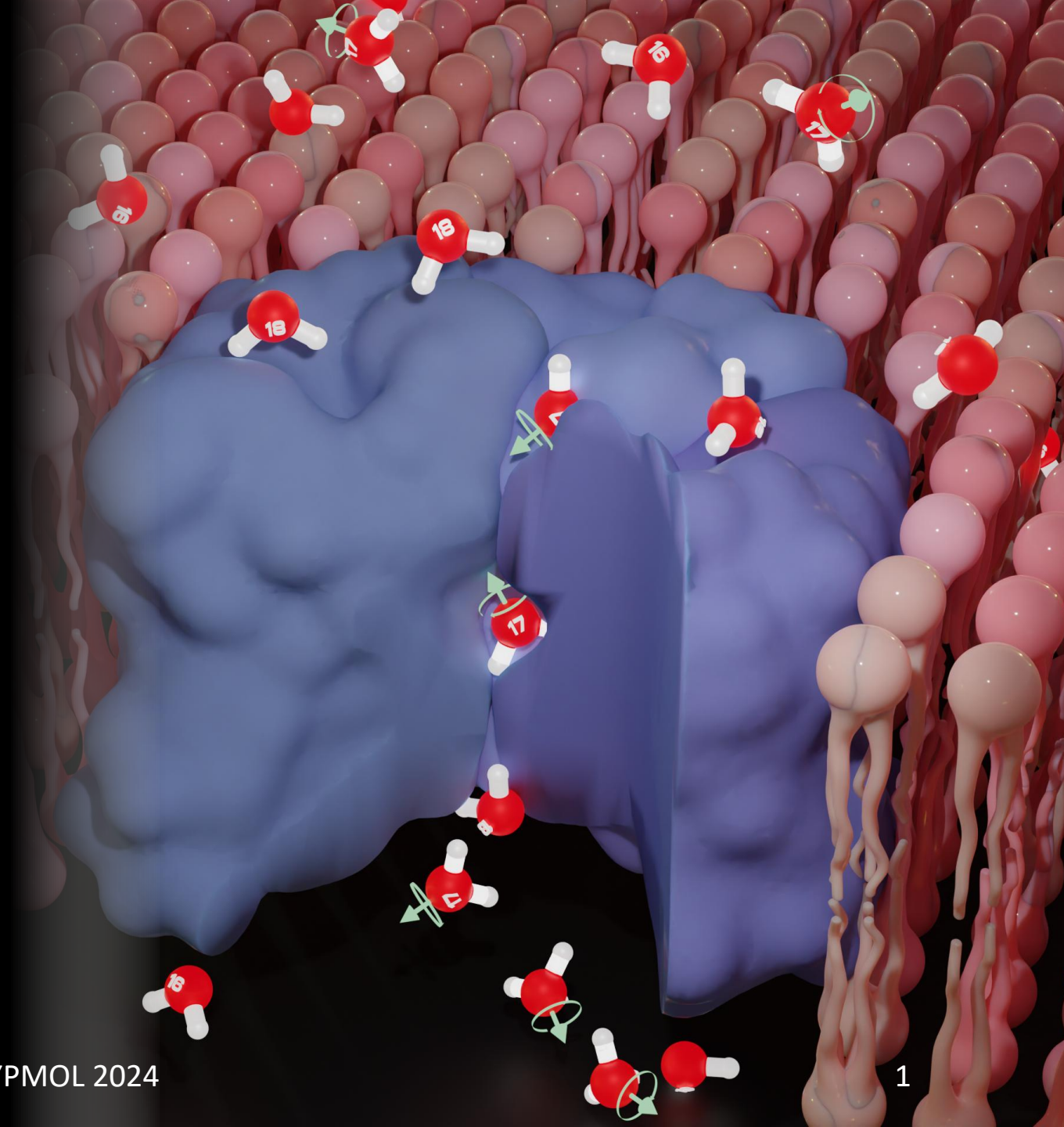
CISS effect relations to nuclear spin and chiral phonons

Yossi Paltiel
The Hebrew University of Jerusalem, Israel



THANKS

Our Current Group: Prof. Yossi Paltiel, Dr. Shira Yochelis, Dr. Ohad Golan (poster chiral cooling), Lilach Baran, Dror Negbi, Daniel Goldberg, Roei Maman, Sheli Muzafe, Yael Kapon, Avi Schneider, Naama Goren, Meital Ozery, Offek Marelly, Chana Fridman, Ofek Vardi, Naama Mordus Sa, Nir Yuran, Omer Shoseyov, Gur Aminadav, Daniel Voignac.

