclay, France*
L. Kronik and S. Sarkar, *Weizmann Institute*



Quantum Interference: Charge transport

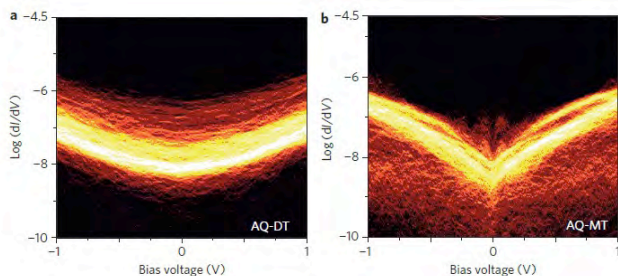
nature
nanotechnology

LETTERS

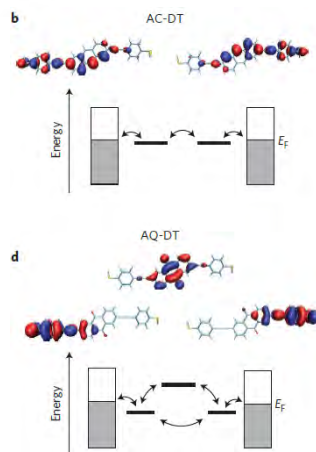
PUBLISHED ONLINE: 25 MARCH 2012 | DOI: 10.1038/NANO.2012.37

Observation of quantum interference in molecular charge transport

Constant M. Guédon¹, Hennie Valkenier², Troels Markussen³, Kristian S. Thygesen³, Jan C. Hummelen² and Sense Jan van der Molen^{1*}



Destructive quantum interference



NANO LETTERS

Letter

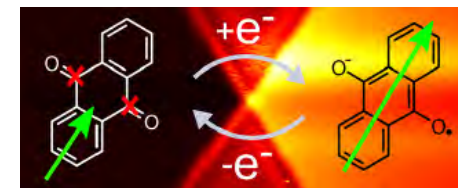
pubs.acs.org/nanolett

Electric-Field Control of Interfering Transport Pathways in a Single-Molecule Anthraquinone Transistor

Max Koole,[†] Jos M. Thijssen,[†] Hennie Valkenier,[‡] Jan C. Hummelen,[‡] and Herre S. J. van der Zant^{*,†}

[†]Kavli Institute of Nanoscience, Delft University of Technology, Lorentzweg 1, 2628 CJ, Delft, The Netherlands

[‡]Stratingh Institute for Chemistry and Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 4, 9747 AG, Groningen, The Netherlands



LETTER

<https://doi.org/10.1038/s41586-018-0197-9>

Comprehensive suppression of single-molecule conductance using destructive σ -interference

Marc H. Garner^{1,9}, Haixing Li^{2,6,9}, Yan Chen^{1,9}, Timothy A. Su^{4,7}, Zhichun Shangquan^{1,5,8}, Daniel W. Paley^{4,5}, Taifeng Liu¹, Fay Ng¹, Hexing Li¹, Shengxiang Xiao^{3a}, Colin Nuckolls^{3,4e}, Latha Venkataraman^{2,4e} & Gemma C. Solomon^{1a}

