

# The Chiral Induced Spin Selectivity: Opportunities and Challenges

**Ron Naaman**

Department of Chemical and Biological Physics,  
Weizmann Institute, Israel

# Chiral Molecules

Even though homochirality in biological organisms represents an entropy reduction, that increases the organisms Gibbs free energy, the question:

**“Why nature kept chirality so persistently through evolution?”**

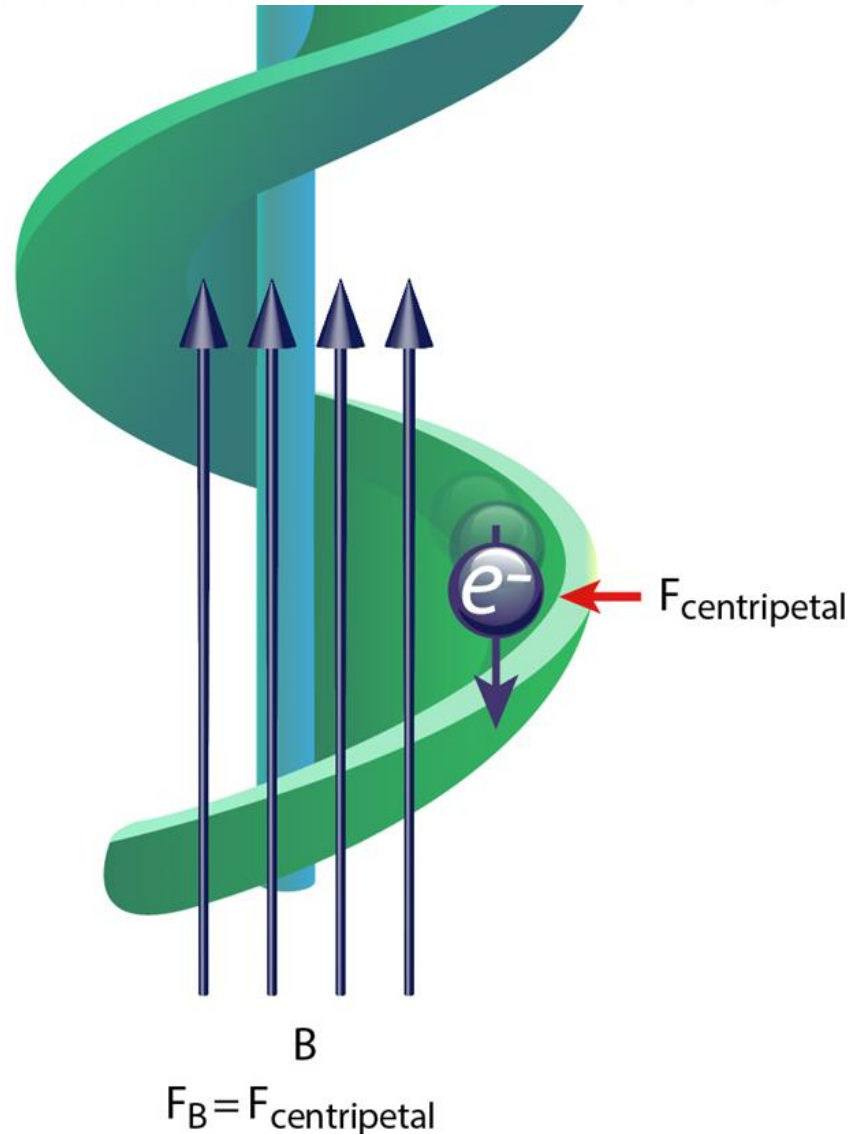
- Spin specific properties are assumed to require either ferromagnetic or paramagnetic properties.
- It is believed that in general the electron spin is not coupled in a significant way to the molecular frame.

**We found that chiral molecules have unique electronic and spintronic properties despite being usually closed shell systems - namely singlet.**

# The Chiral Induced Spin Selectivity (CISS) Effect

Please note:

The sign of the preferred spin depends on the sign of the velocity and of the electric field (E).

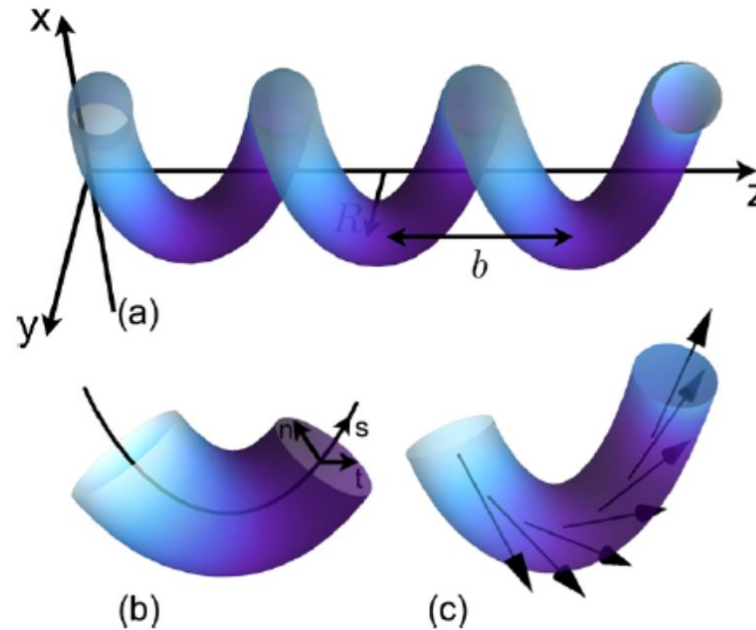


# Momentum conservation

The electron moving in helical potential must exchange momentum with the system

**In solids**, that have momentum with the system

**In insulators/metal** therefore momentum that have angular momentum



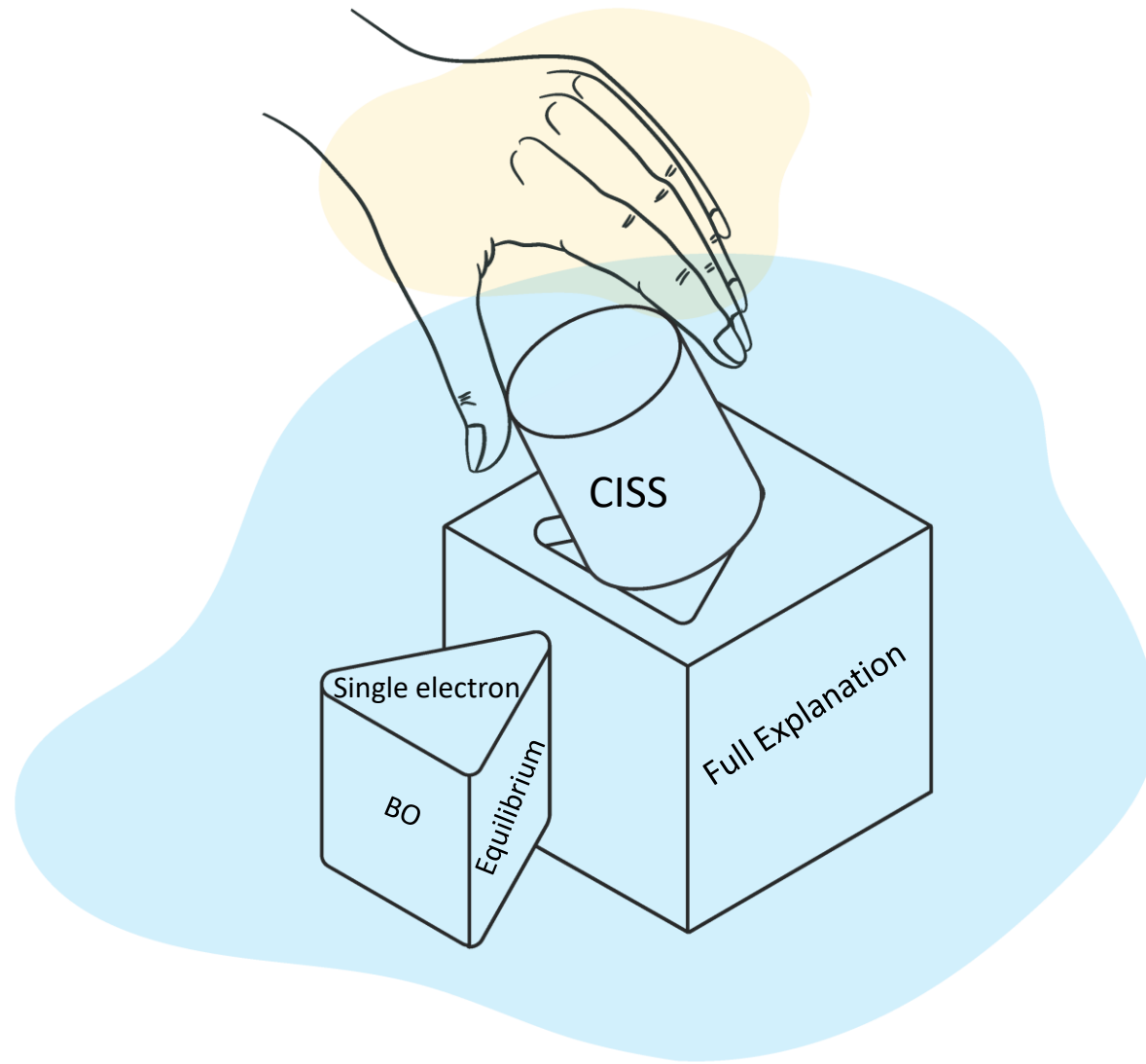
ns can exchange

are localized and  
energy vibrations  
ons.

Works by:

Joe Subotnik: Phys. Rev. B **106**, 184302 (2022); *Nat. Comm.* **12**, 700 (2021); *Phys. Chem. C* **127**, 14155 (2023).

Jonas Fransson: Nano Lett., 21, 3026 (2021); Phys. Rev. **B** 102, 235416(2020)



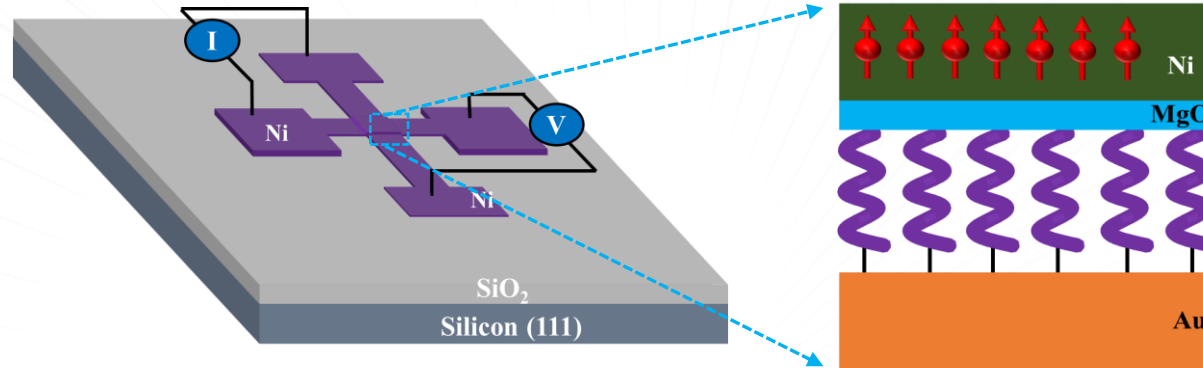
## Hence:

- While for electrons moving in straight line phonons/vibrations are interfering with the straight path, in chiral potentials they are essential (especially if there are no unlocalized electrons).
- The CISS samples the electrons that **did interact** with the vibrations/phonons.

