WEIZMANN INSTITUTE OF SCIENCE

Chirality, Spin, and Phonons- The Right Combination

Ron Naaman
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Weizmann Institute, Israel

The Chirality Induced Spin Selectivity (CISS) Effect

Any motion of electrons in chiral medium depends on the electrons' spin.

Which spin is preferred depends on the handedness of the system and the direction of the electron's motion.

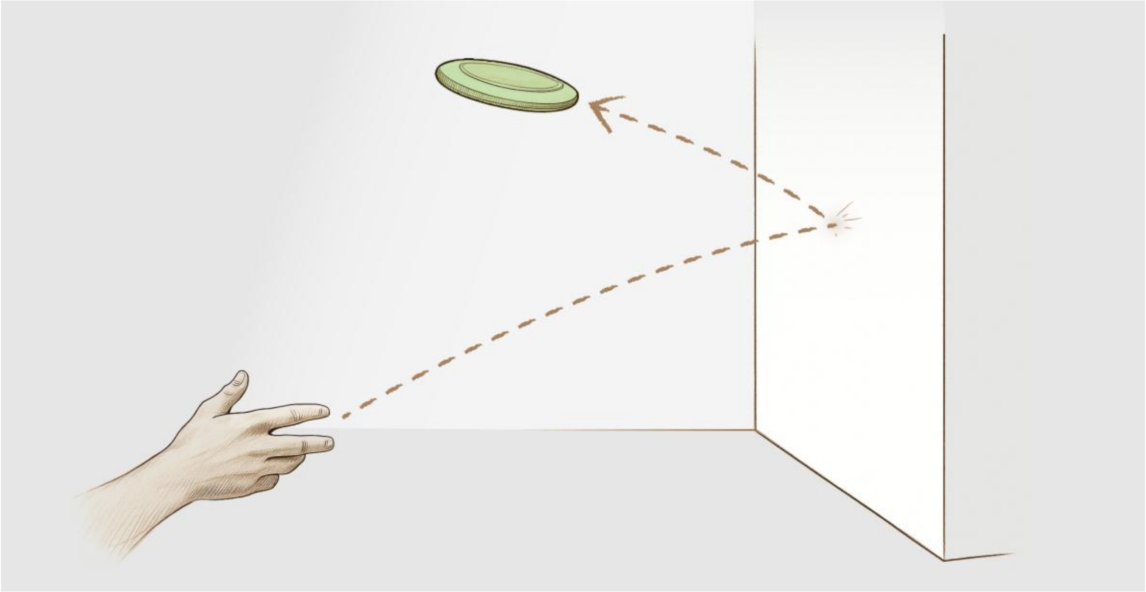
The CISS effect provides-

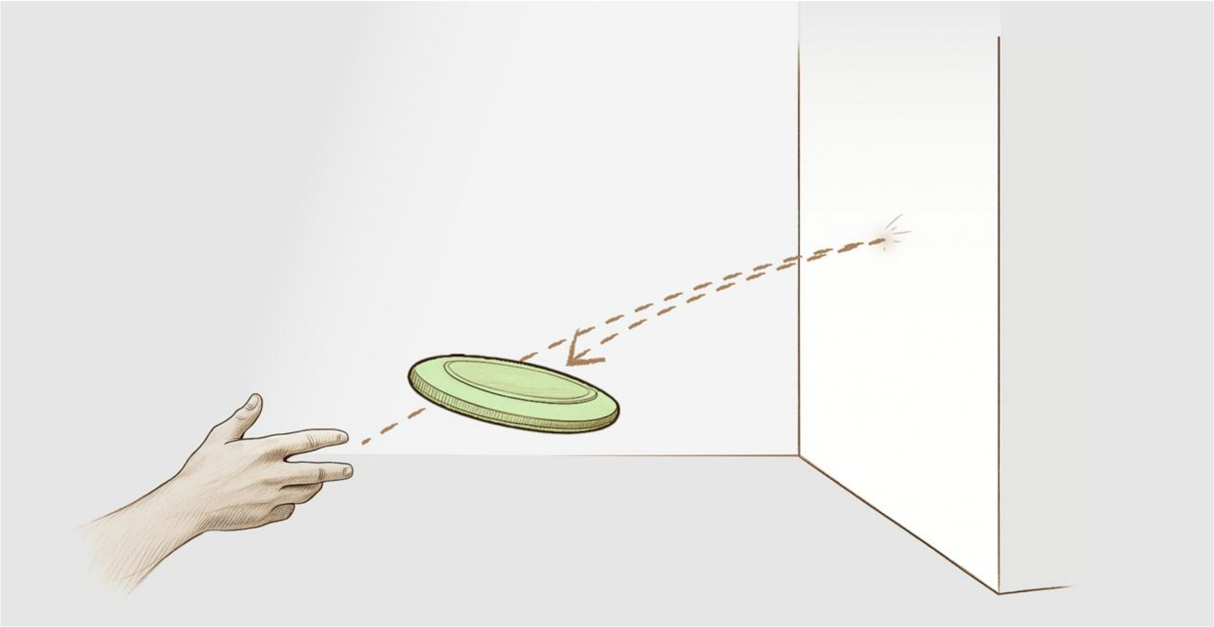
Spin polarized electrons, at room temperature, without ferromagnet using nanometric "device".

The Freesbee effect

What is required for the effect ?

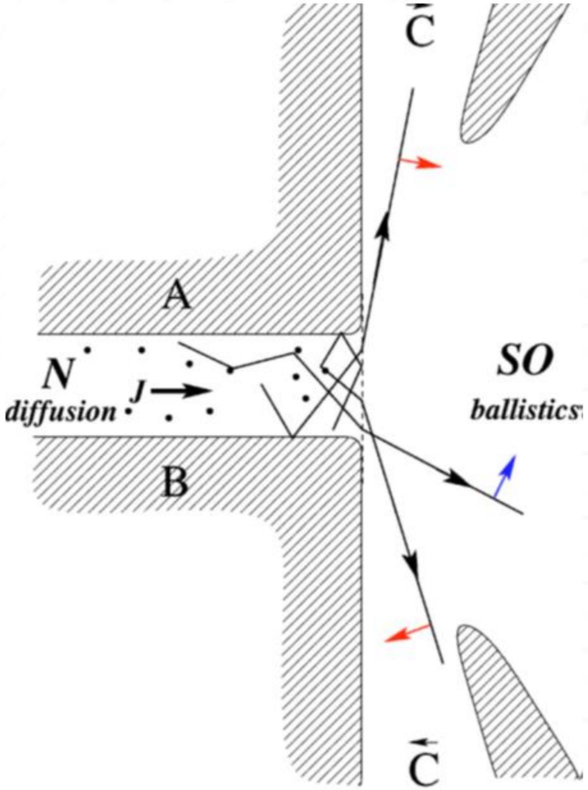
- Angular momentum
- Friction- Spin orbit coupling +dissipation.



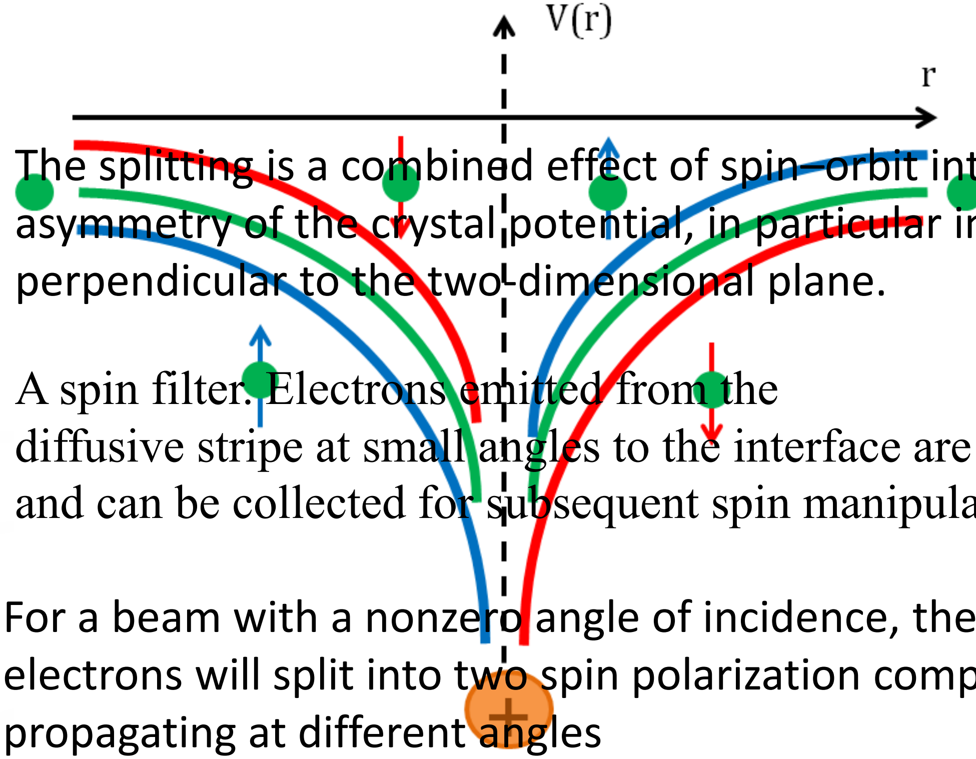


Spin polarization at room temperature without ferromagnet

Rashba scattering



Mott scattering



The splitting is a combined effect of spin–orbit interaction and asymmetry of the crystal potential, in particular in the direction perpendicular to the two-dimensional plane.

A spin filter. Electrons emitted from the diffusive stripe at small angles to the interface are spin polarized and can be collected for subsequent spin manipulations.