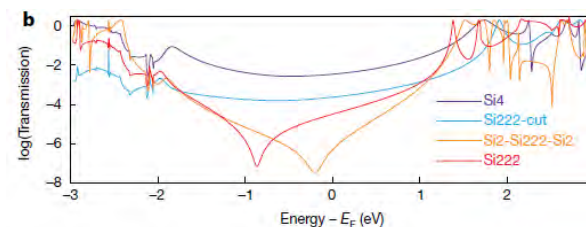
LETTERS

<https://doi.org/10.1038/s41565-018-0258-0>

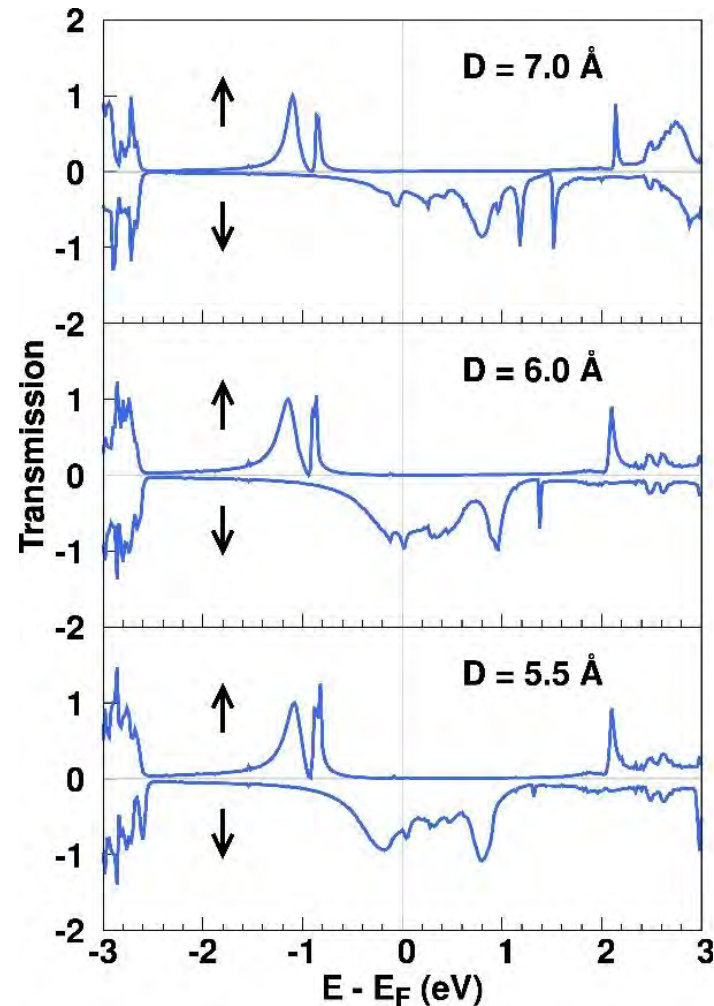
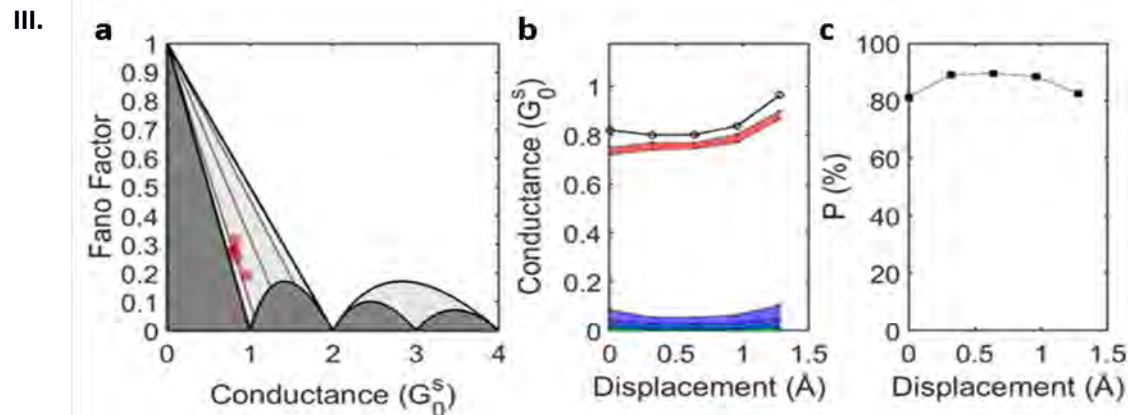
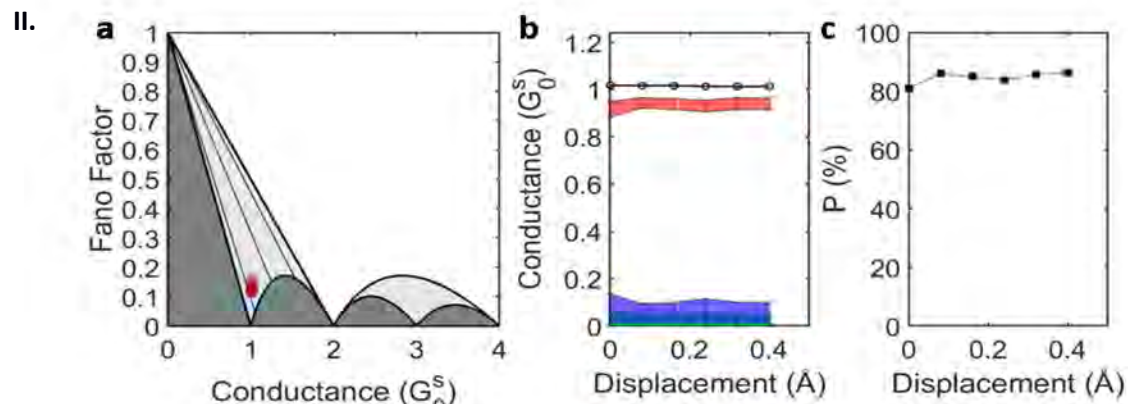
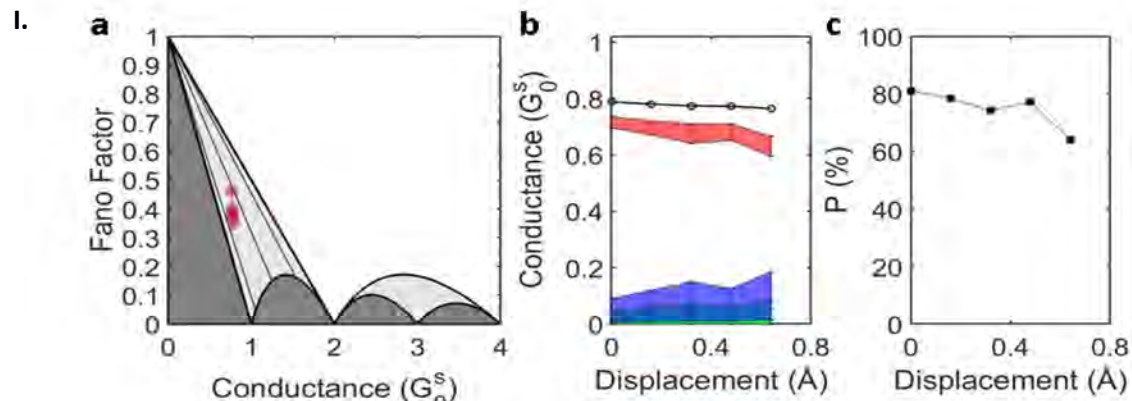
nature
nanotechnology