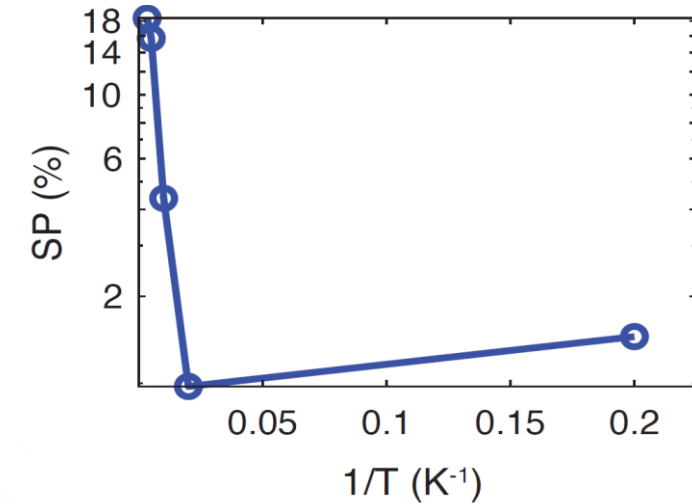
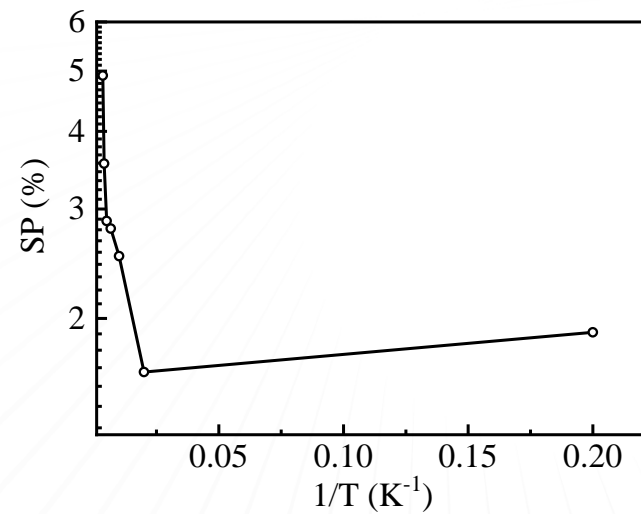
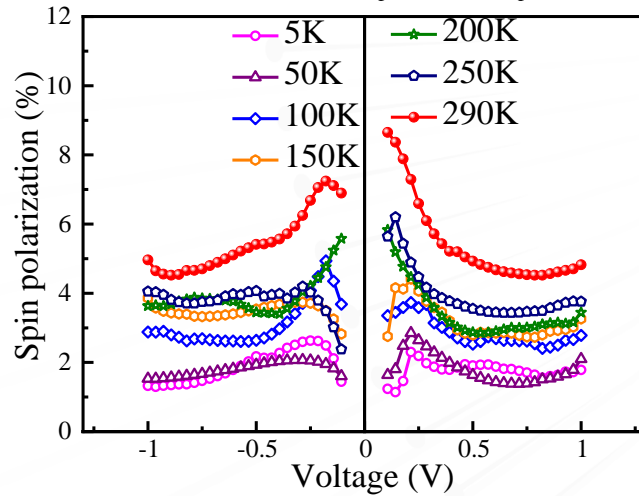
Longlong Zhang, Yuying Hao, Wei Qin, Shijie Xie, Fanyao Qu, PHYSICAL REVIEW B 102, 214303 (2020). Role of polarons.

Gui-Fang Du, Hua-Hua Fu, Ruqian Wu. PHYSICAL REVIEW B 102, 035431 (2020) Role of phonons in DNA

# The role of phonons



$$\text{Spin polarization (\%)} = (I_{\text{up}} - I_{\text{down}}) / (I_{\text{up}} + I_{\text{down}}) * 100$$

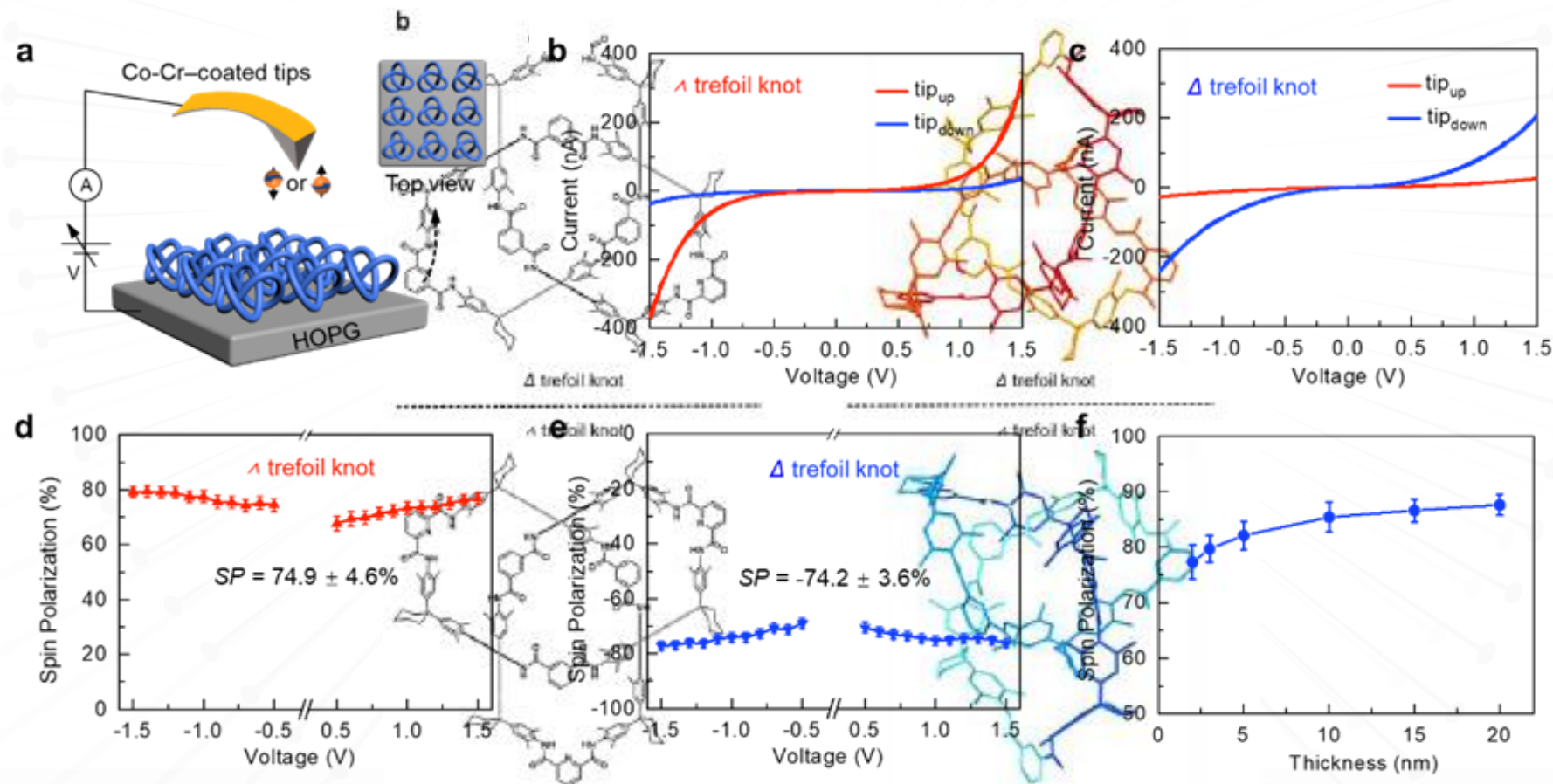


Theory by:  
**Jonas Fransson**, Uppsala University

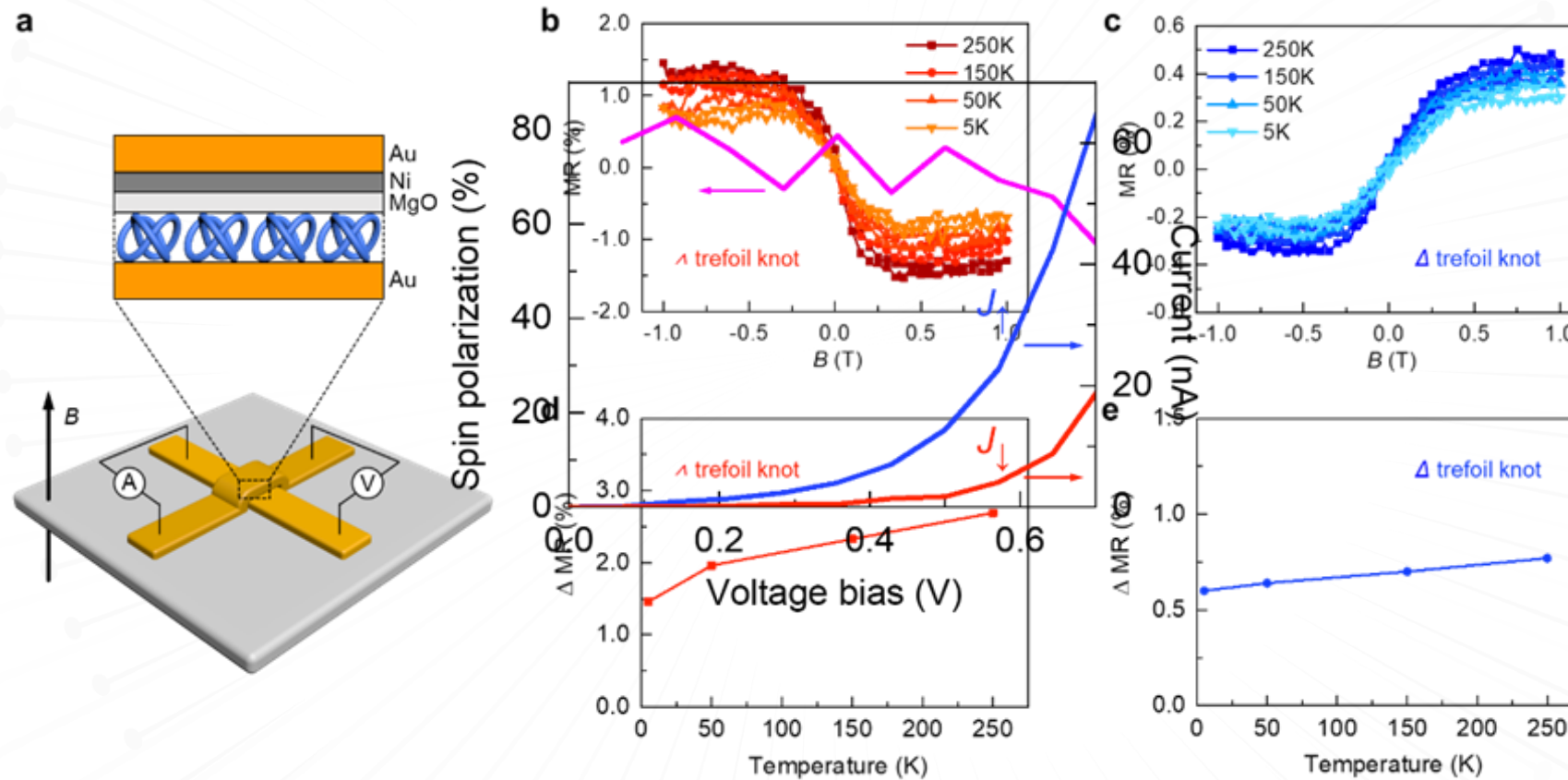


# Highly conductive topologically chiral molecular knots as efficient spin filters

D.-Y. Zhang, Y. Sang, T. K. Das, Z. Guan, N. Zhong, C.-G. Duan, W. Wang, J. Fransson, R. Naaman, H.-B. Yang, *J. Am. Chem. Soc.* 145, 26791–26798 (2023).