For a beam with a nonzero angle of incidence, the transmitted electrons will split into two spin polarization components propagating at different angles

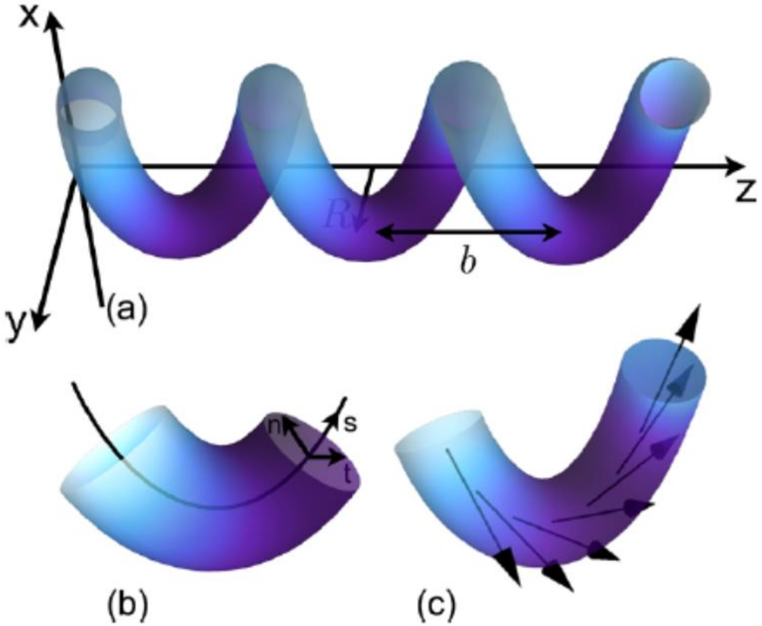
M. Khodas, A. Shekhter, and A.M. Finkel'stein, PRL, 92 086602 (2004)
A. Shekhter, M. Khodas, and A. M. Finkel'stein, PHYSICAL REVIEW B 71, 125114 s2005d
Kohda et al. Nat. Comm. 3, 1082 (2012)

Momentum conservation

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

In solids, that ha ns can exchange momentum with t

In insulators/m are localized and therefore moment ency vibrations that have angular 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);

- While for electrons moving in straight line, interaction with 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 electrons/vibrations/phonons.
- The interaction with the system introduces two important effects-

The role of polarizability,

Dissipation

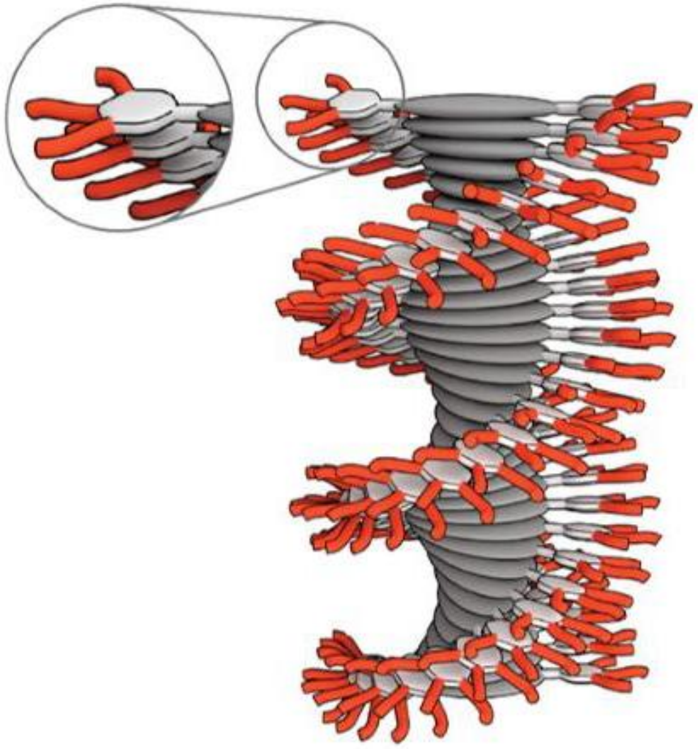
Longlong Zhang, Yuying Hao, Wei Qin, Shijie Xie, Fanyao Qu, PHYSICAL REVIEW B 102, 214303 (2020). Role of polarons.

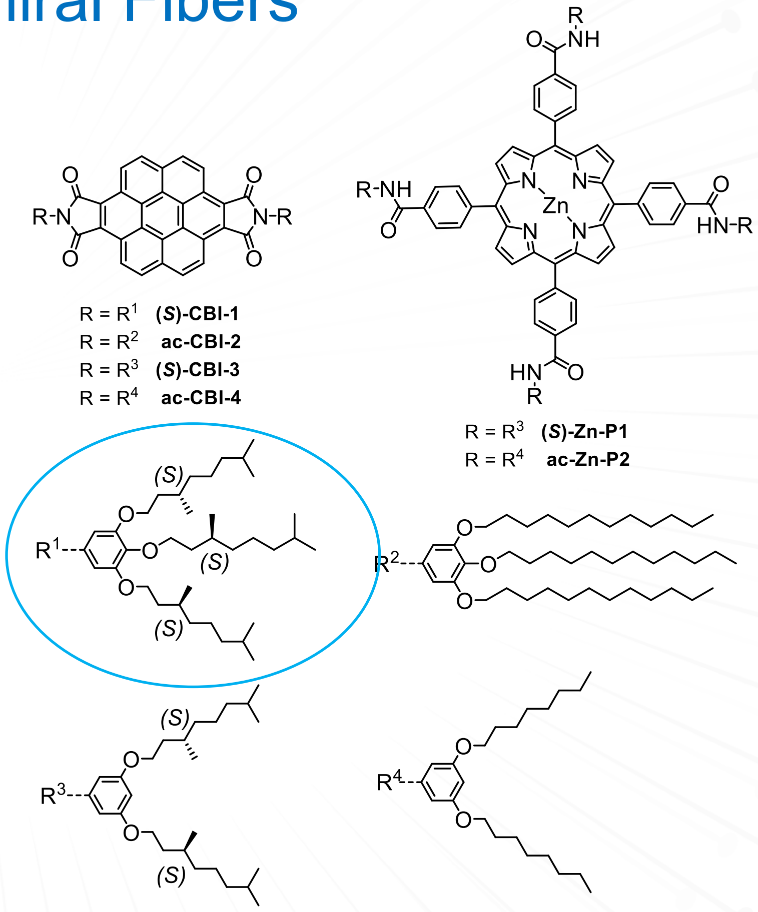
Gui-Fang Du, Hua-Hua Fu, Ruqian Wu. PHYSICAL REVIEW B 102, 035431 (2020) Role of phonons in DNA

CISS and Optical Activity

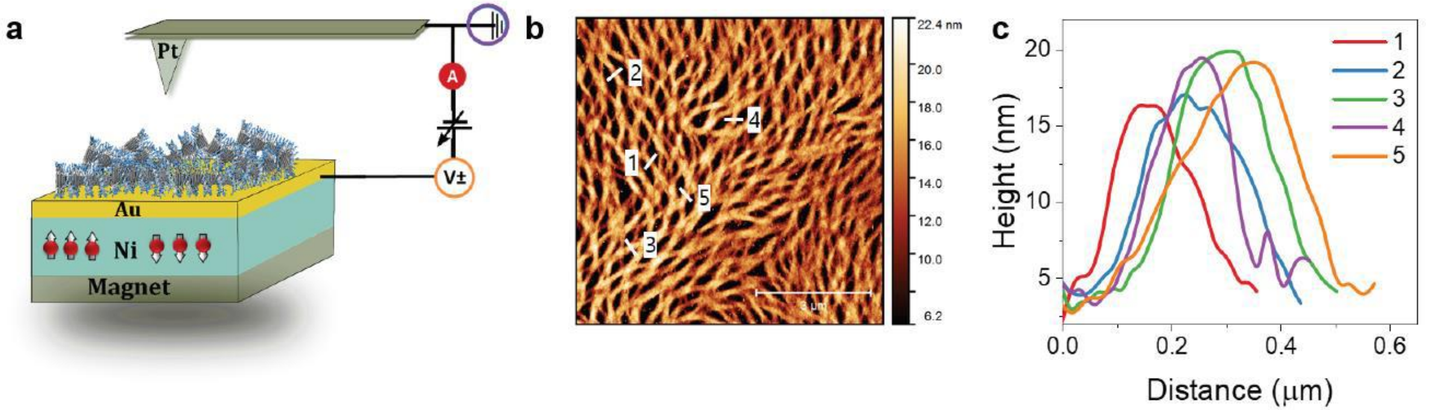
In collaboration with E.B. Meijer- Eindhoven

Chiral and Achiral Fibers



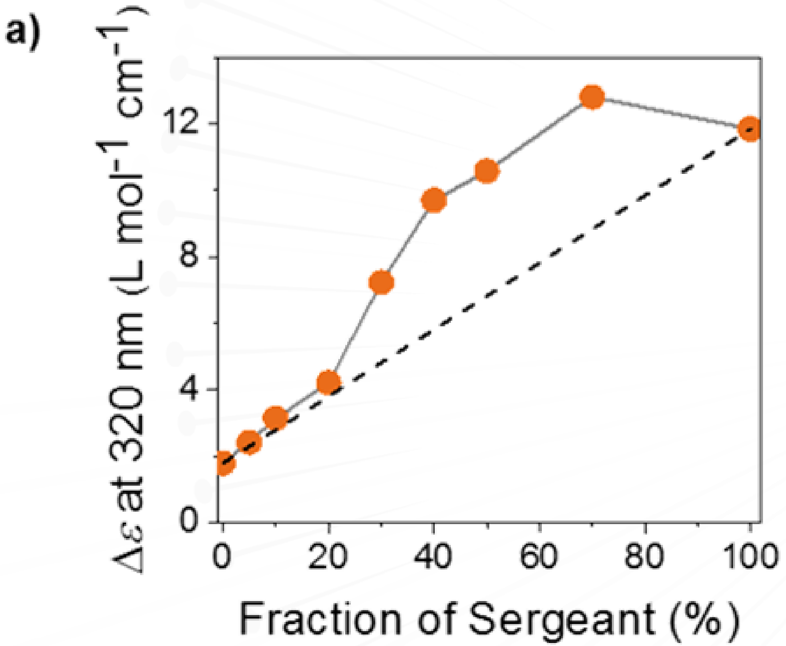


C. Kulkarni, A. K. Mondal, T. K Das, G. Grinbom, F. Tassinari, M. F. J. Mabesoone, E. W. Meijer, R. Naaman, *Adv. Mat.* 1904965 (2020).


a
Pt
A
V±
Au
Ni
Magnet
b
22.4 nm
20.0
18.0
16.0
14.0
12.0
10.0
6.2
c
Height (nm)
Distance (μm)
1
2
3
4
5