Mechanically controlled quantum interference in graphene break junctions

Sabina Caneva¹, Pascal Gehring¹, Víctor M. García-Suárez^{2,3}, Amador García-Fuente², Davide Stefani¹, Ignacio J. Olavarria-Contreras¹, Jaime Ferrer^{1,2,3*}, Cees Dekker¹ and Herre S. J. van der Zant^{1*}



Non monotonic stretching dependence

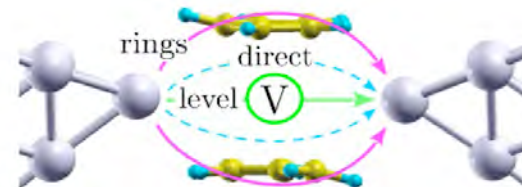
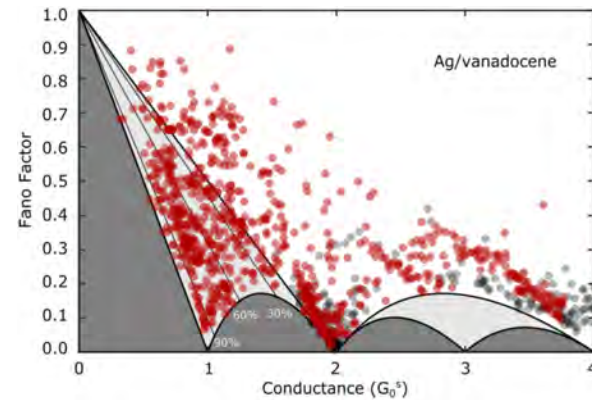
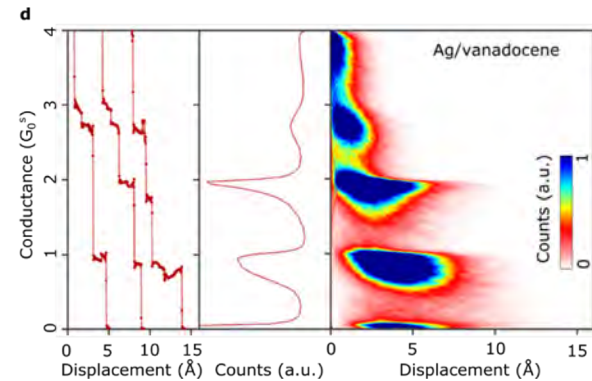


Conclusions

- Ag-Vanadocene-Ag junction
Conductance $\sim 1e^2/h$

- Suppression of Shot Noise
Spin filtering $\sim 100\%$, Ballistic Spin channel

- Spin dependent quantum interference



Acknowledgments



Oren Tal



Sudipto Chakraborti



Nadav Genossar



Lev Khmel'nitsky



Ran Vardiman

Collaborators

Calculations:

A. Smogunov and D. Li, Université Paris-Saclay, France

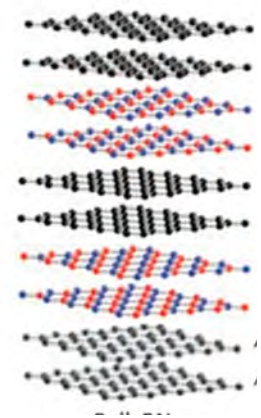
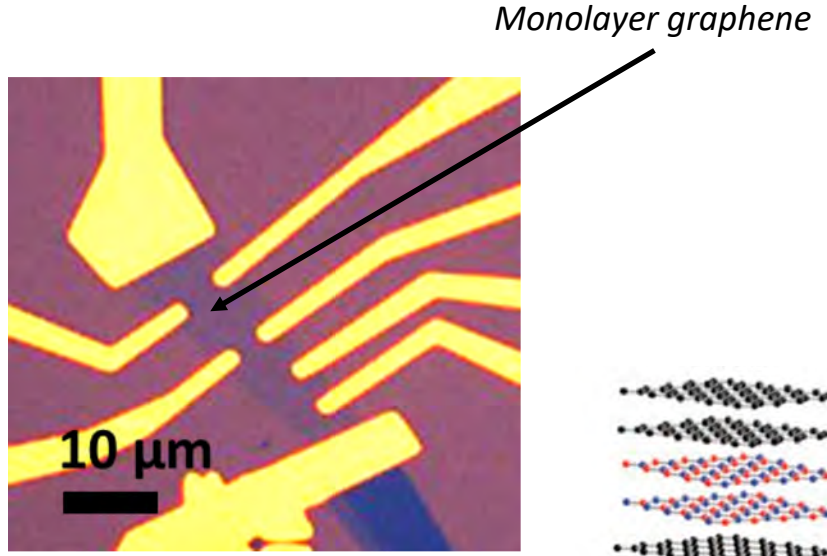
L. Kronik and S. Sarkar, Weizmann Institute



Ref. Nature Communication (Accepted for publication)

Current Research

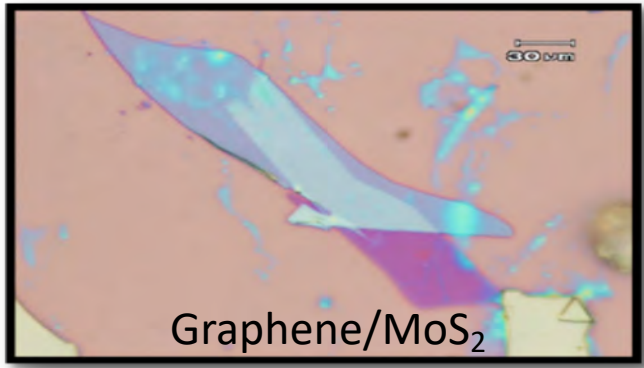
- 2D materials: Graphene, MoS_2 , WSe_2 , Carbon Nanotube and nanowires.
- Low temperature Physics
- Topological Insulator
- Charge and spin transport
- Molecular electronics
- Noise Measurements
- Quantum Hall effect
- Bio electronics