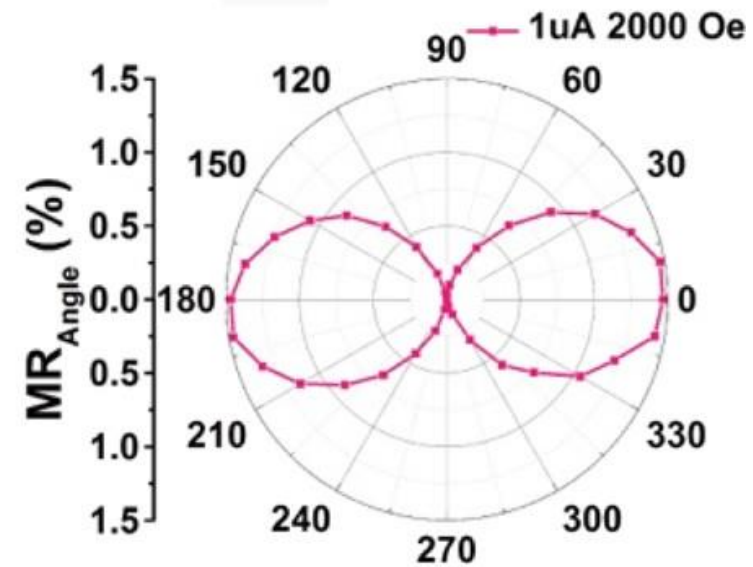
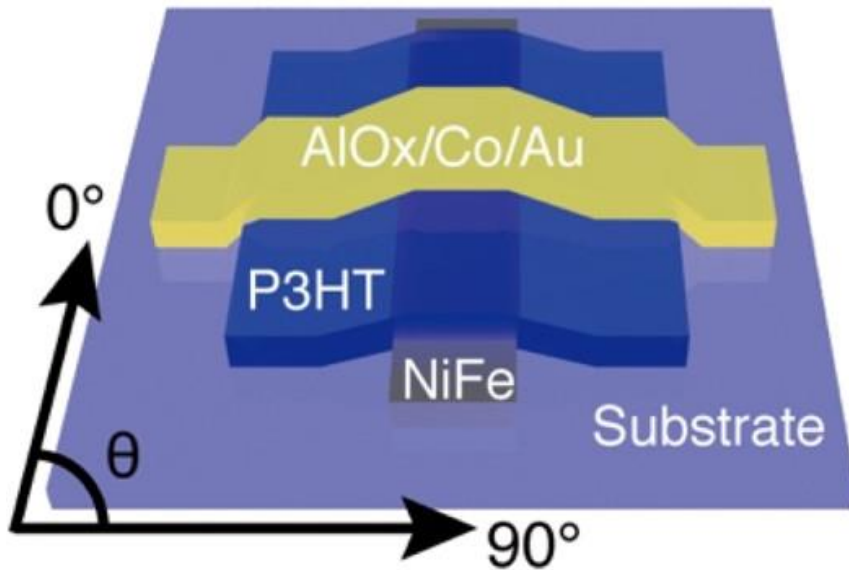


# Almost no temperature dependent



Electron-electron interaction allows changing momentum

# Anisotropic Magnetoresistance in Spintronics Devices

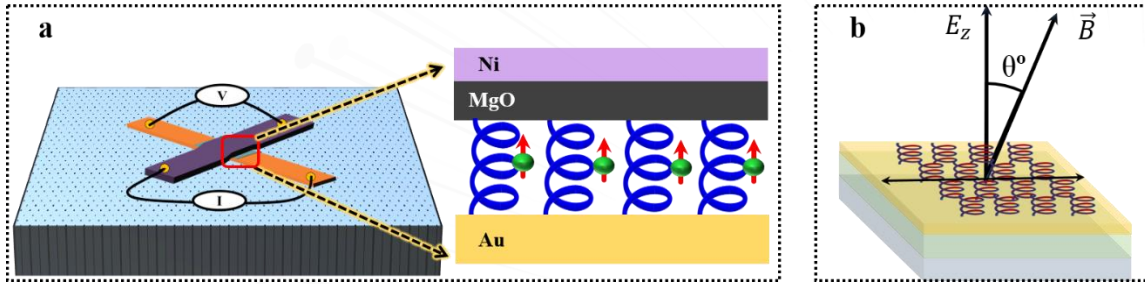


Anisotropic Magnetoresistance in NiFe-Based Polymer Spin Valves

Shuaishuai Ding, Yuan Tian, Huanli Dong, Daoben Zhu, and Wenping Hu

ACS Appl. Mater. Interfaces 2019, 11, 11654–11659

# The Effect of Angle Dependent Magnetic Moment of the Substrate.

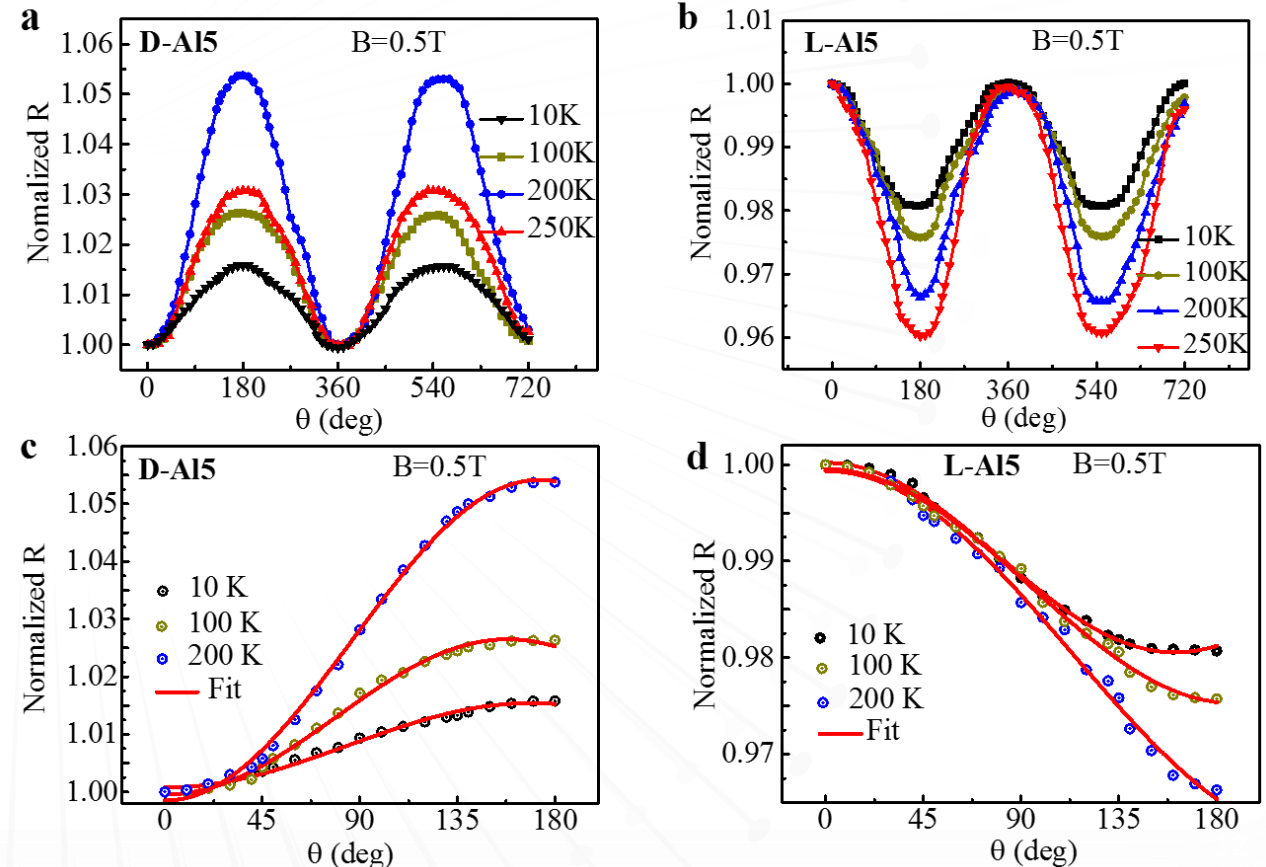


T. K. Das, R. Naaman, J. Fransson, *Adv. Mat.*, 2313708 (2024).

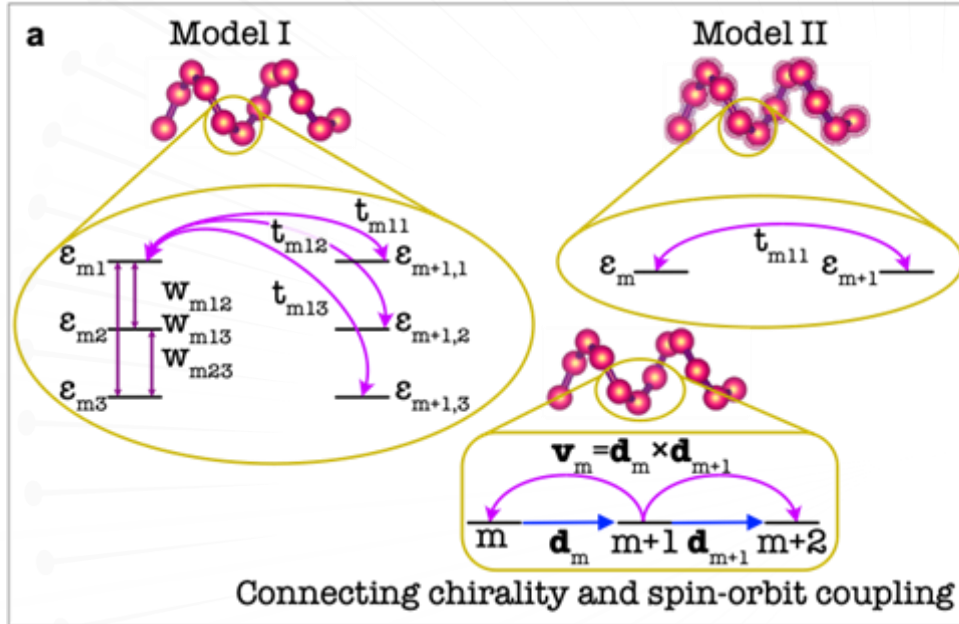
The angle dependent resistance curves were fitted to

$$R = R_{\perp} + (R_{\parallel} - R_{\perp})\cos^2 \theta/2$$

Like in GMR.