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

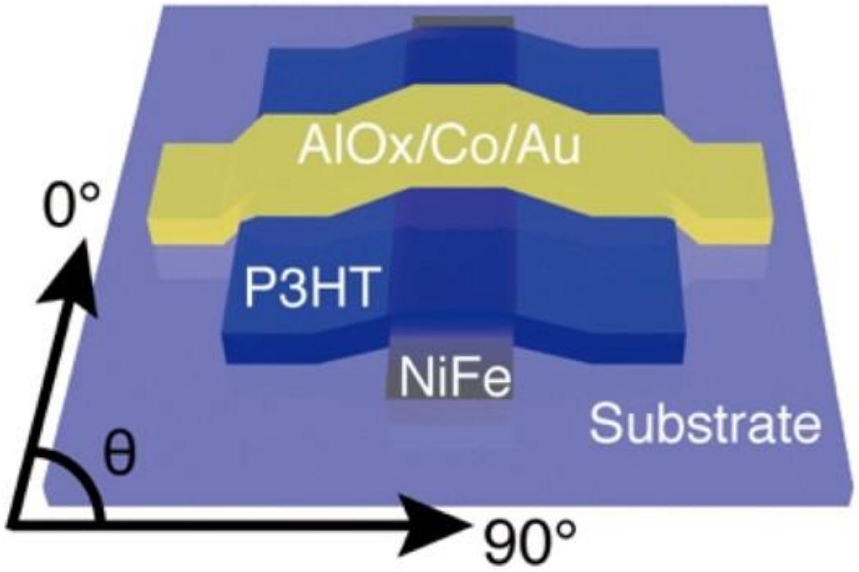
Correlation between the CISS and Optical Activity

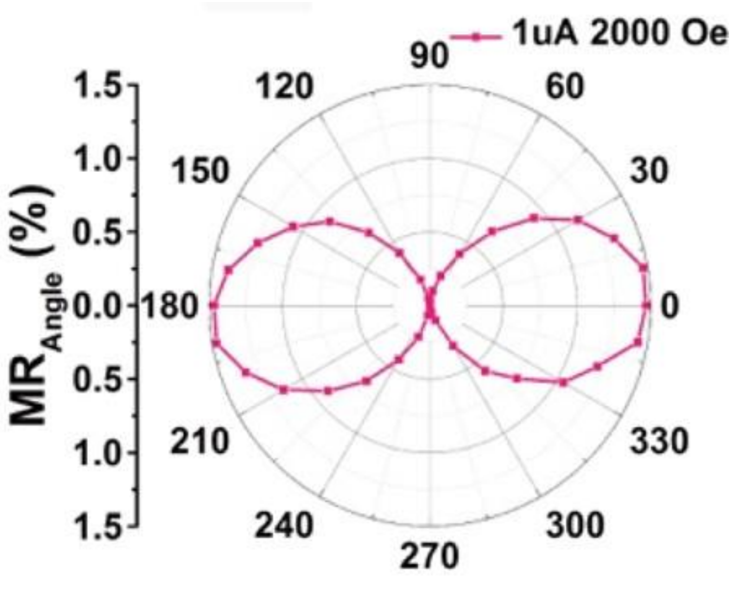
What do we mean by optical activity ?

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

D. Amsallem, A. Kumar, R. Naaman, **O. Gidron**, *Chirality* 1-7. (2023).

Anisotropic Magnetoresistance in Spintronics Devices

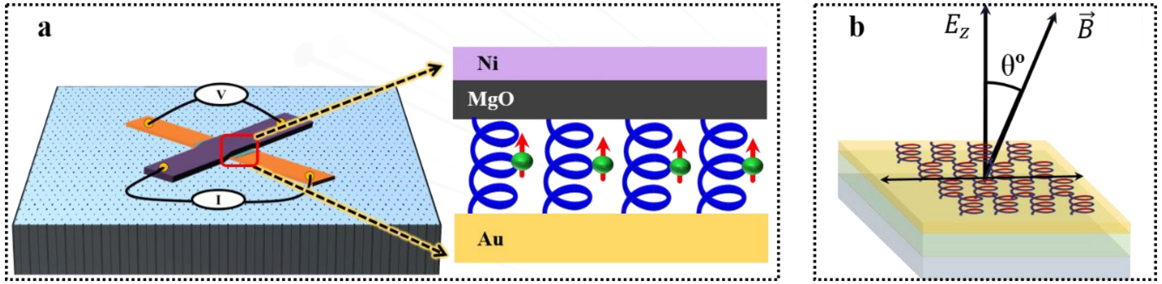




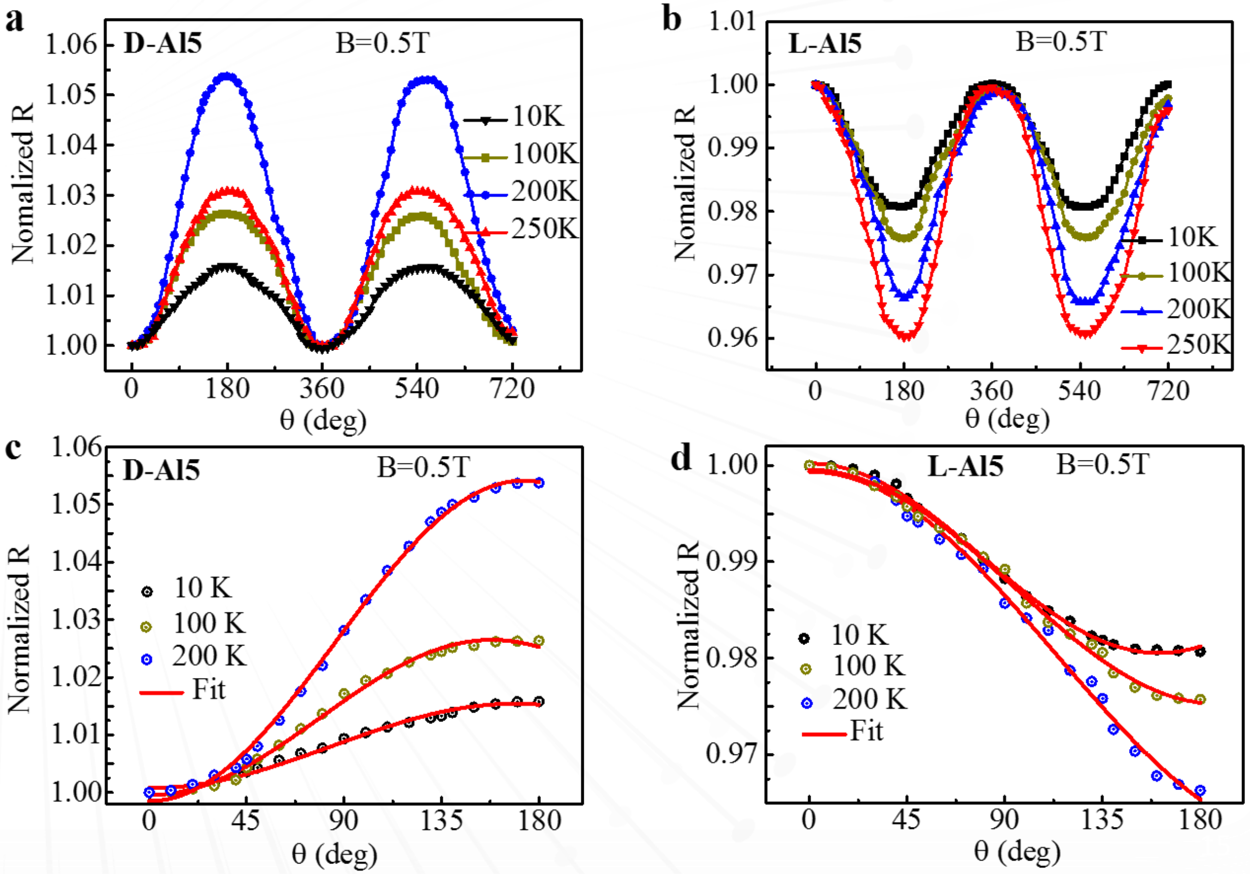
Anisotropic Magnetoresistance in NiFe-Based Polymer Spin Valves
Shuaishuai Ding, Yuan Tian, Huanli Dong, Daoben Zhu, and Wenping Hu

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

Anisotropic Magnetoresistance in CISS



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

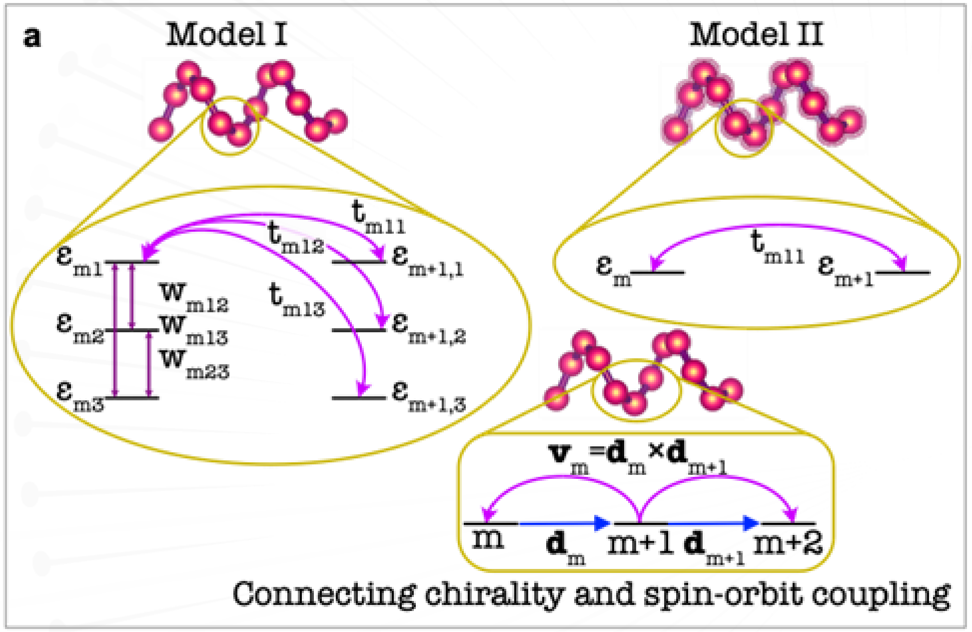


The angle dependent resistance curves were fitted to

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

Like in GMR.