Example of a Graphene Field Effect Transistor

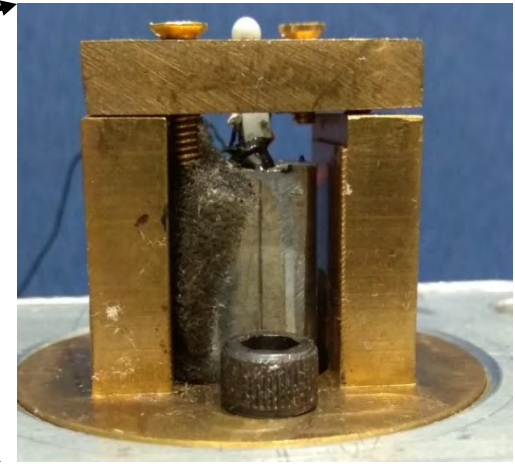
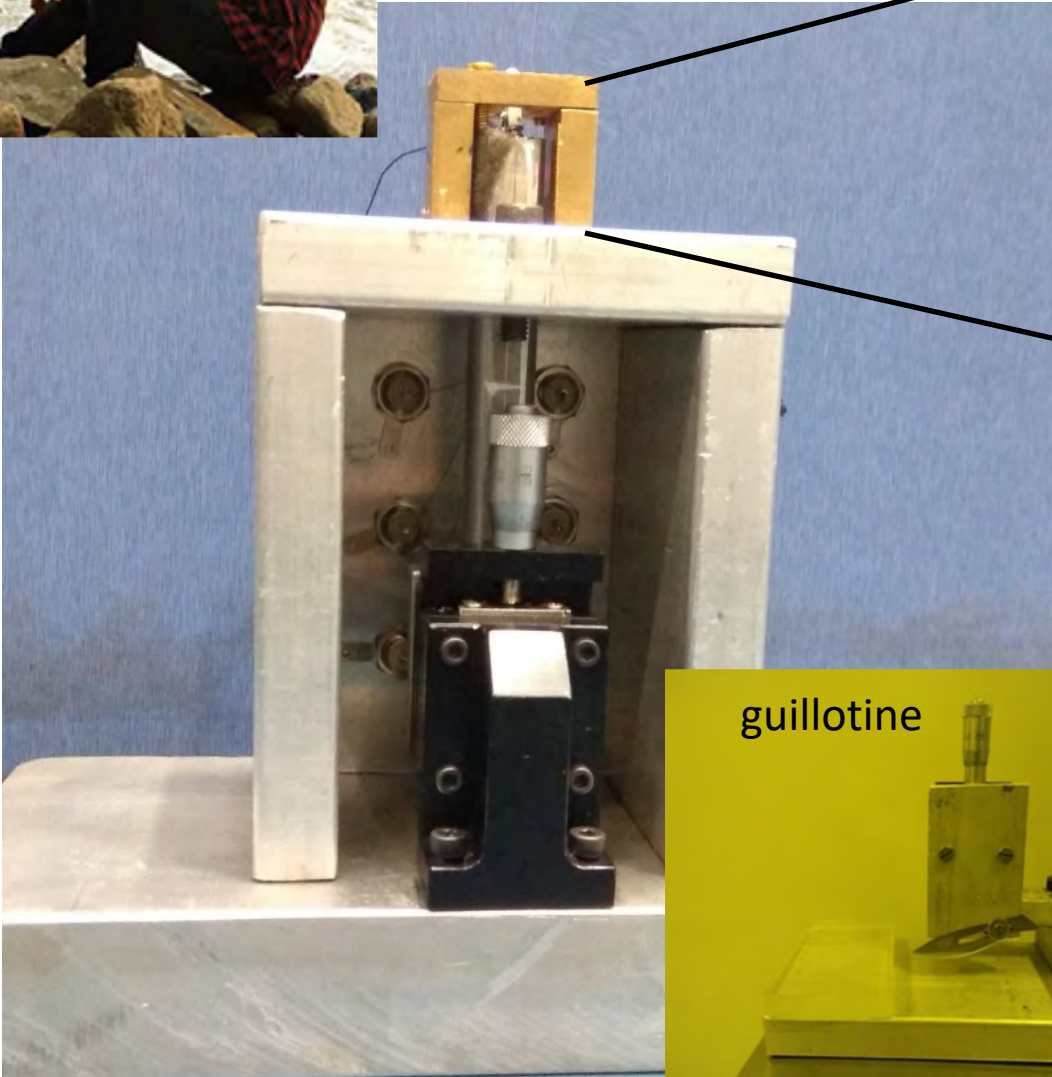