# Theory by Jonas Fransson



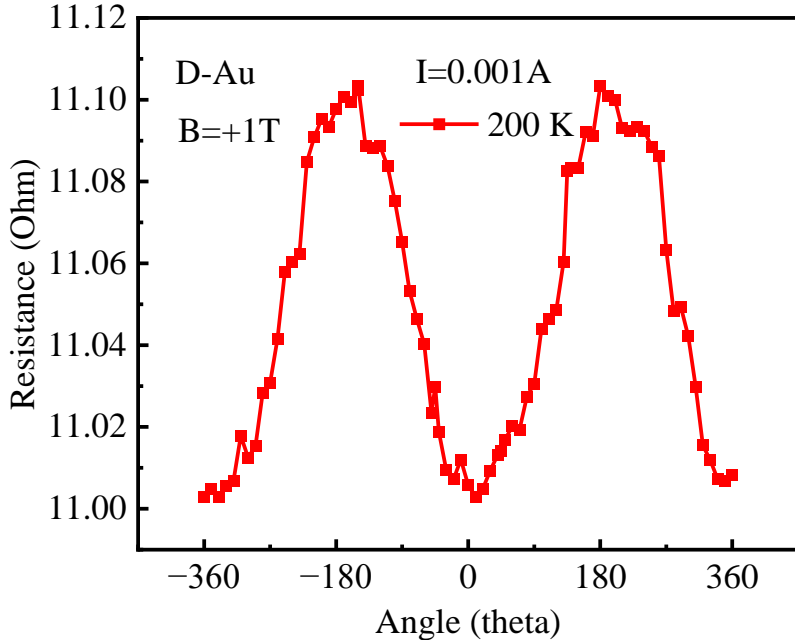
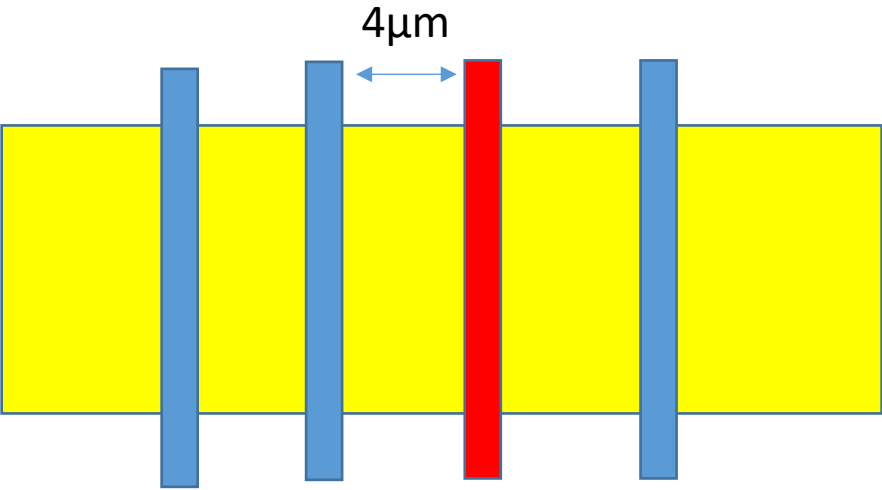
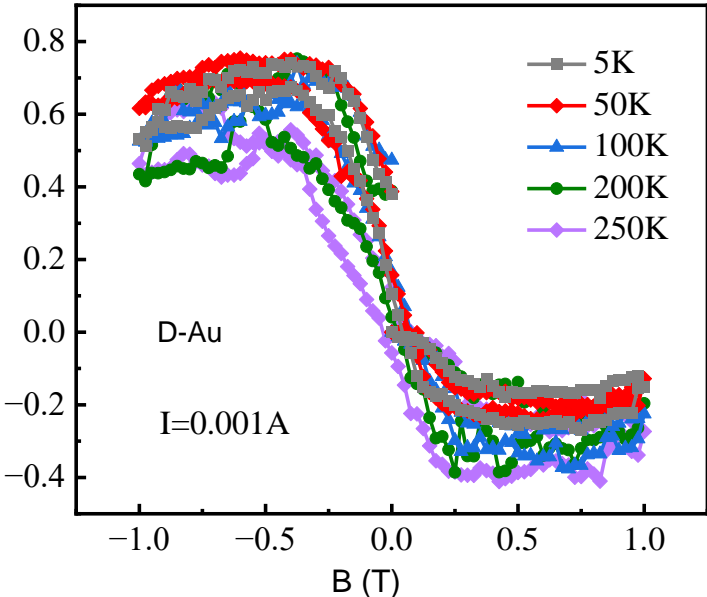
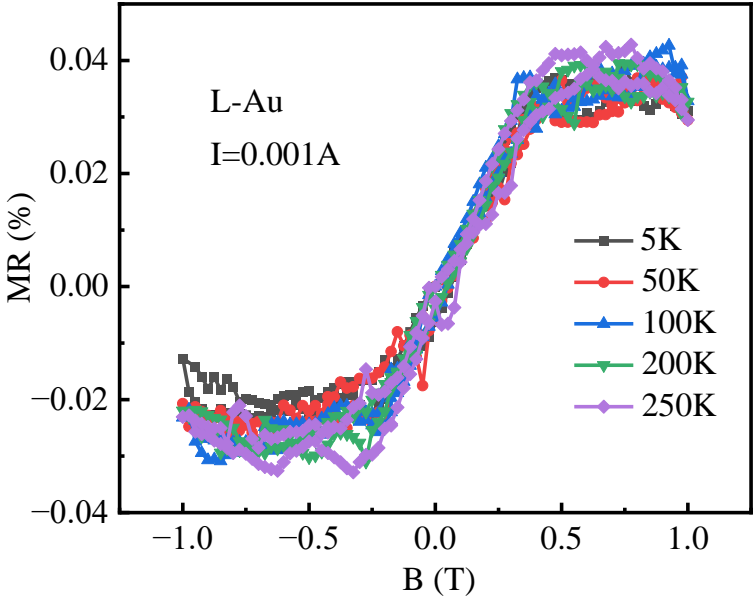


# Conclusions from the simulation of the angle dependent

- SOC in the lead/s can induce spin polarization but no angle dependent.
- SOC in the molecule and electron-electron interactions result in angle dependent, but not like the experimental results.
- Only SOC in the molecule+electron-electron+phonons with dissipation produce the experimental results.

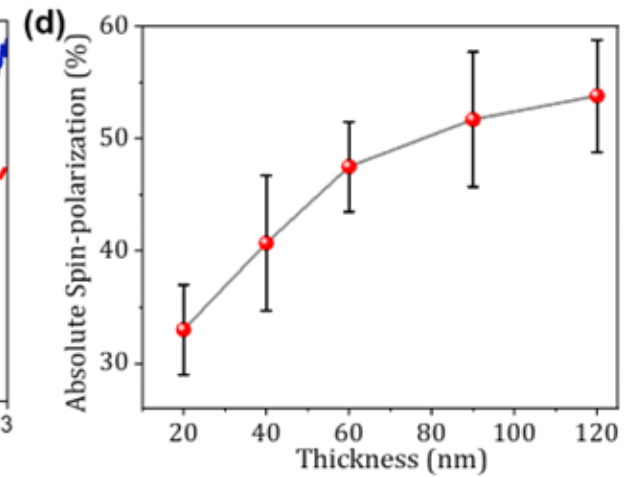
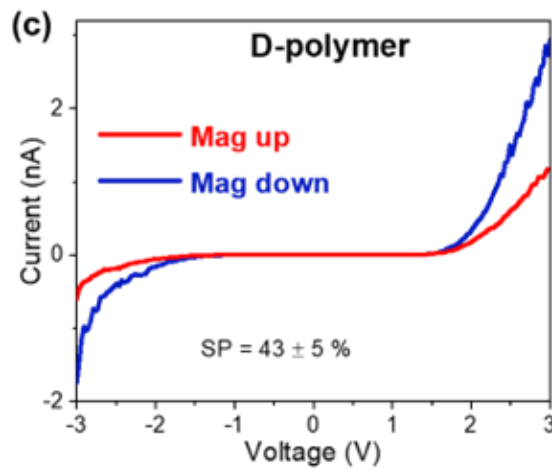
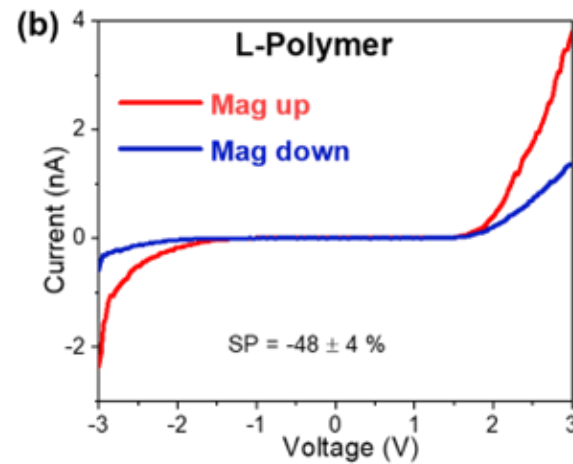
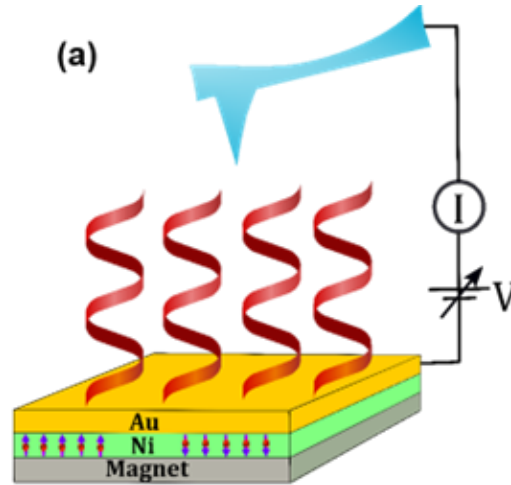
Long range spin transport at  
room temperature.

# Chiral Gold film- about 200 nm thick



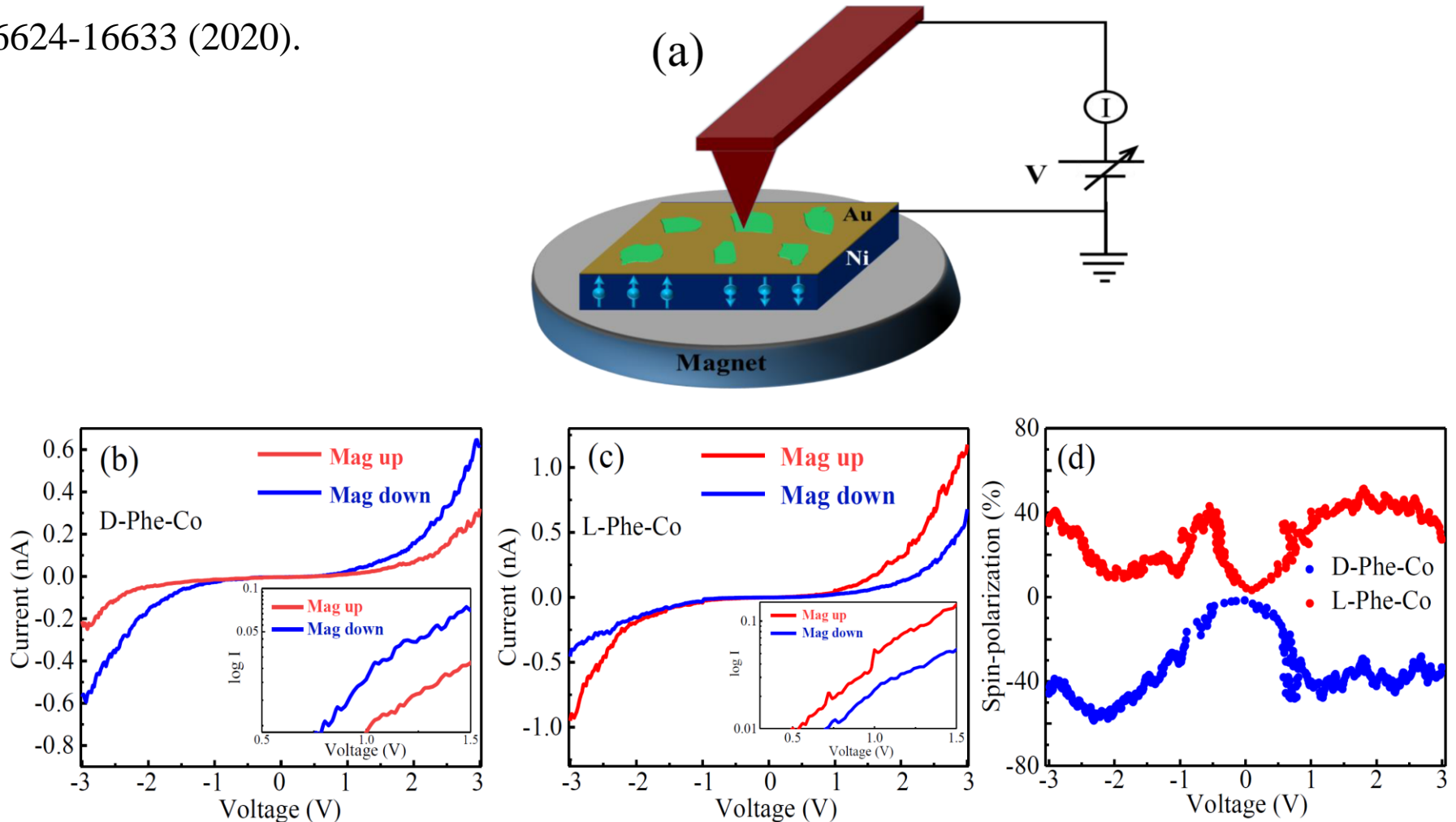


# Polymer film



# 300 nm thick Cu-phenylalanine crystals

*ACS Nano* **14**, 16624-16633 (2020).