Theory by Jonas Fransson



Conclusions from the simulation of the angle dependent

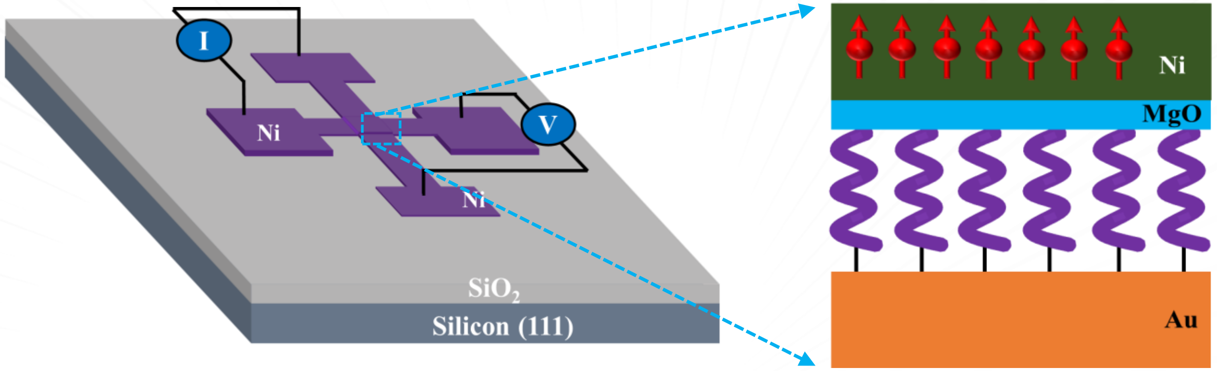
- SOC in the lead/s can induce spin polarization but no angle dependent.
- SOC in the molecule and electron-electron interactions result in angle dependent, but not the same as observed experimentally.
- Only SOC in the molecule **and** electron-electron **and** electron-phonons **and** dissipation, produces the experimental results.

These conclusions are consistent with the works of

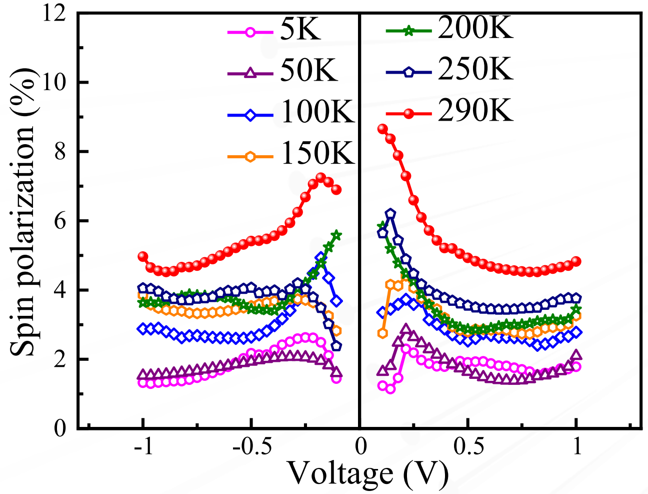
Dali Sun and Dave Waldeck: *Sci Adv.* 2024, 10, eadn3240.

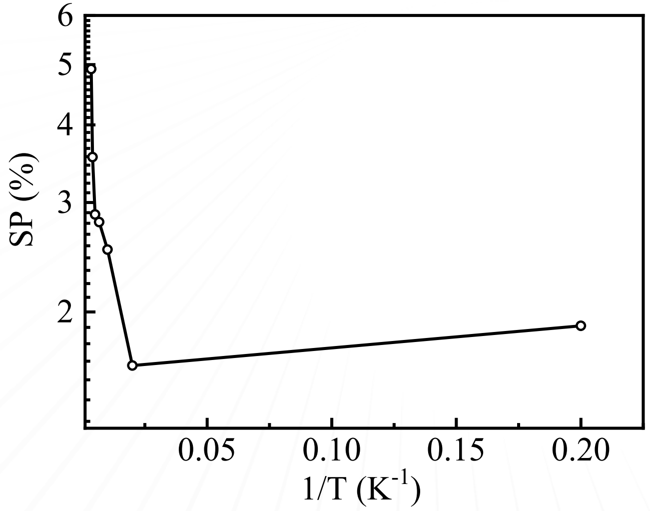
Angela Wittman and Yossi Paltiel: Chiral-induced unidirectional spin-to-charge conversion, *Sci. Adv.*11,eado4285 (2025).