Dr. Shira Yochelis

Previous members

Dr. Oren Ben Dor, Dr. Eran Katzir, Dr. Guy Koplovitch, Dr. Ohad Westrich, Dr. Amir Ziv, Dr. Nir Sukenik, Dr. Yuval Koldney, Dr. Hen Alpern, Dr. Tzuriel Metzger, Eytan Avigad, Yuval Shifris, Shoshan Vortman, Amitai Meir

Collaborators;

Ron Naaman, Nir Keren, Oded Millo, Oded Shoseyov, Dave Waldeck, Thomas Baczewski, Christoph Tegenkamp, Michael Therien, Furkan Ozturk, Jonas Fransson.

SPIN PHENOMENA INTERDISCIPLINARY CENTER SPICE

Thanks to **Martina Basini, ETH Zurich**
Dominik Juraschek, TU Eindhoven
Shuichi Murakami, University of Tokyo
Angela Wittmann, JGU

Gordon Research Conferences

frontiers of science

Chiral Molecule as an Electron Spin Filter

Announcing the 2025 Gordon Research Conference on:

Electron Spin Interactions with Chiral Molecules and Materials

Chiral Spin Filtering and Its Manifestations From Molecules to Devices

August 3-8 2025 GRC

Chair: C. Herrmann, Y. Paltiel
Vice Chair: M. Lingenfelder, V. Mujica

August 2 - 3 2025 GRS

Chair: Y. Kapon, N. Sukenik

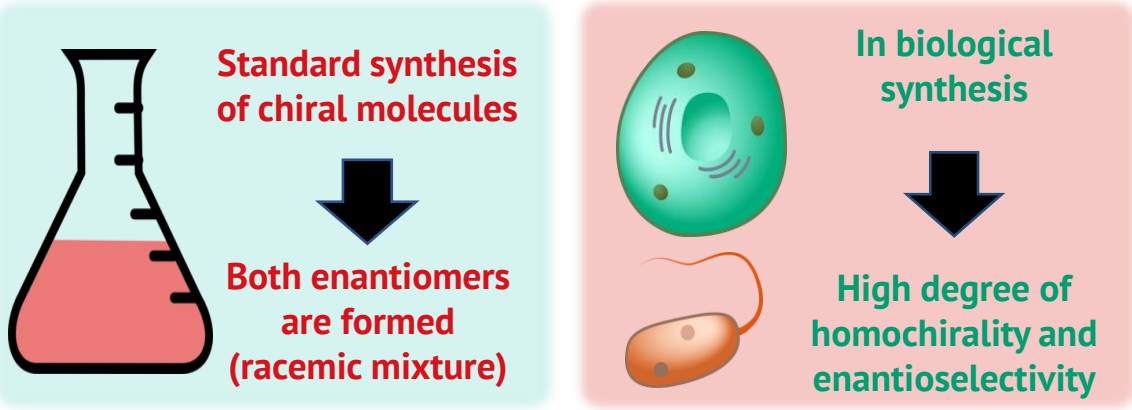
Southern New Hampshire University, Manchester NH USA

Meeting Description: *This meeting will emphasize chiral induced spin-selectivity and its manifestations in Chemistry, Biology, and Physics. Among other subjects, quantum spin chemistry and green energy production will be discussed. Invited speakers represent a variety of scientific disciplines, and the Conference format aims to bring together researchers from the forefront of the field, to provide opportunities for junior scientists, and to encourage collaborations. The GRS conference before the GRC will supply a generic introduction about the CISS effects to young scientists.*