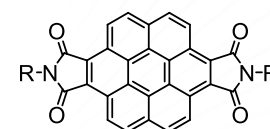
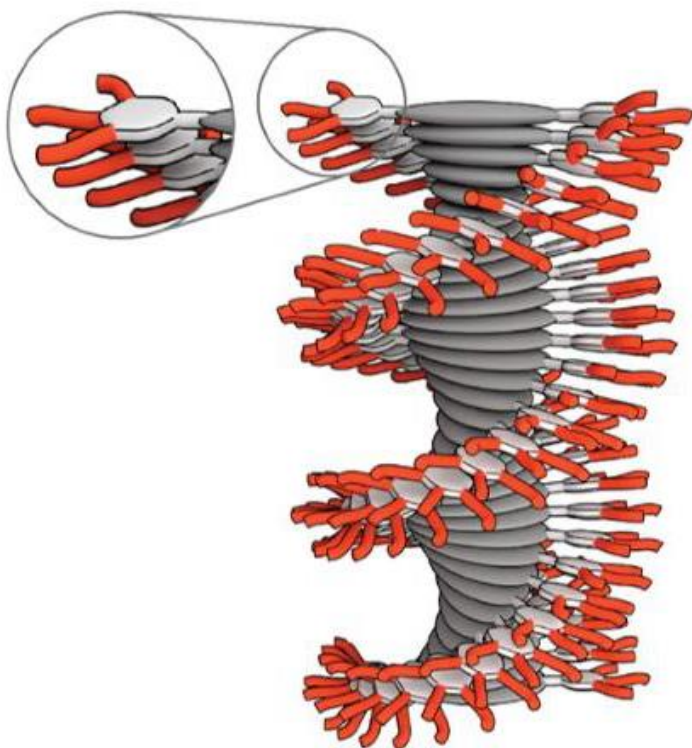


**What other properties the theory should explain?**

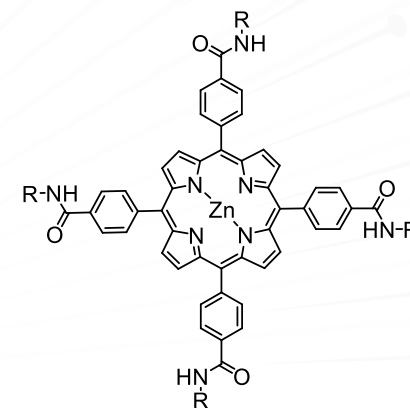
# CISS and Optical Activity

In collaboration with E.B. Meijer- Eindhoven

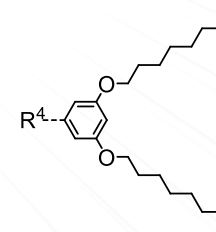
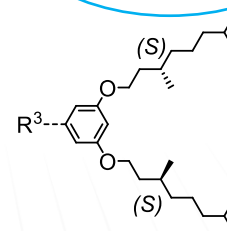
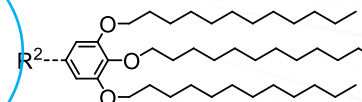
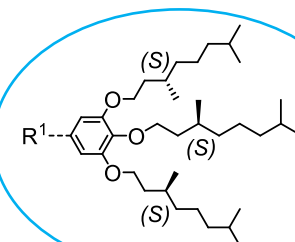
## Chiral and Achiral Fibers



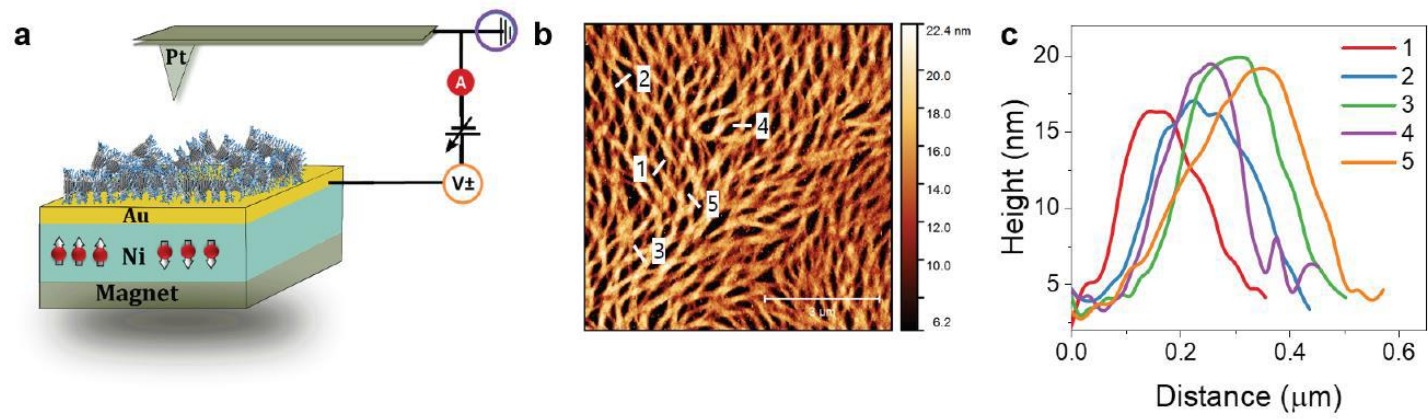
R = R<sup>1</sup> (S)-CBI-1  
R = R<sup>2</sup> ac-CBI-2  
R = R<sup>3</sup> (S)-CBI-3  
R = R<sup>4</sup> ac-CBI-4



R = R<sup>3</sup> (S)-Zn-P1  
R = R<sup>4</sup> ac-Zn-P2

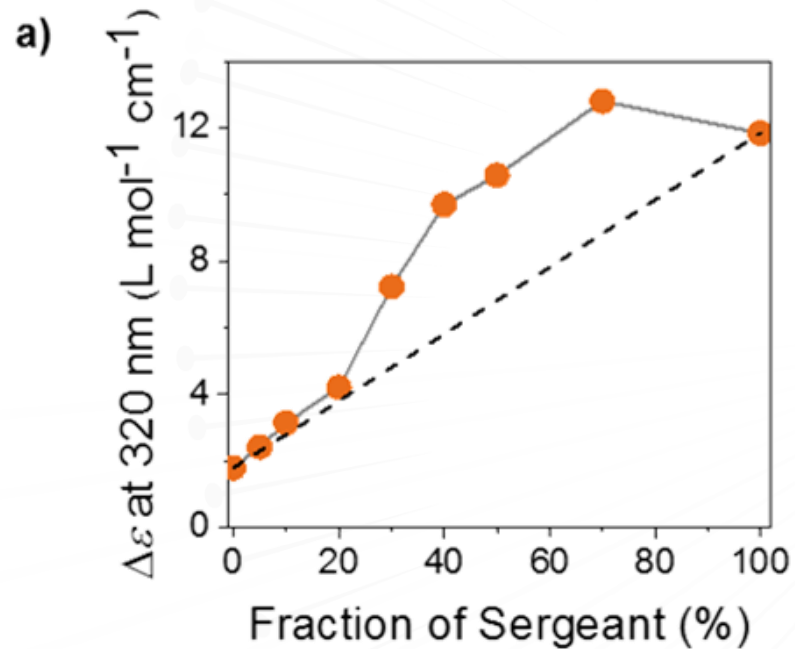


C. Kulkarni, A. K. Mondal, T. K Das, G. Grinbom, F. Tassinari, M. F. J. Mabesoone, E. W. Meijer, R. Naaman, *Adv. Mat.* 1904965 (2020).



# Sergeant and Soldier (S&S) principle for CBI-35 system

Intensity of the CD peak at 320 nm



There is correlation between the optical activity  
and the spin polarization

# Correlation between the CISS and Optical Activity

What do we mean by optical activity ?

**The CISS effect is related to the asymmetry factor ( $g$ ) of the molecules, namely to the anisotropic polarizability.**

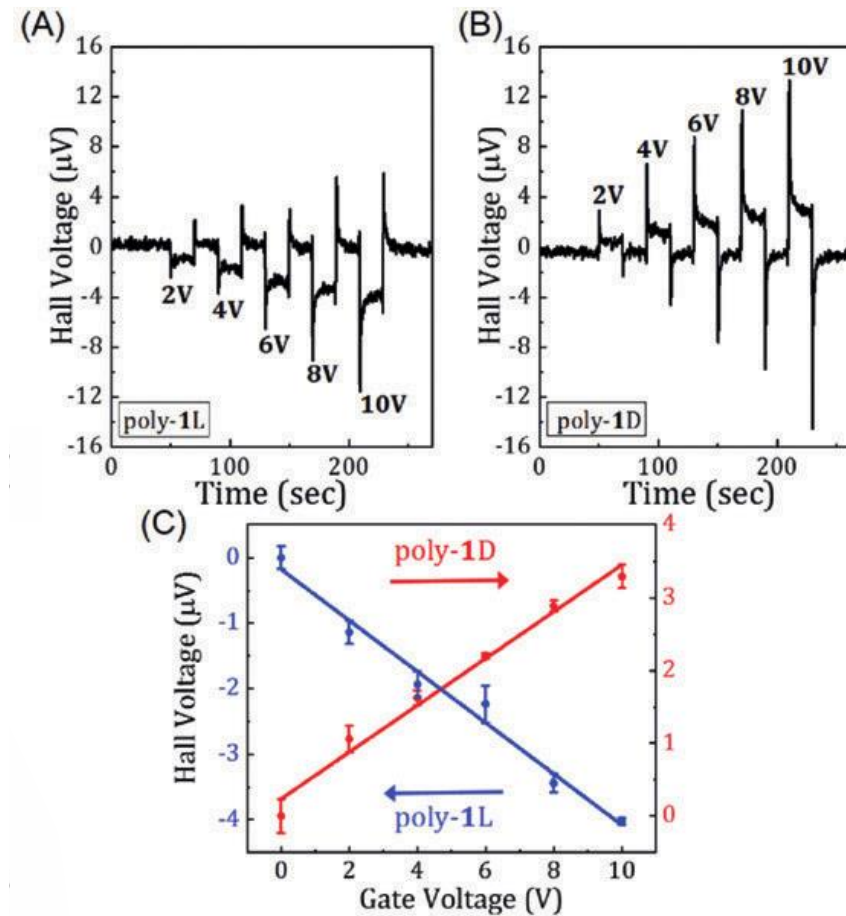
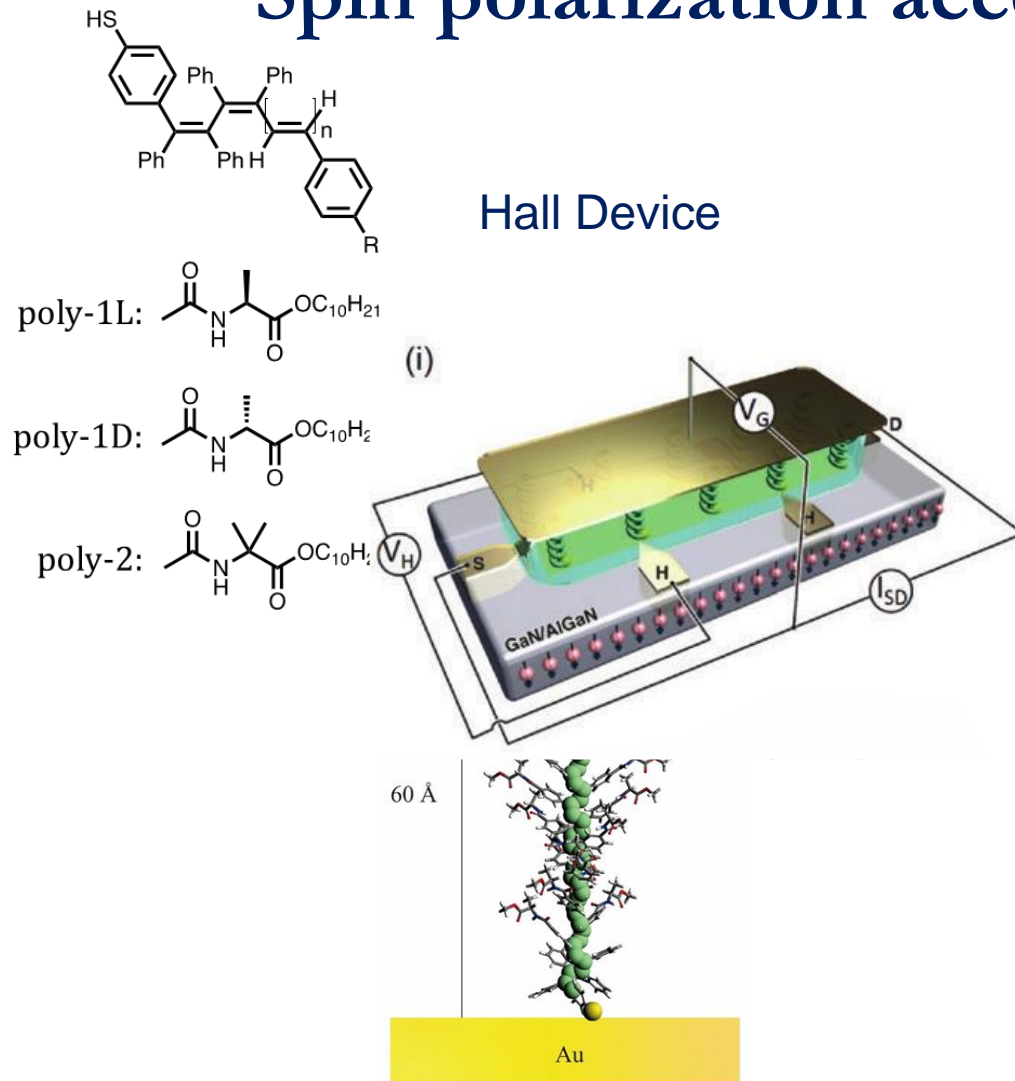
The CISS effect is correlated with optical activity

Optical Activity is a “non-localized” property.