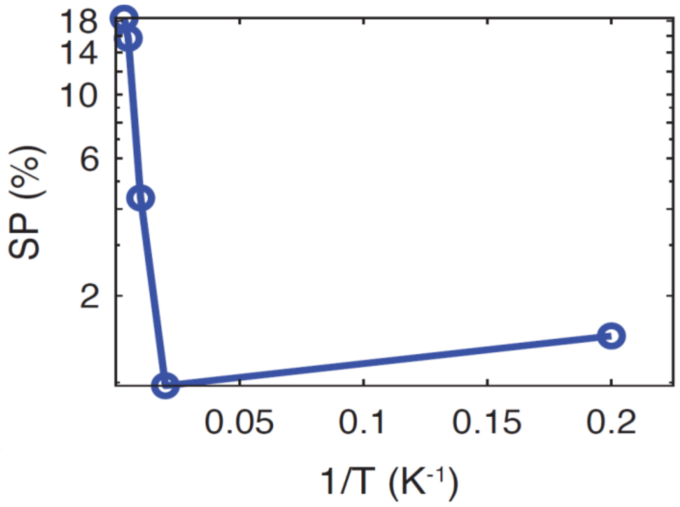
The role of phonons



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





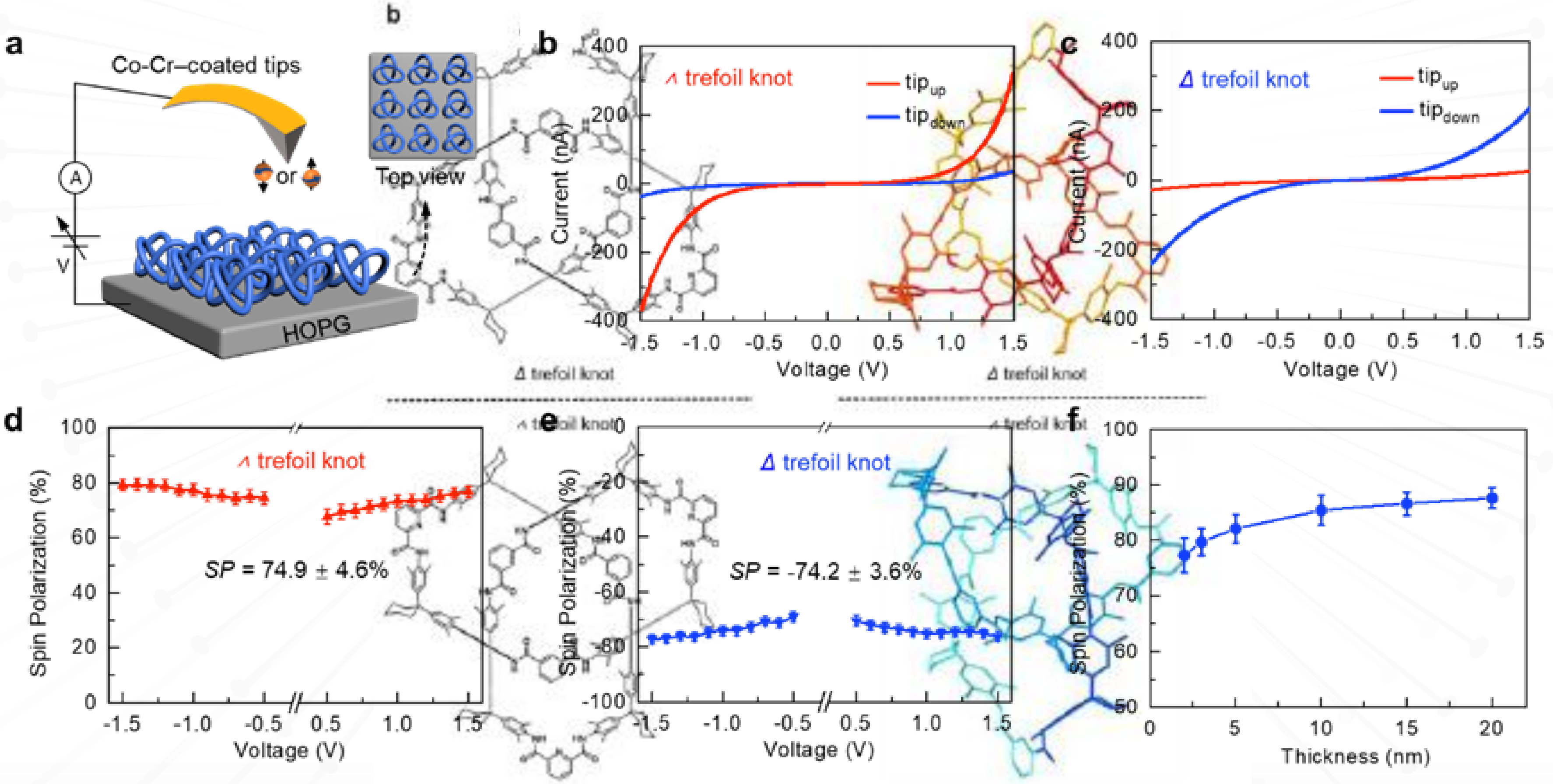


Theory by:
Jonas Fransson, Uppsala University

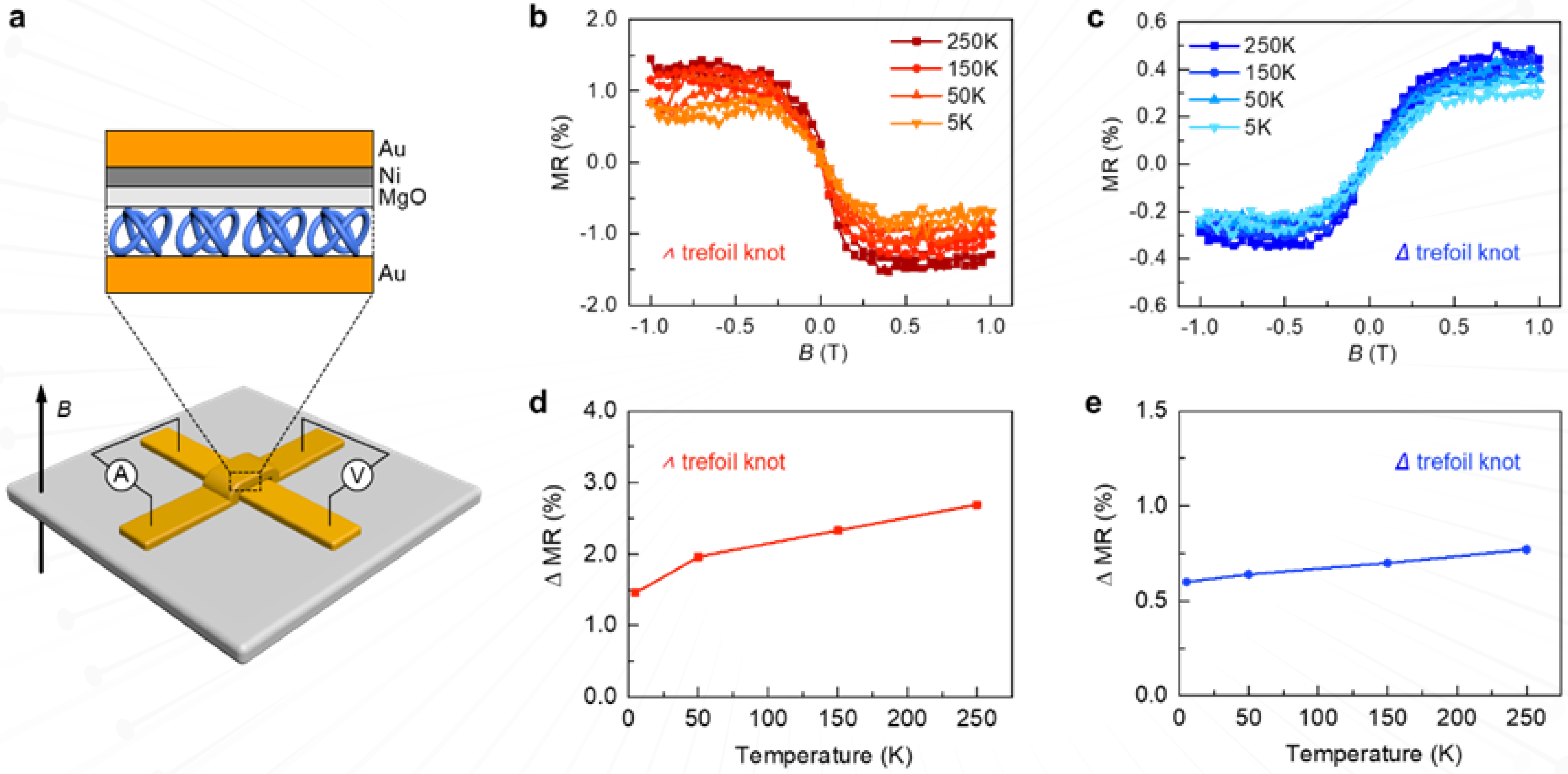
T. K. Das, **F. Tassinari,** R. Naaman**, J. Fransson,** *J. Phys. Chem. C*, **126**, 3257 (2022).

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

The role of chiral phonons:

The effect of vibrations on the SOC: For introducing the vibrations we follow Fransson and expand the electric field by the vibrational coordinates, namely go beyond the BO approximation. Then we get for the first term in the expansion:

$$E(Q) = E(Q_0) + \frac{1}{2}\left(\frac{\delta E}{\delta Q} Q\right)_{Q_0} + \cdots. \qquad (1)$$

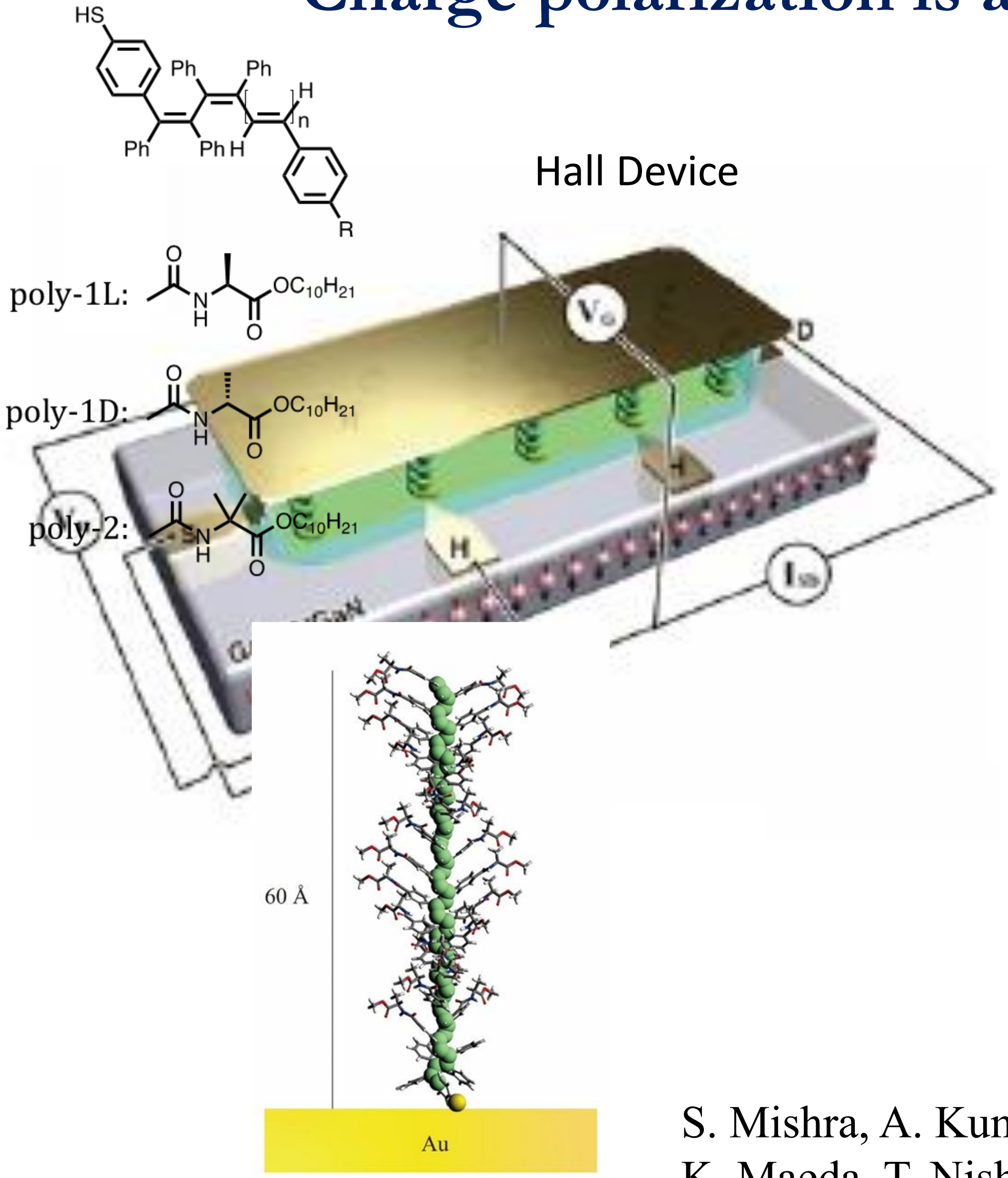
The matrix elements for the first correction term will be:

$$\langle \psi_i | \delta E / \delta Q | \psi_i \rangle \langle \varphi_i | Q | \varphi_{i+1} \rangle \qquad (2)$$

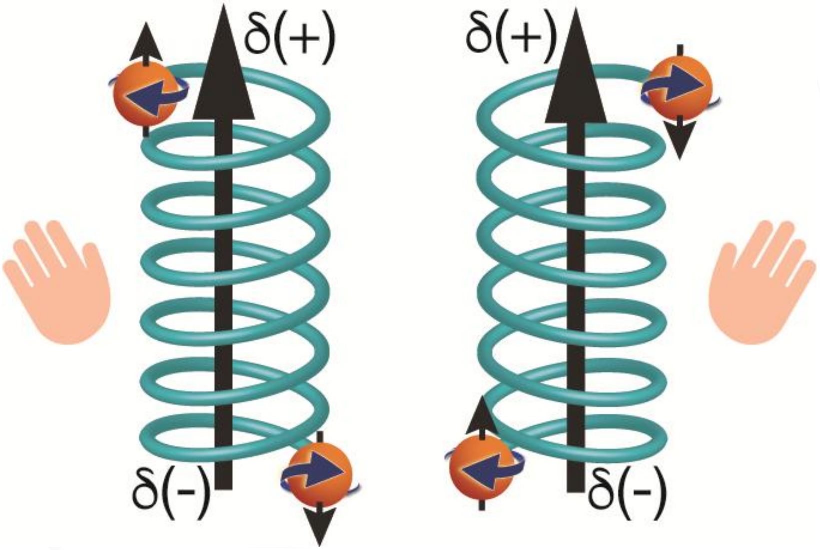
When ψ_i and φ_i are the electronic and vibrational BO states respectively.

From equation 2 we learn that in order it to be nonzero the symmetry of the vibration should be the same as of the electric field. Namely for chiral electric field we must have chiral vibration.