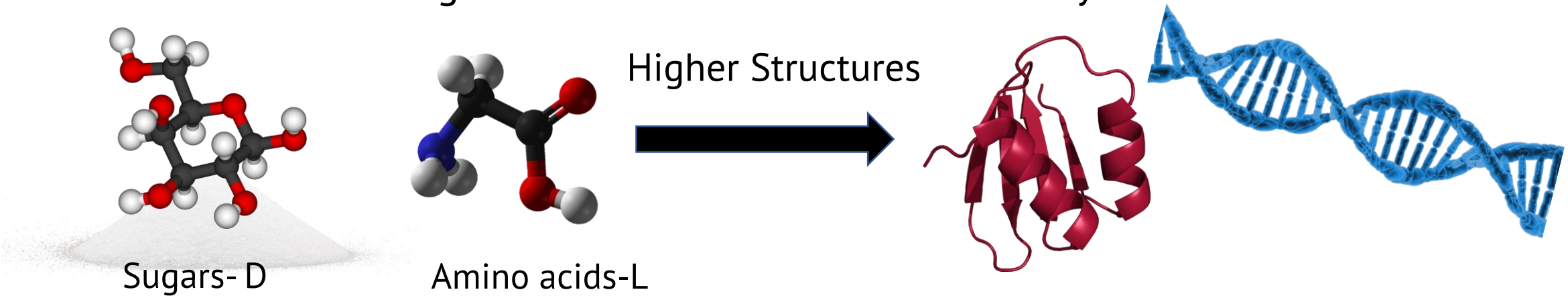
Topics: The Role of Chiral Induced Spin-Selectivity in Chemical Reactions; Spin-Selectivity in Chiral Materials, Chiral spintronics; Chiral Induced Spin Selectivity on Surfaces; Coherent and entangled spin chemistry, Green energy and spin, Chiral Molecules and Magnetism; Chiral Interfaces of Electronic Materials; Mechanistic understanding of Chiral Induced Spin Selectivity, Chirality and Spin in Biology.

More details and online application are available at:
https://www.grc.org/electron-spin-interactions-with-chiral-molecules-and-materials-conference/2025/

Life Is Chiral

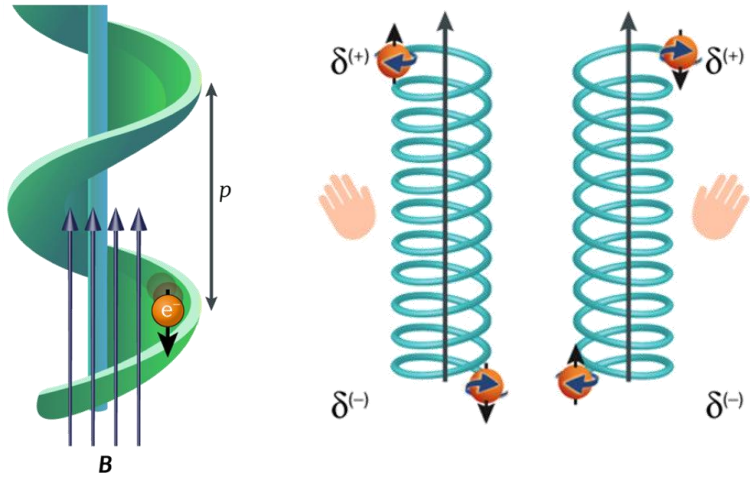


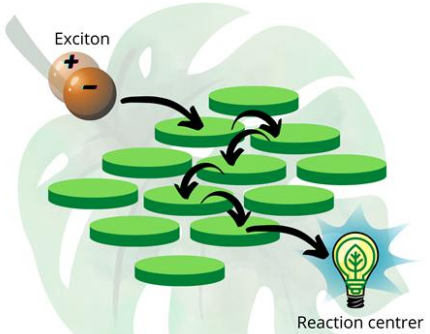
- All of life's building blocks are homochiral – exist only as one enantiomer



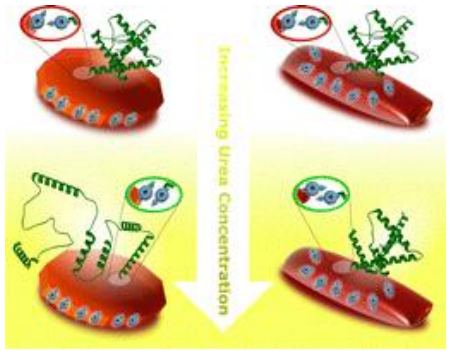
Electron Spin in Biology

The Chiral Induced Spin Selectivity Effect
CISS

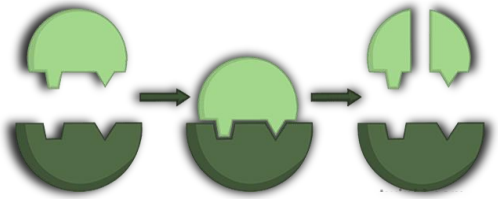




Photosynthesis



Protein structural stability



Biorecognition

Not yet studied for nuclear spin!