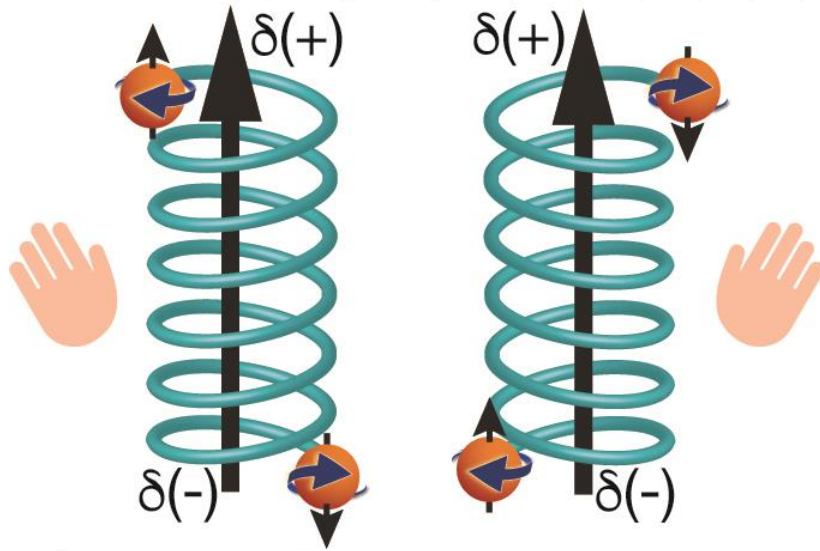
Hence CISS is a “non localized” effect.



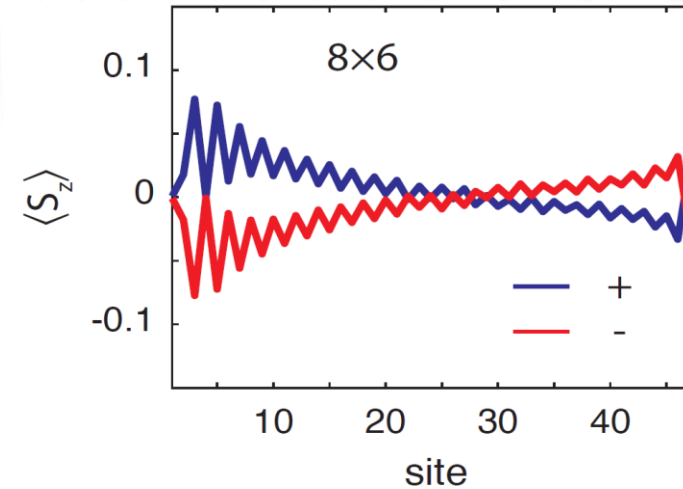
# Spin polarization accompanied charge polarization



S. Mishra, A. Kumar Mondal, E. Z. B. Smolinsky, R. Naaman, **K. Maeda**, **T. Nishimura**, **T. Taniguchi**, **T. Yoshida**, **K. Takayama**, **E. Yashima**, *Angew. Chemie* **59**, 2–8 (2020)



Theoretical verification:

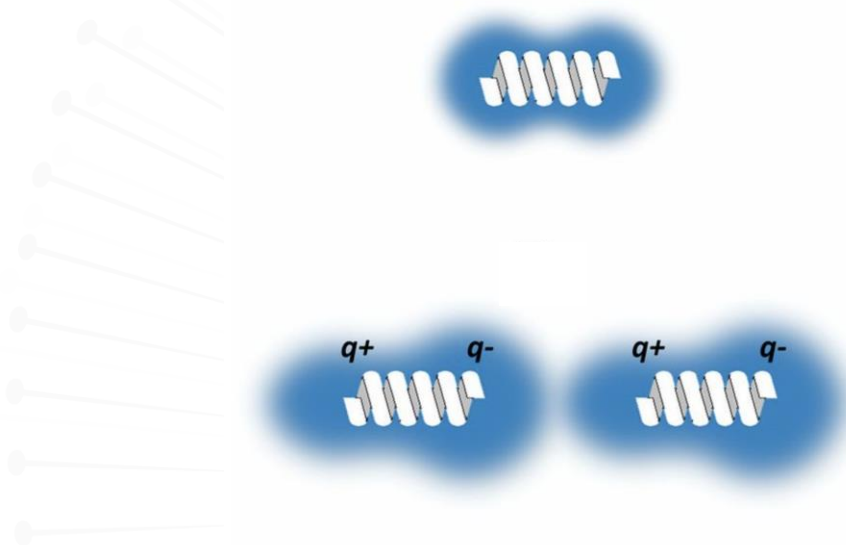


Jonas Fransson, Uppsala University.

*Phys. Rev. B*, 2020, 102, 235416; *Nano Lett.* 2021, 21, 3026.

- Upon electron being transferred through chiral system, the entanglement in the singlet state brakes.
- The electron's spin is strongly coupled to the molecular frame.

# Enhancement of Enantiorecognition



In chiral molecules charge polarization is accompanied by transient spin polarization.

This introduces new electronic interaction term which is enantio-specific when two chiral molecules interact.

A. Kumar, E. Capua, M. K. Kesharwani, J. M. L. Martin, E. Sitbon, D. H. Waldeck, R. Naaman, *PNAS*, **114**, 2474–2478 (2017).

# Importance of Spin Polarization in Protein Activity

S. Mishra, S. Pirbadian, A. K. Mondal, M. Y. **El-Naggar**, R. Naaman, Spin-Dependent Electron Transport through Bacterial Cell Surface Multiheme Electron Conduits, *J. Am. Chem. Soc.* **141**, 19198-19202 (2019).

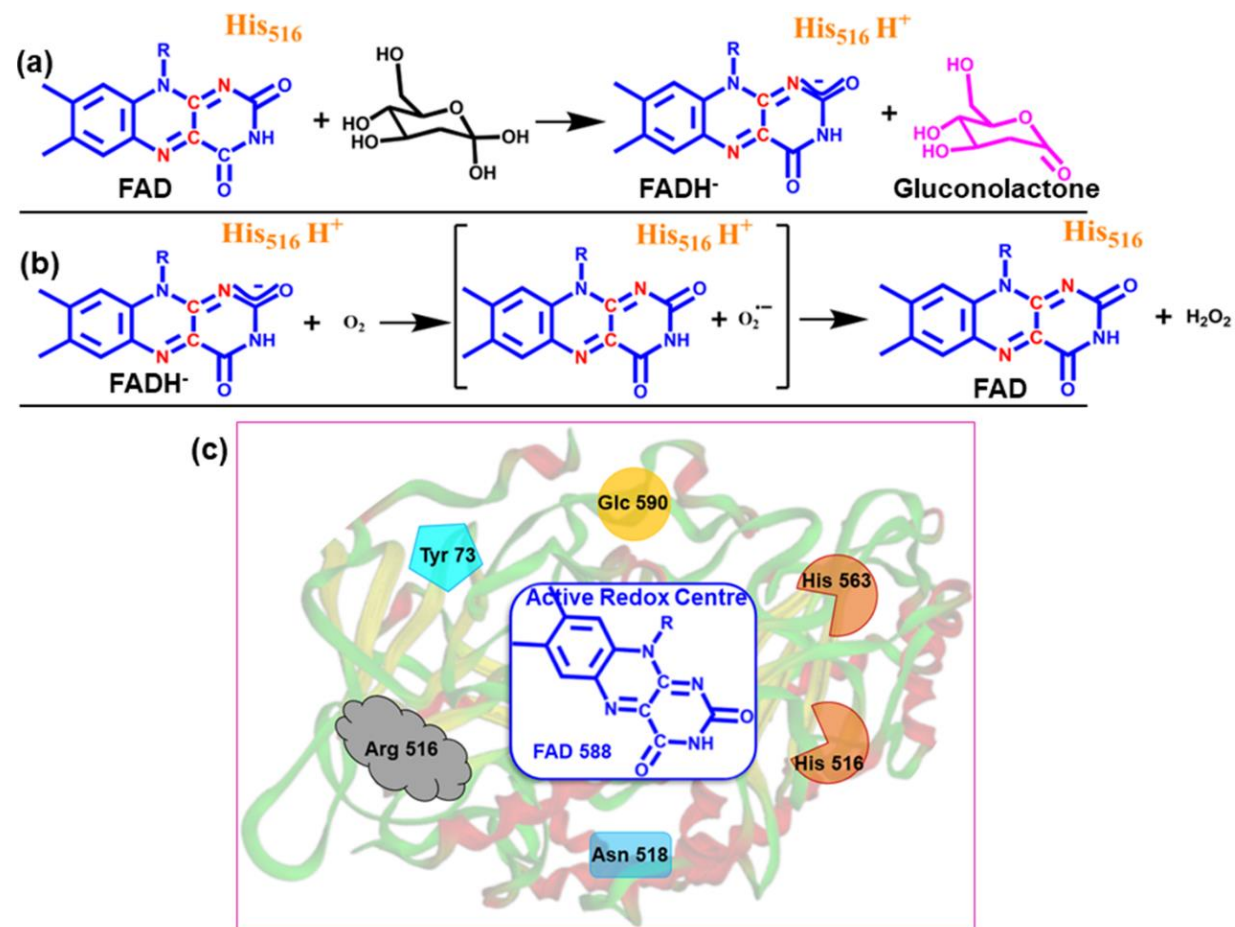
C. Niman, N. Sukenik, T. Dang, J. Nwachukwu, M. Thirumurthy, A. Jones, R. Naaman, K. Santra, T. Das, Y. Paltiel, L. Baczewski, M. **El-Naggar**. Bacterial Extracellular Electron Transfer Components are Spin Selective, *J. Chem. Phys.* **159**, 145101 (2023).