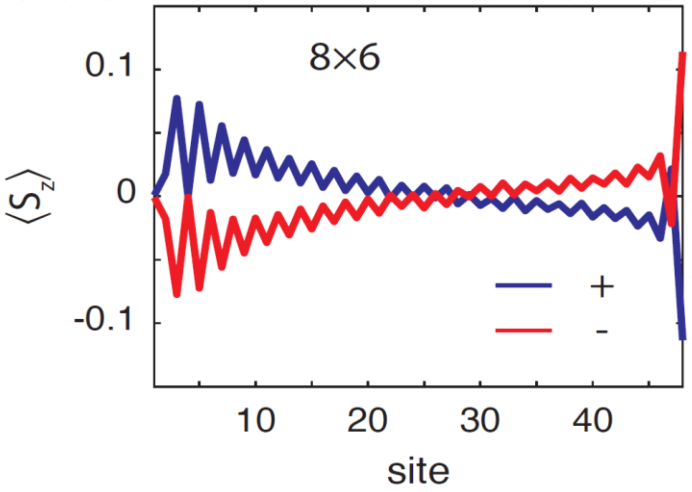
Charge polarization is accompanied by spin polarization



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 electrons being redistributed in chiral systems, the entanglement in the singlet state brakes, at list partially.

- The electron’s spin is strongly coupled to the molecular frame.

Spin polarization accompanied the charge polarization

- EPR studies (M. Wasielewski) verify the spin polarization without any substrate. (Hannah J. Eckvahl et al. , Science 382,197-201(2023). Hannah J. et al, J. Am. Chem. Soc. 2024, 146, 34, 24125–24132)

- Enantioselective interaction between chiral molecules.

- Interaction with ferromagnets-

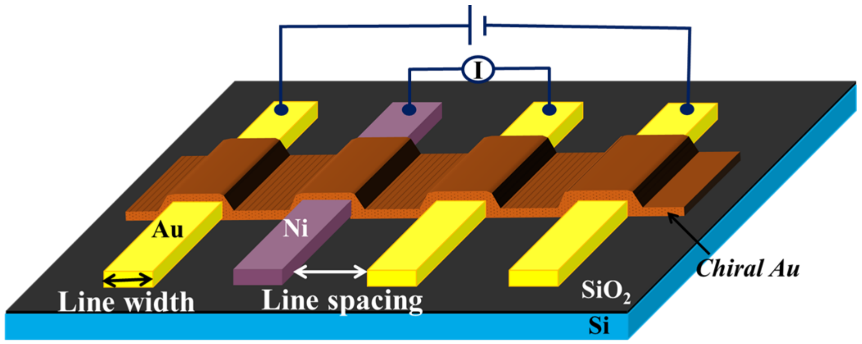
enantioselective separation, switching of the magnet direction by adsorption

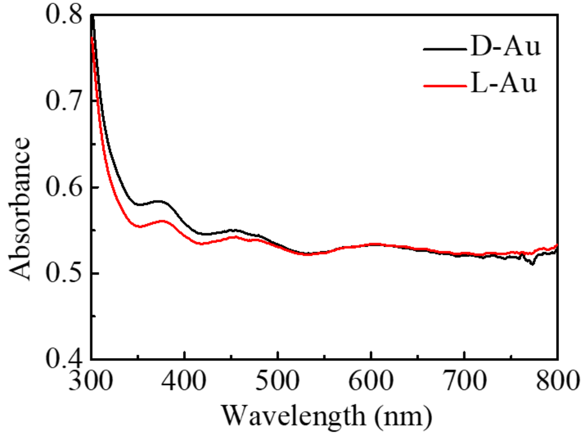
- Adsorption of chiral molecules creates “magnetic impurity” in superconductor.

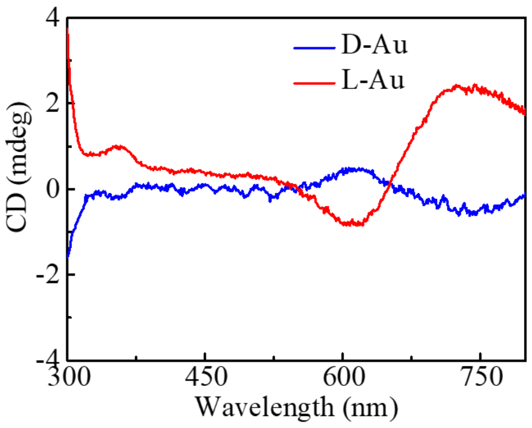
Long range spin transport at room temperature.

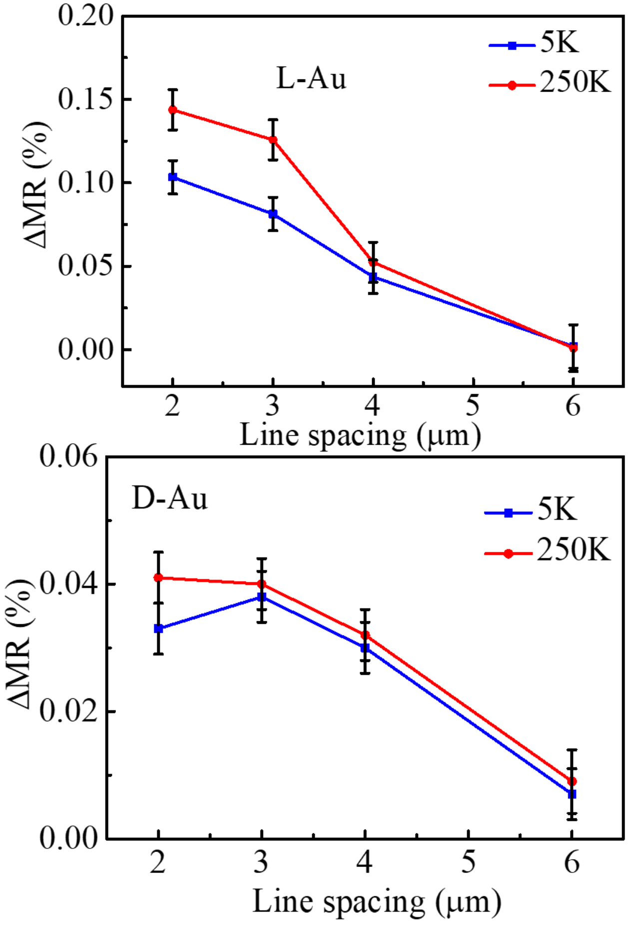
Long Range Magnetoresistance in Chiral Gold and Topological-Anomalous Hall effect.

Tapan Kumar Das, Offek Marelly, Shira Yochlis, Yossi Paltiel, Jonas Fransson Adv. Mat. 2506523 (2025).



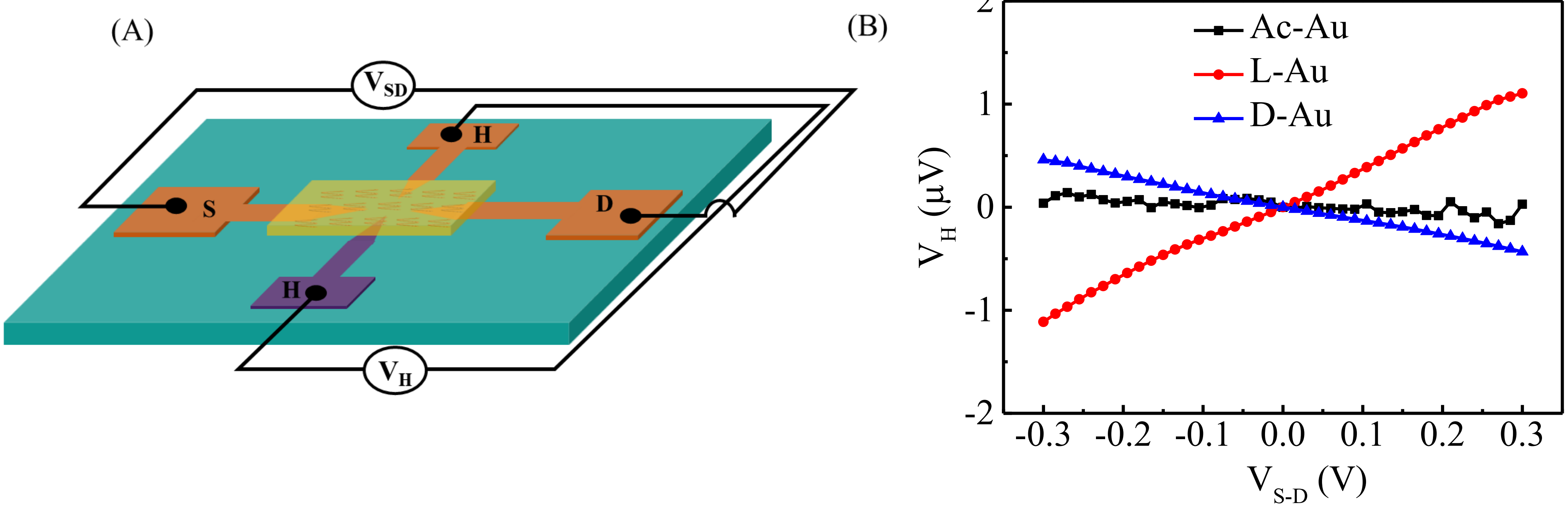






$\Delta MR\ (\%) = MR(\%)_{1T} + MR(\%)_{-1T}$.

Hall Signal



$$S = Wexp[-(k_D - k_B)t]$$

The Anomalous Topological Hall Effect

Theory by Jonas Fransson

The “effective spin orbit coupling” is a result of anisotropic polarizability.

In chiral systems spin information can be transferred for long distance exceeding microns.