Graphene

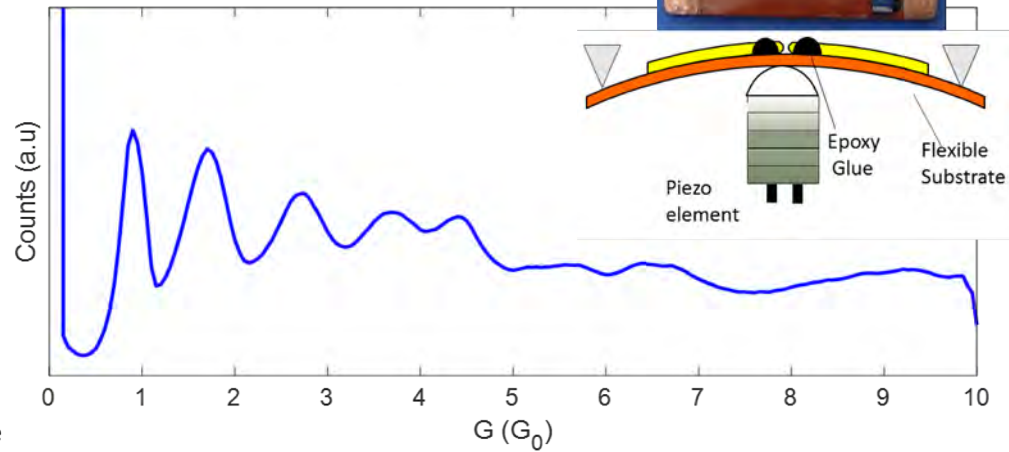
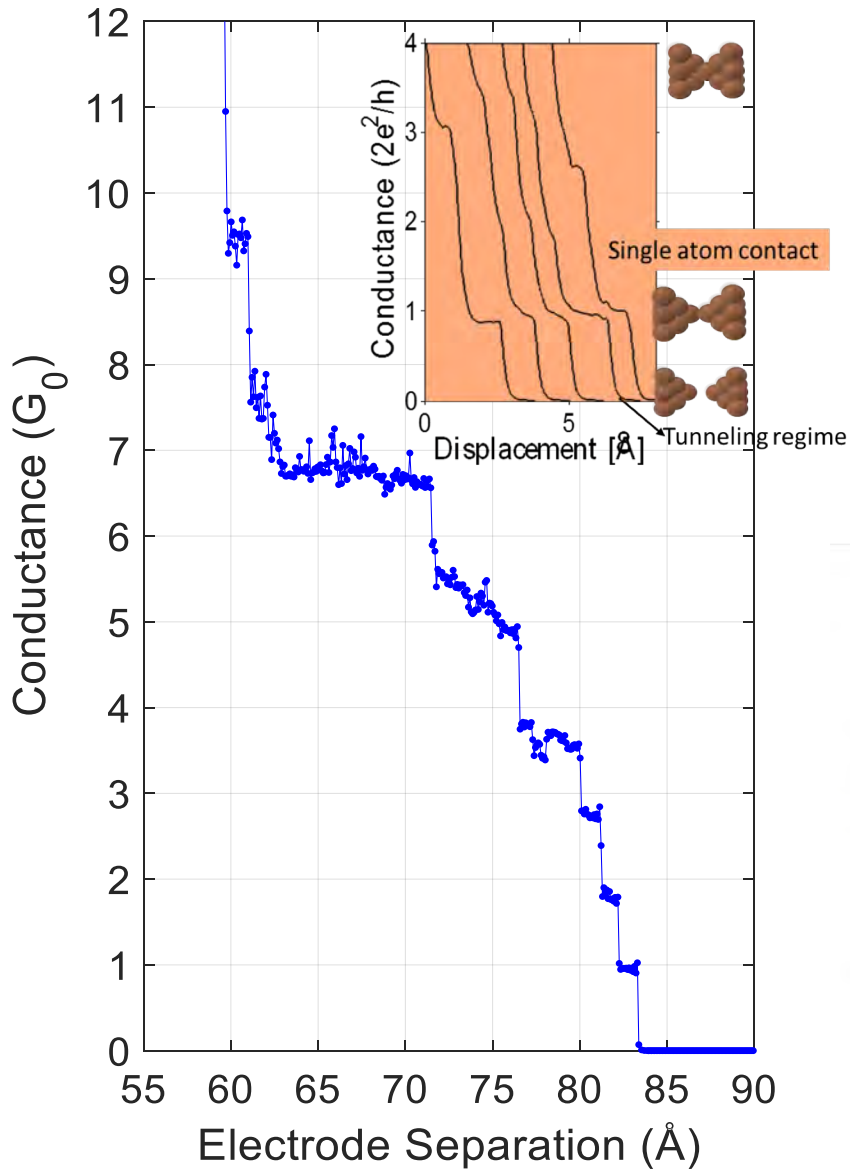
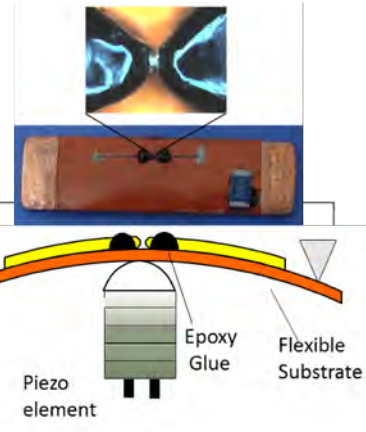