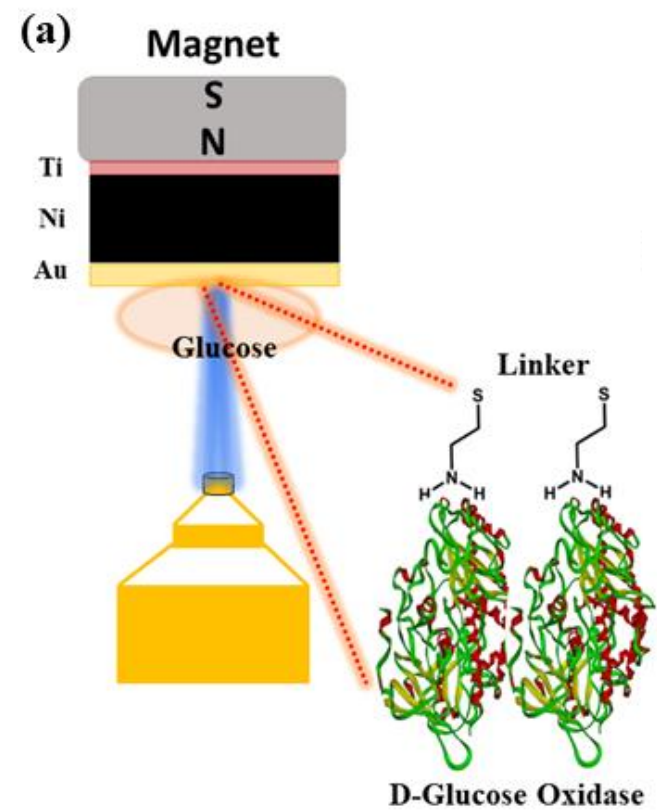
K. Banerjee-Ghosh, S. Ghosh, H. Mazal, I. Riven, G. Haran, R. Naaman, *JACS* **142**, 20456–20462 (2020).

S. Ghosh, K. Banerjee-Ghosh, D. Levy, I. Riven, R. Naaman, G. Haran, *J. Phys. Chem. Lett.* **12**, 2805-2808 (2021).

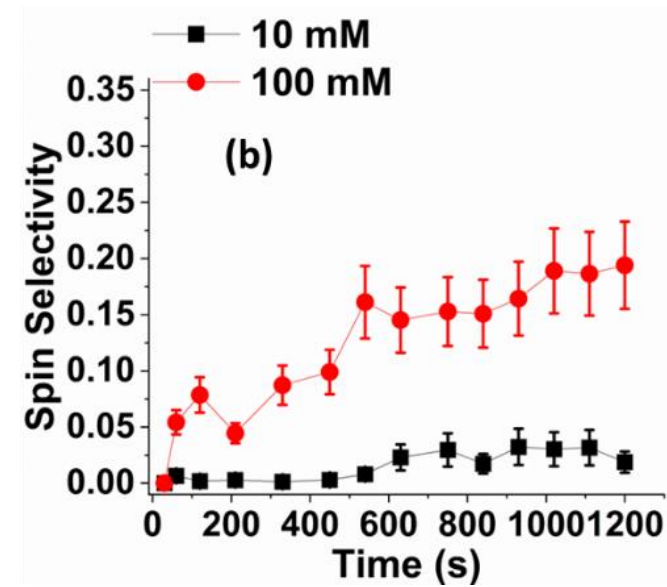
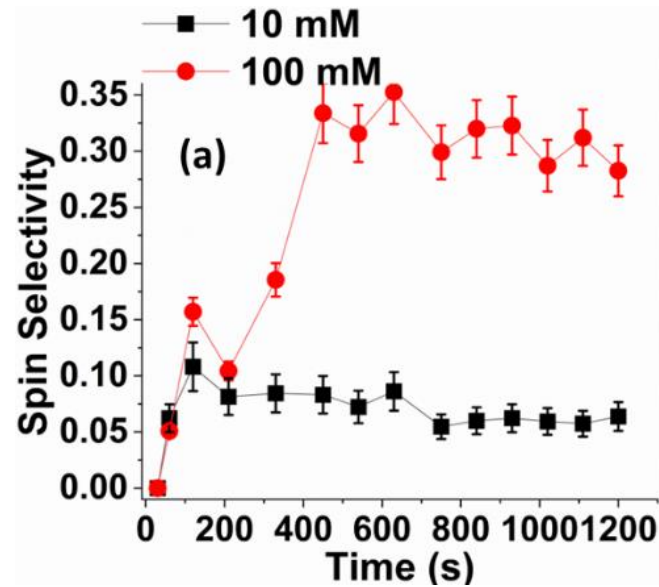
# The Importance of Spin-Polarized Charge Reorganization in the Catalytic Activity of D-Glucose Oxidase

Naupada Preeyanka, Qirong Zhu, Tapan-Kumar Das, and Ron Naaman, *PhysChemPhys* e202400033 (2024).





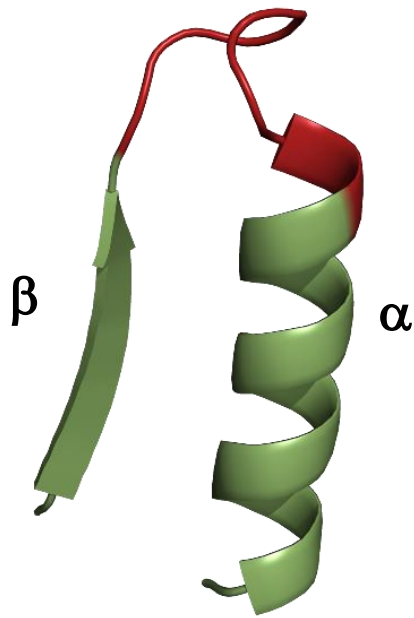




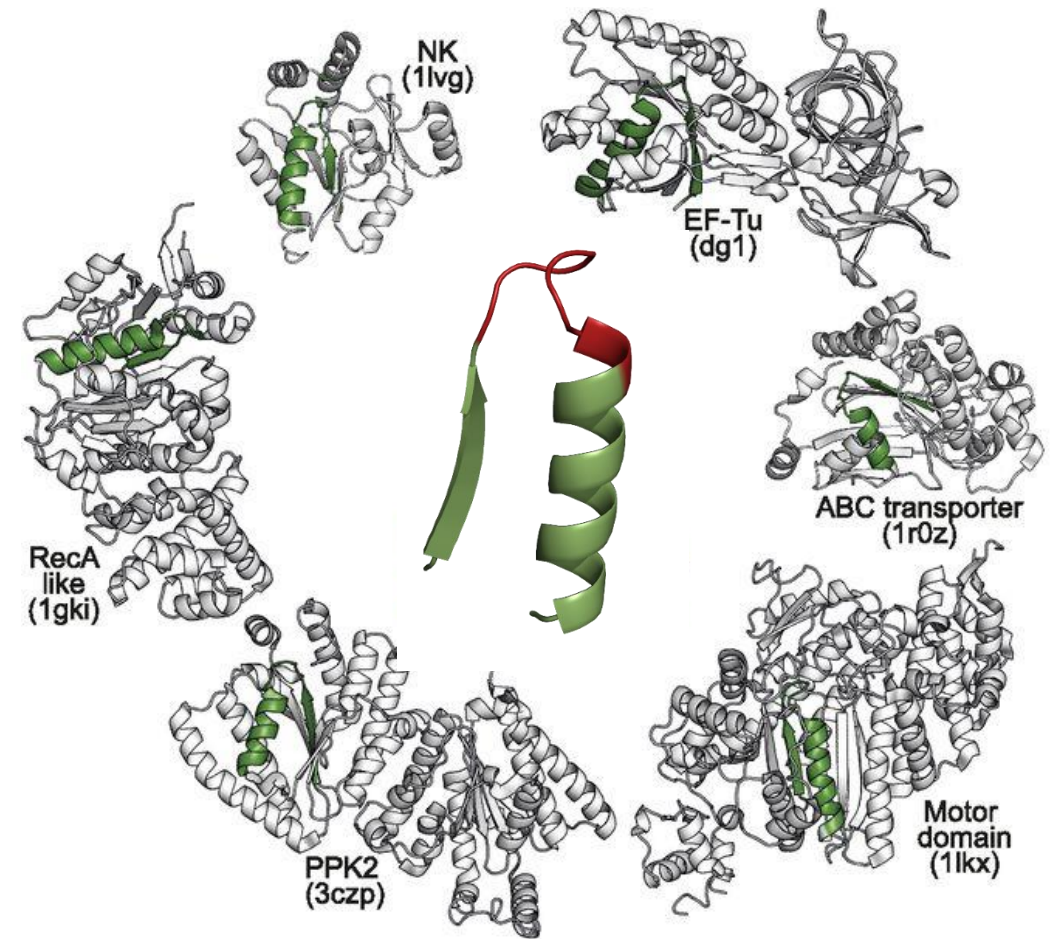
The spin selectivity of the kinetics of the reaction of GOx in the presence of (a) D-glucose and (b) L-glucose for glucose concentrations of 10 mM and 100 mM (black and red, respectively).

# The P-loop motif & P-loop NTPases

P-loop or Walker A motif  
**GxxGxGK(T/S)**



Embedded in a  $\beta$ -(P-loop)- $\alpha$  element

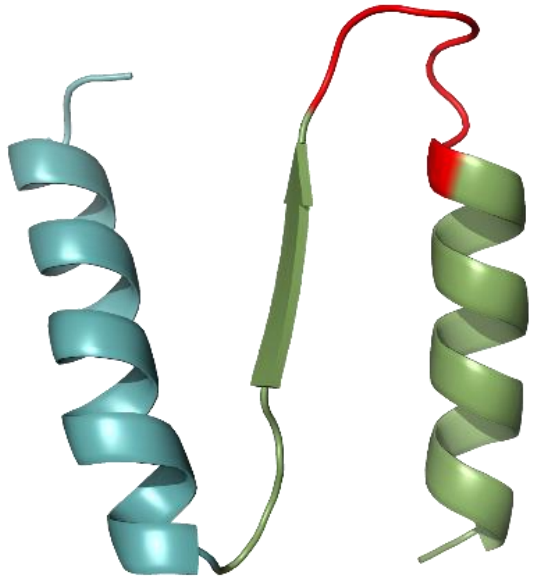


Functionally diverse, abundant and **ancient**

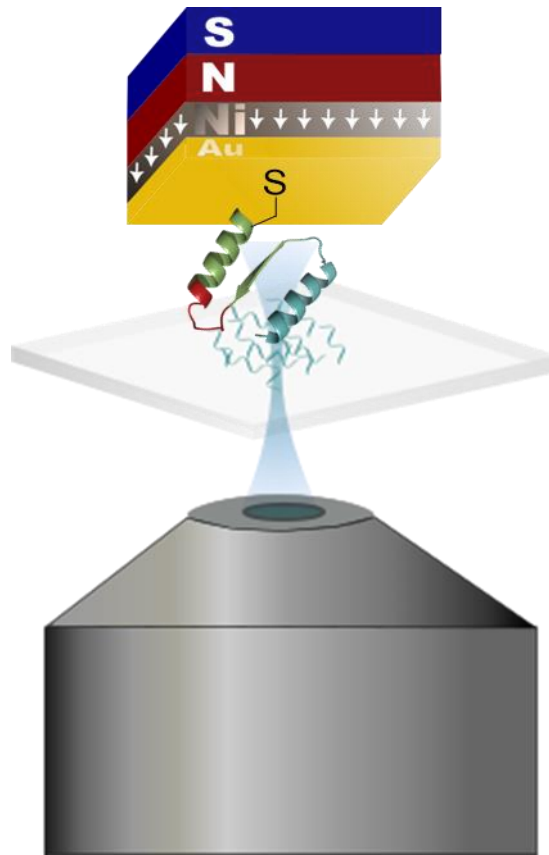


# The role of spin in protein-DNA interaction

**Pratik Vyas, Kakali Santra,** Naupada Preeyanka, Anu Gupta, Orit Weil-Ktorza, Qirong Zhu, Liam M. Longo, Jonas Fransson, Norman Metanis, and Ron Naaman