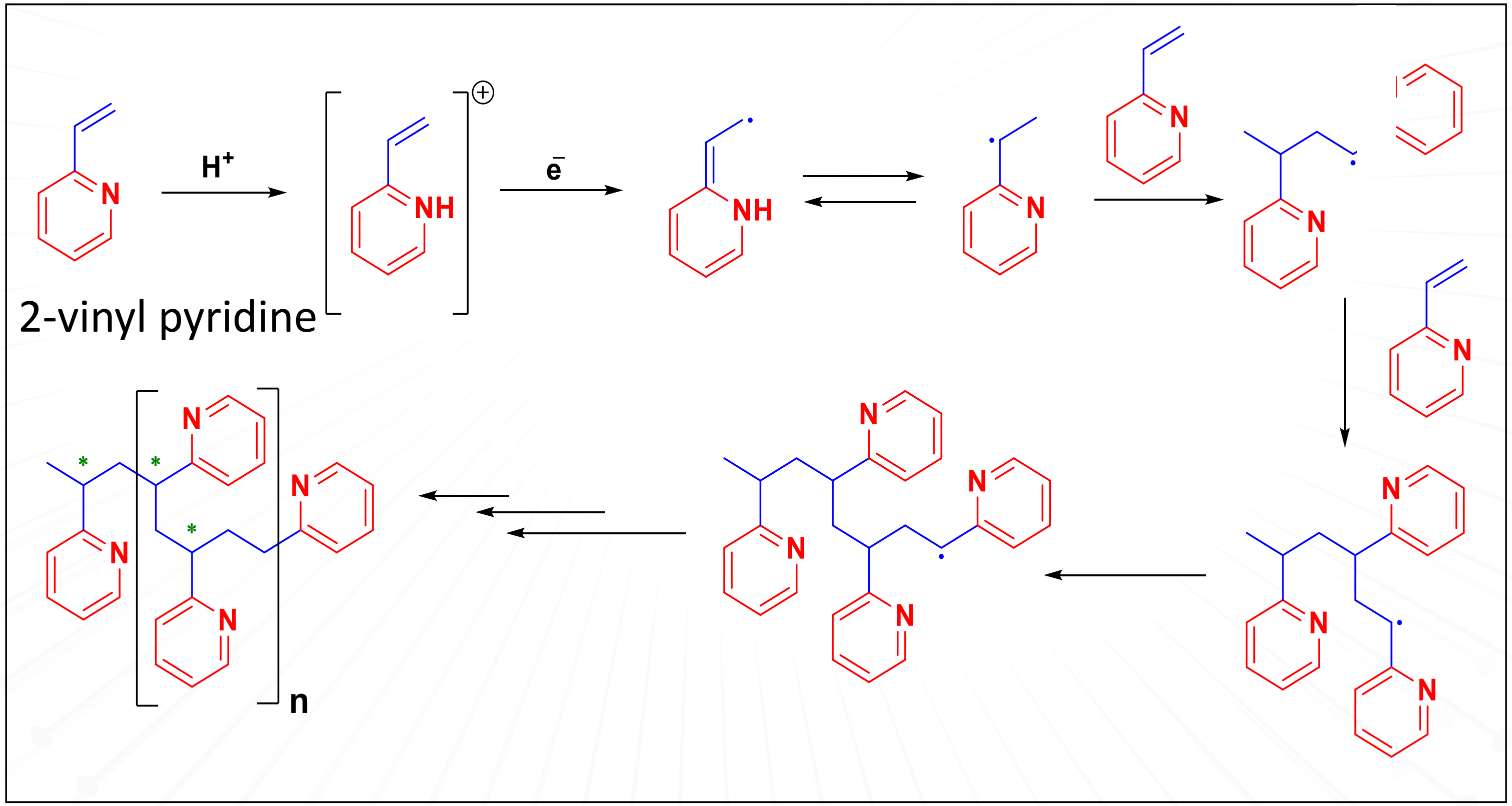
There are two competing processes-
Spin randomization and spin polarization.

This property makes chiral metals ideal as interconnectors in spintronics.

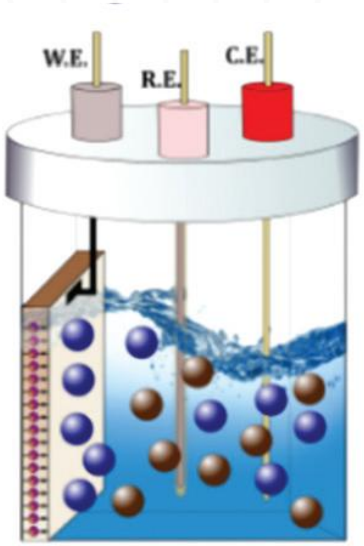
Breaking symmetry

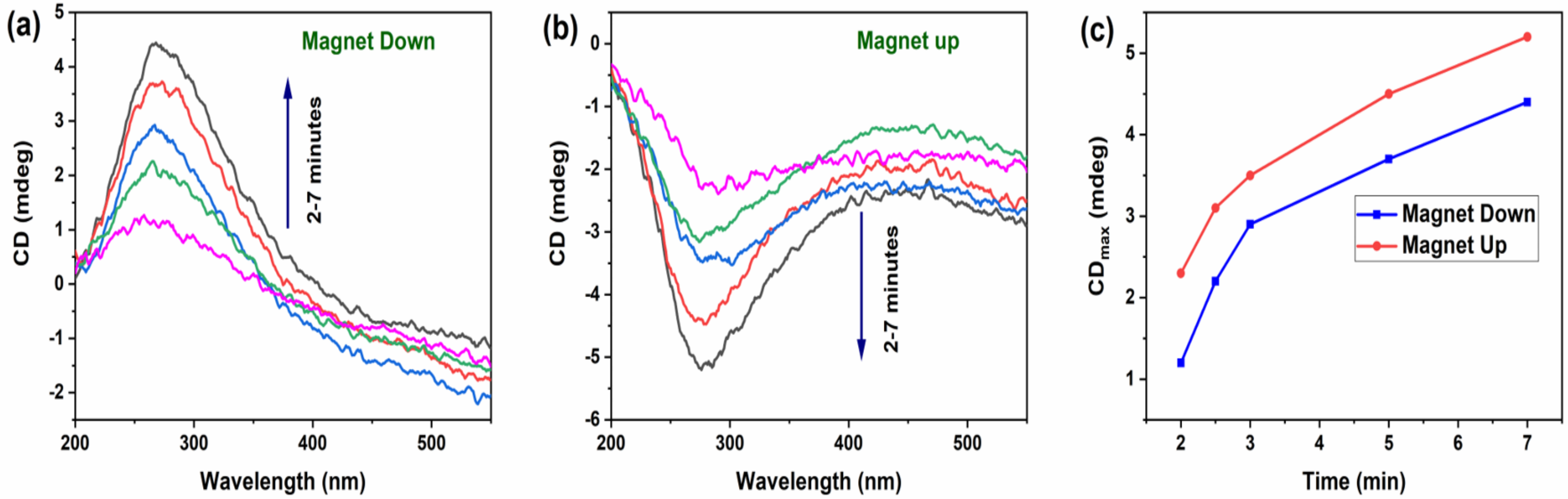
Applying Spin Polarized Electrons for Inducing Asymmetric synthesis

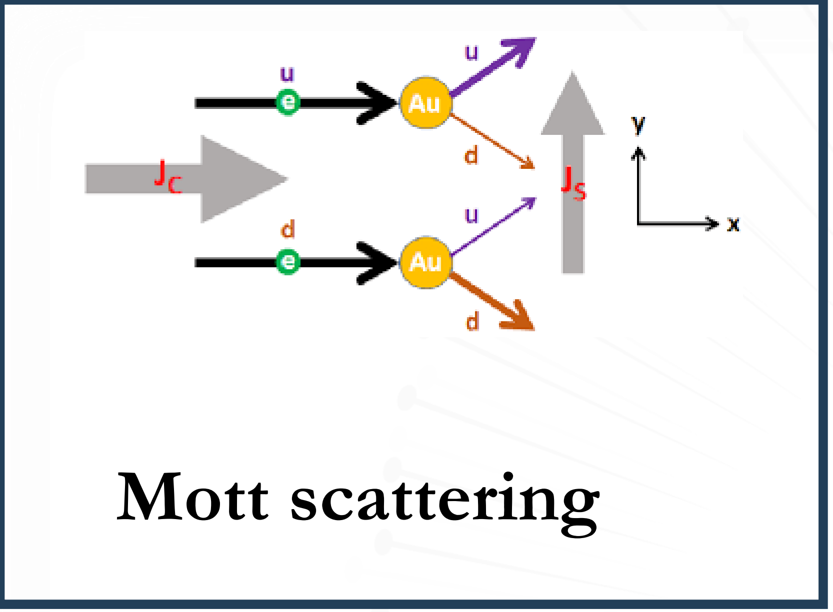
D. K. Bhowmick, T. K. Das, K. Santra, A. K. Mondal, F. Tassinari, R. Schwarz, C. E. Diesendruck, R. Naaman, *Science Adv.* **8**, eabq2727 (2022).

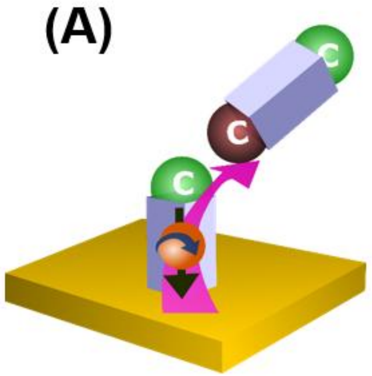


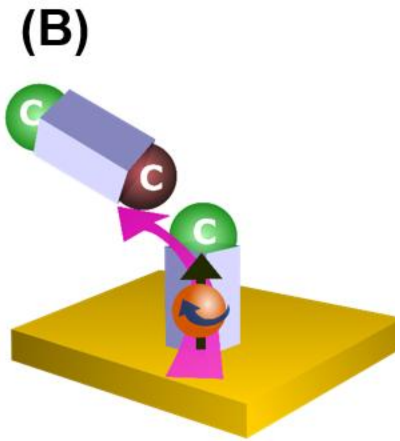
ee=55%


W.E.
R.E.
C.E.


(a)
Magnet Down
2-7 minutes
CD (mdeg)
Wavelength (nm)
(b)
Magnet up
2-7 minutes
CD (mdeg)
Wavelength (nm)
(c)
Magnet Down
Magnet Up
CDmax (mdeg)
Time (min)







Spin polarized electrons behave as chiral reagents

Importance of Spin Polarization in Protein Activity

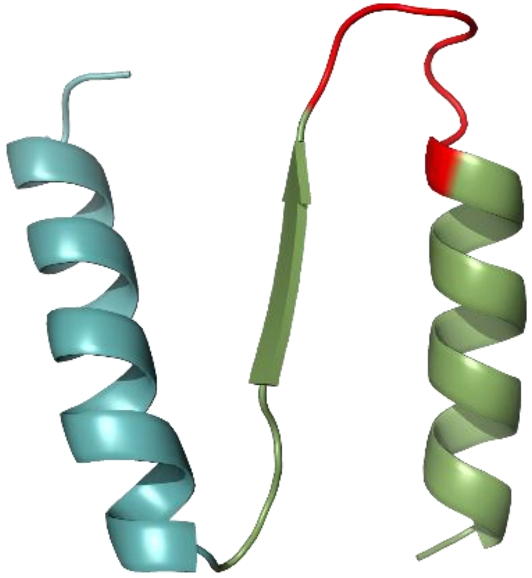
S. Mishra, S. Pirbadian, A. K. Mondal, M. Y. **El-Naggar**, R. Naaman, Spin-Dependent Electron Transport through Bacterial Cell Surface Multiheme Electron Conduits, *J. Am. Chem. Soc.* **141**, 19198-19202 (2019).