Graphene/ MoS_2

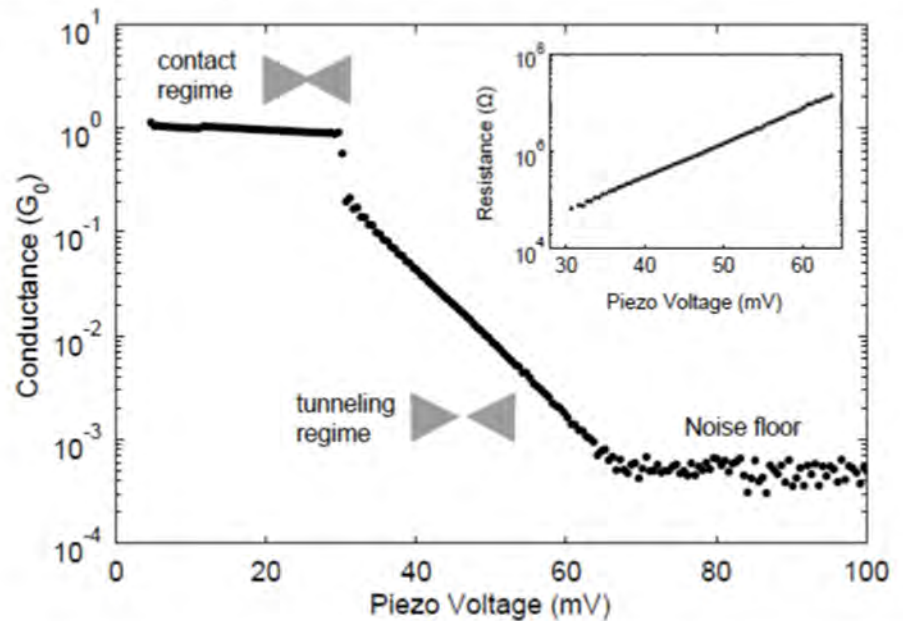
Room temperature MCBJ set up at SNBNCBS



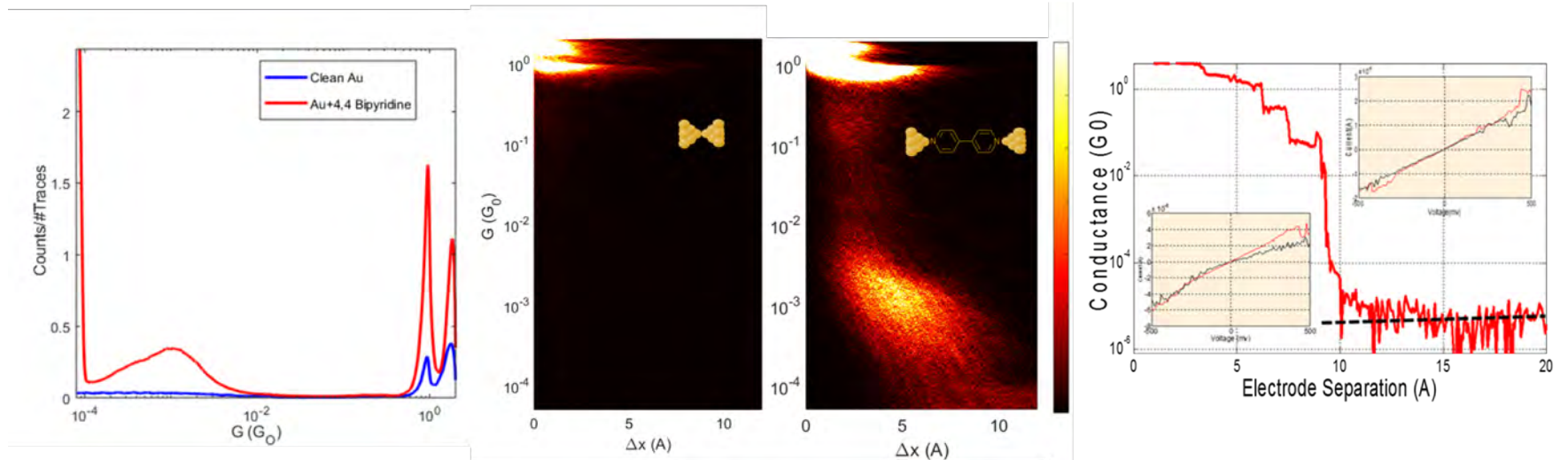
Atomic Gold junction



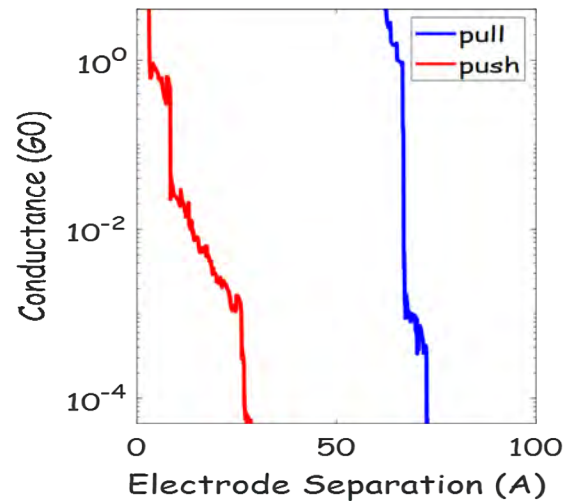
Length Calibration



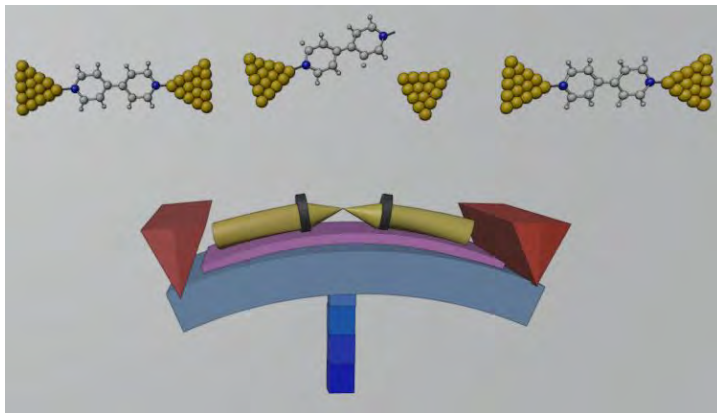
Gold-4,4 BiPyridine junction



Conductance Trace



Breaking and making process?



Group Members



Shubhadip
Moulick

Hybrid 2D devices



Shubhrasish
Mukherjee



Biswajit
Pabi

Single Molecular
transport