**N-αβα prototype**  
**α<sub>2</sub>β<sub>1</sub>-(P-loop)-α<sub>1</sub>**

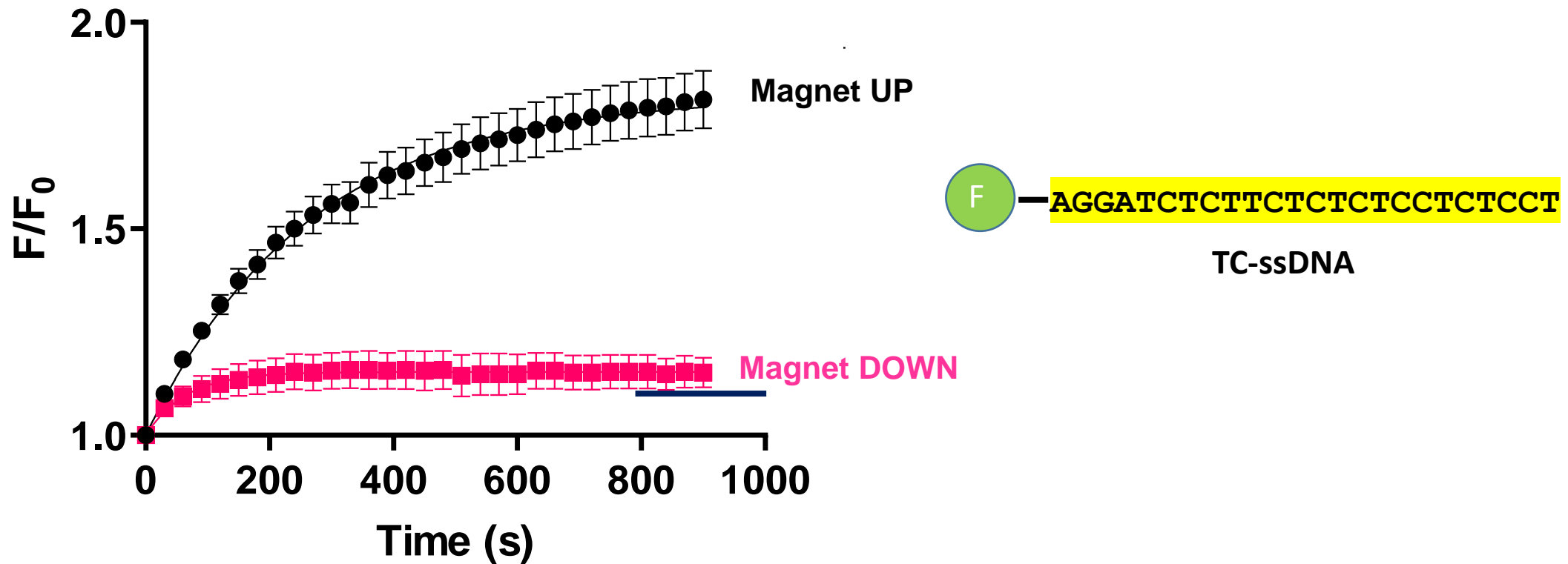


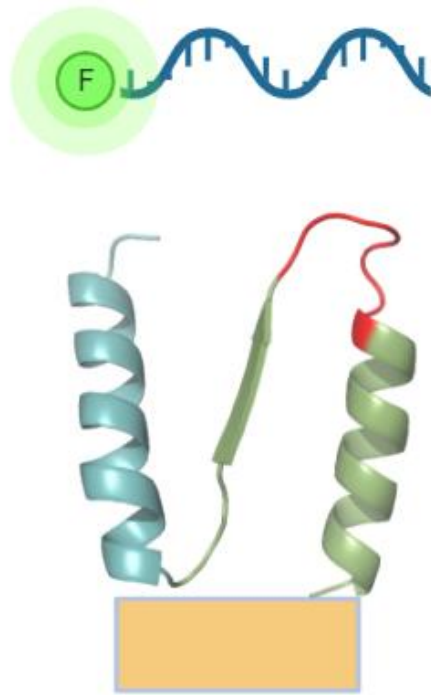
It is hypothesized that proteins and enzymes emerged via duplication and fusion of relatively short ‘seeding’ peptides with simple secondary structures.

Romero MLR, Rabin A, **Tawfik DS**. Functional Proteins from Short Peptides : Dayhoff s Hypothesis Turns 50. *Angew Chem Int Ed Engl.* 2016;1980:15966-15971.

**Vyas P**, Malitsky S, Itkin M, **Tawfik D**. On the origins of enzymes: Phosphate-binding Polypeptides Mediate Phosphoryl Transfer to Synthesize ATP. *J Am Chem Soc.* 2023;Accepted.

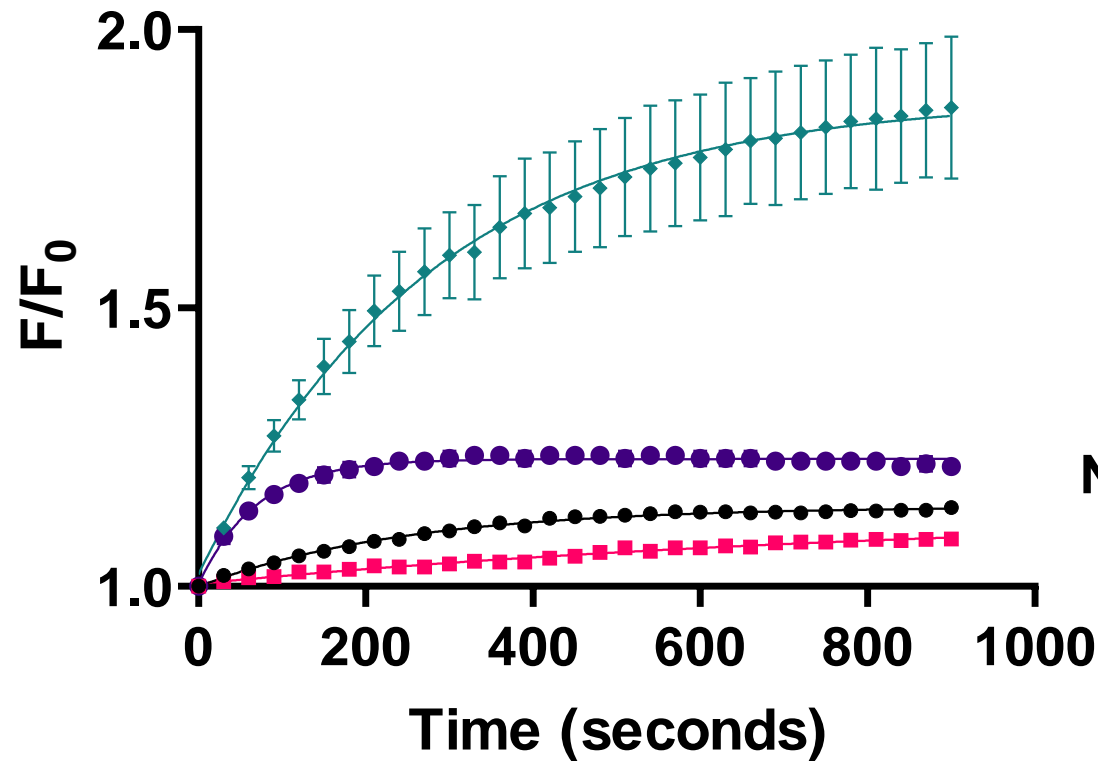
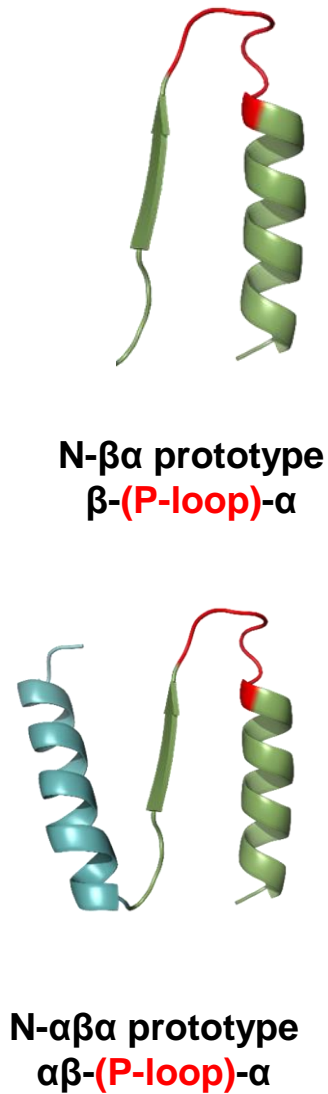
# ssDNA binding function is 'spin-selective'





The “effective polarizability” of the protein affects the binding to the DNA.

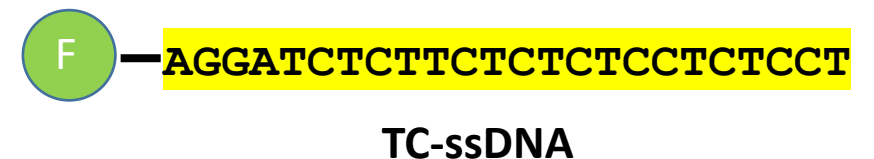
Even motifs that are not in immediate contact with the active site, affect the binding strength.



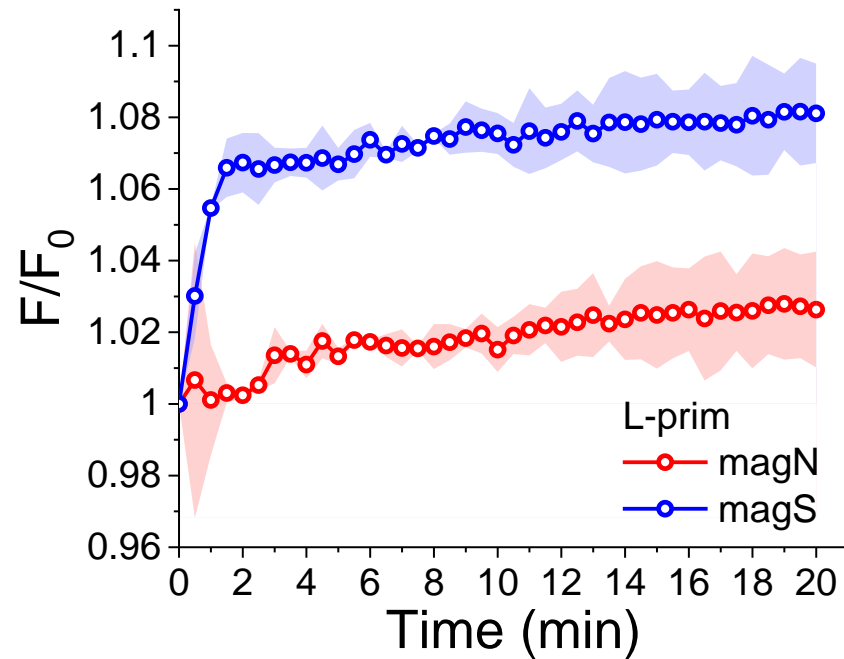
N-αβα + Magnet UP

N-αβα + Magnet DOWN

N-βα + Magnet UP & N-βα + Magnet DOWN



# Effect of spin on the interaction between primordial protein and double helix DNA



Prof. Norman Metanis  
Hebrew University, Jerusalem

Dr. Kakali Santra

## L-Primordial(29-60) Sequence

CSIERIRRASVEELTEVPGIGPRLARRILERL

## Sequence for DNA binding:

Top strand

5'-6-FAM/TAGATCGATCGC-3'

Bottom strand

5'-GCGATCGATCTA-3'

The interaction between the DNA and the protein  
does **NOT** depend on the spin.

The polarizability of the protein IS.

# Conclusions

1. The CISS effect enables long range electron transfer.
2. Spin selective chemistry is enabled and spin-controlled reactions (like hydrogen evolution and oxygen reduction) are enabled.
3. Spin long range transport enables spin-interconnect.
4. Enantio-recognition is enhanced.
5. Enantio-separation is enabled by spin polarized surfaces.
6. The model for the mechanism of the CISS effect requires non-BO interactions and introducing of many electrons effects.





A. K. Mondal



K. Santra



Y. Sang



F. Tassinari



E. Z.  
Smolinsky



S. Mishra



K. Banerjee-  
Ghosh



T.K. Das



A. Kumar



N. Preeyanka



Q. Zhu



P. Vyas



D. Bhowmick



A. Kumar

# Thank you



Funded by  
the European Union