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).

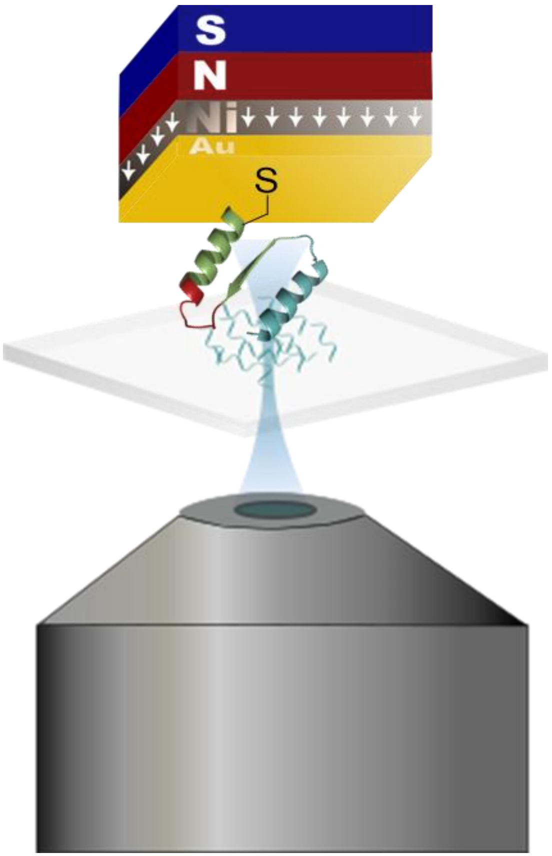
S. Ghosh, K Banerjee-Ghosh, D. Levy, D. Scheerer, I. Riven, J. Shin, H. B. Gray, R. Naaman, G. Haran, Control of protein activity by photoinduced spin polarized charge reorganization, *PNAS* **119**, e2204735119 (2022).

The role of spin in protein-DNA interaction



N-αβα prototype
$\alpha_2\beta_1$-(P-loop)-α_1

P. Vyas, K. Santra, N. Preeyanka, A. Gupta, O. Weil-Ktorza, Q. Zhu, L. M. Longo, J. Fransson, N. Metanis, R. Naaman, J. Phys. Chem. B, 129, 3978–3987 (2025).

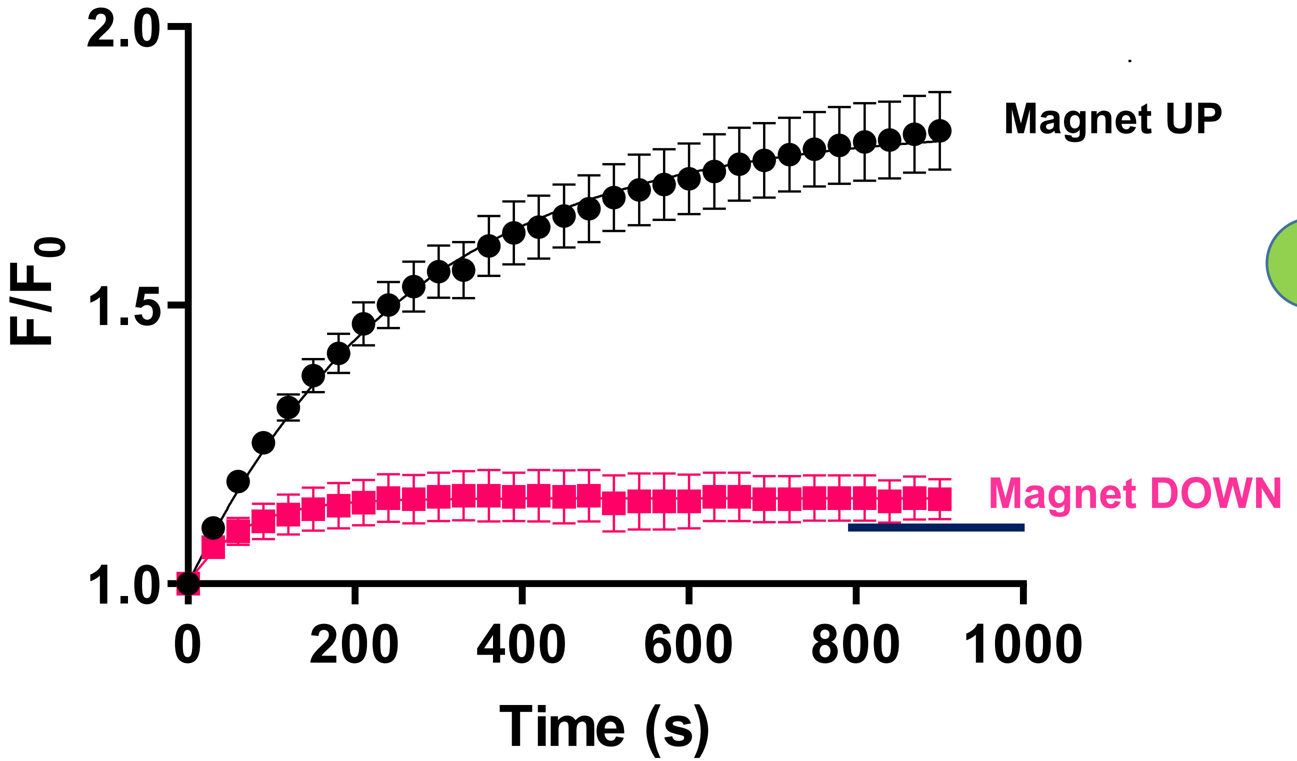


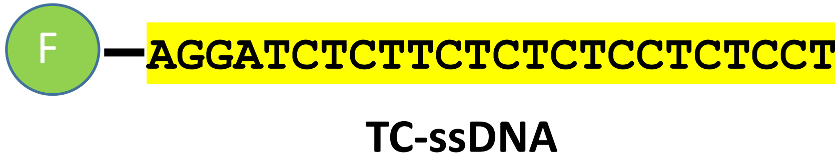
It is hypothesized that proteins and enzymes emerged via duplication and fusion of relatively short 'seeding' peptides with simple secondary structures.

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.

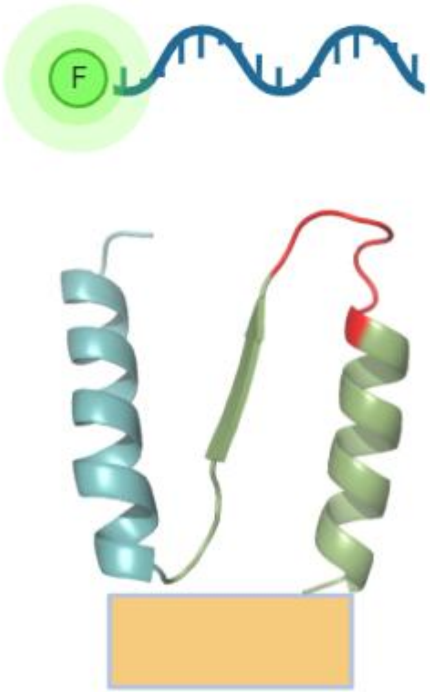
Vyas P, Malitsky S, Itkin M, **Tawfik D**. On the origins of enzymes: Phosphate-binding Polypeptides Mediate Phosphoryl Transfer to Synthesize ATP. J Am Chem Soc. 2023;Accepted.

ssDNA binding function is ‘spin-selective’



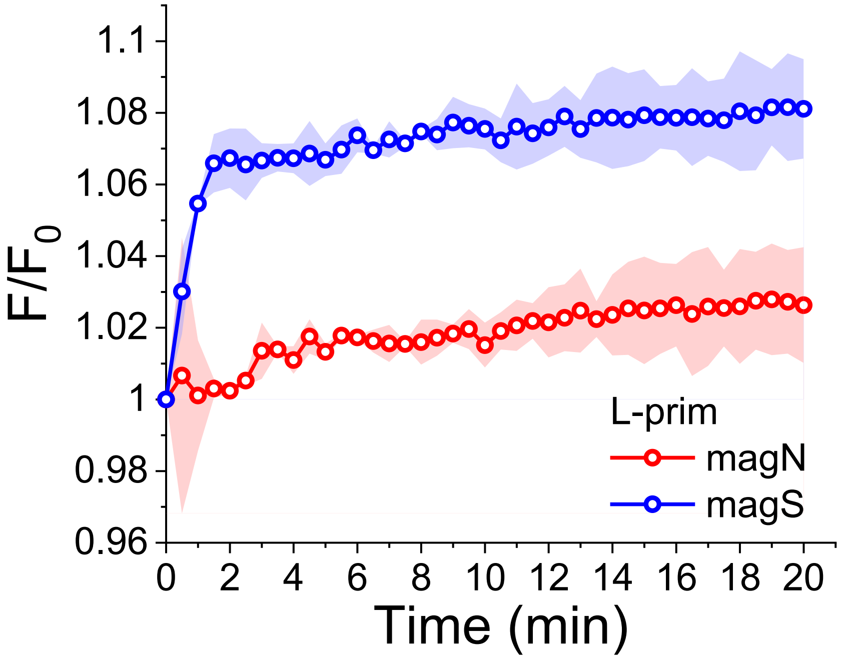


Vyas, Santra and Naaman, in preparation



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

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. Dissipation is an intrinsic process in CISS.

2. Polarizability must be considered as is evident from the correlation between optical activity and spin polarization. The connection is through the anisotropic polarizability of the system.

3. In polarizable system, for a passing electron. there is an effective spin orbit coupling which is much larger than the atomic one.

4. Angular momentum considerations must be included, especially when interaction between electron-phonons/vibrations is involved.

5. Spin long range transport enables spin-interconnect.

5. 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

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