Rafiqul
Alam

Transport in
Topological
Materials



Riju Pal

Spintronics with
2D materials



Post Doc
Buddhadeb Pal

Superconductor-
Ferromagnet
junction



Visiting Fellow
Aditya N Roychoudhury

Vortex dynamics



Tousif
Project Student



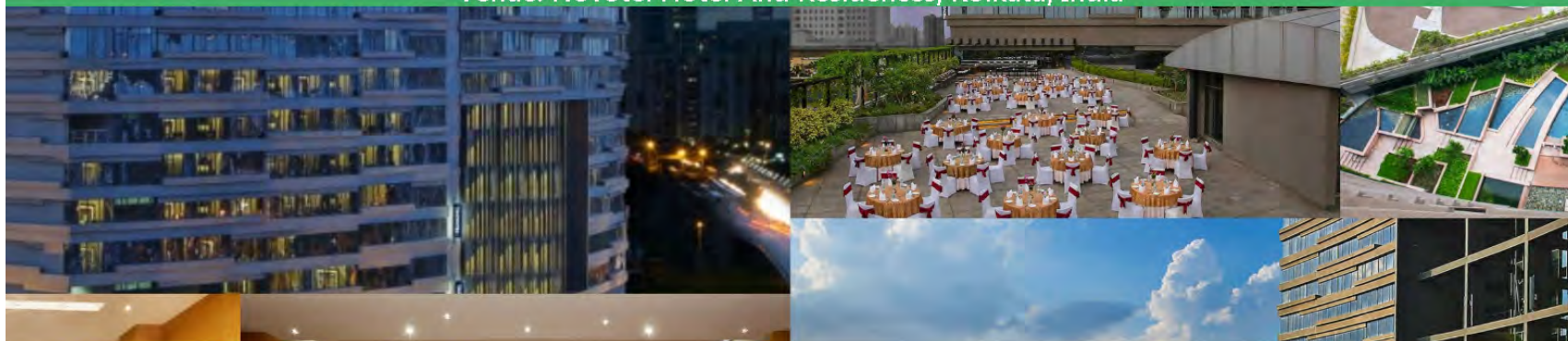
Taniya Basu
Technical assistant
Clean Room

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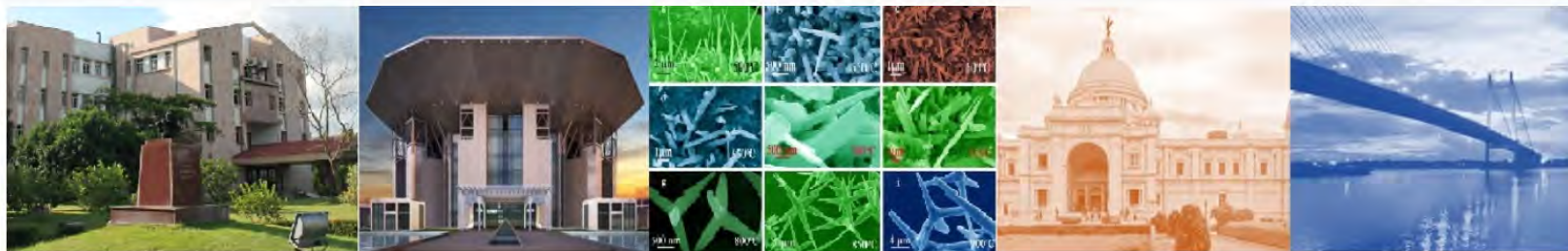


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