Naaman, R. Paltiel Y., Waldeck D., (2019) Nat. Rev. Chem. 3, 250-260

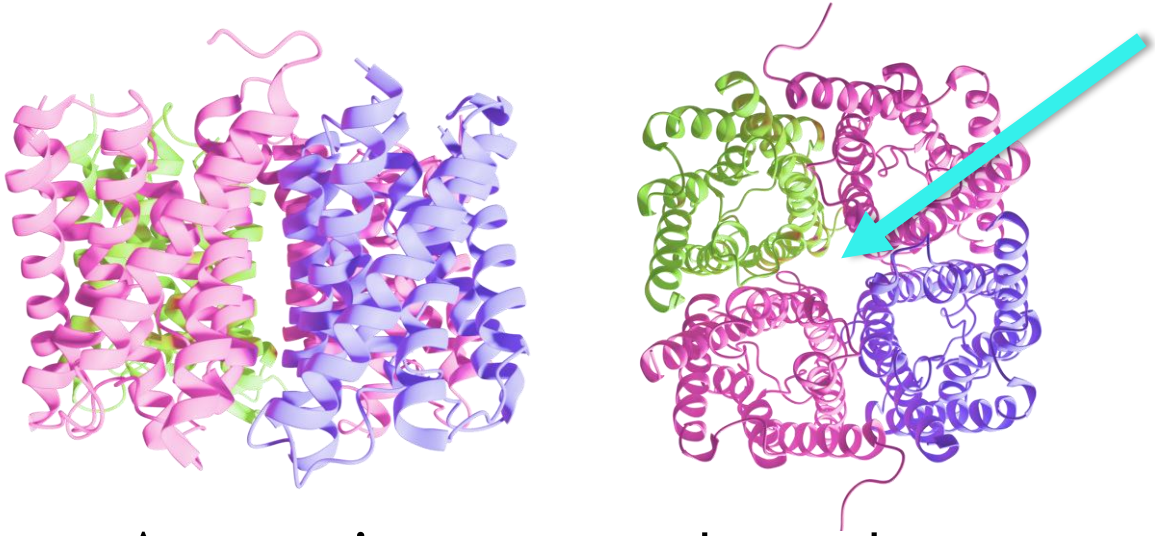
Hadar Manis Levy, et al, Phys. Chem. Chem. Phys., 2022,24, 29176
Kapon, Y., et al. (2021). Chem, 7, 10, 2787-2799

How Can We Check if Nuclear Spin is Involved in Biological Processes?

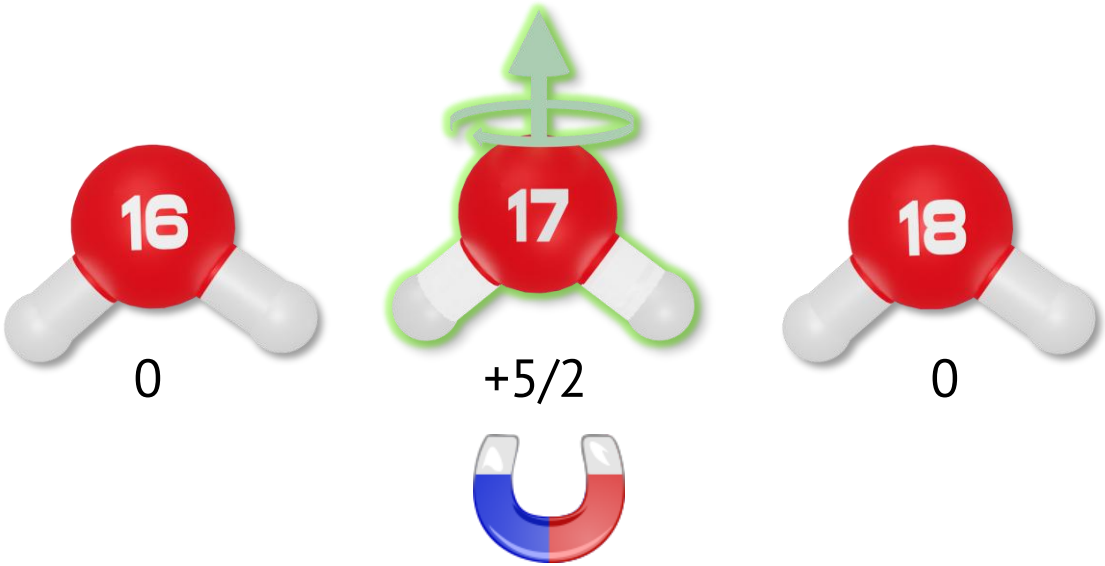
Two examples: protons and ions

Experimental Design

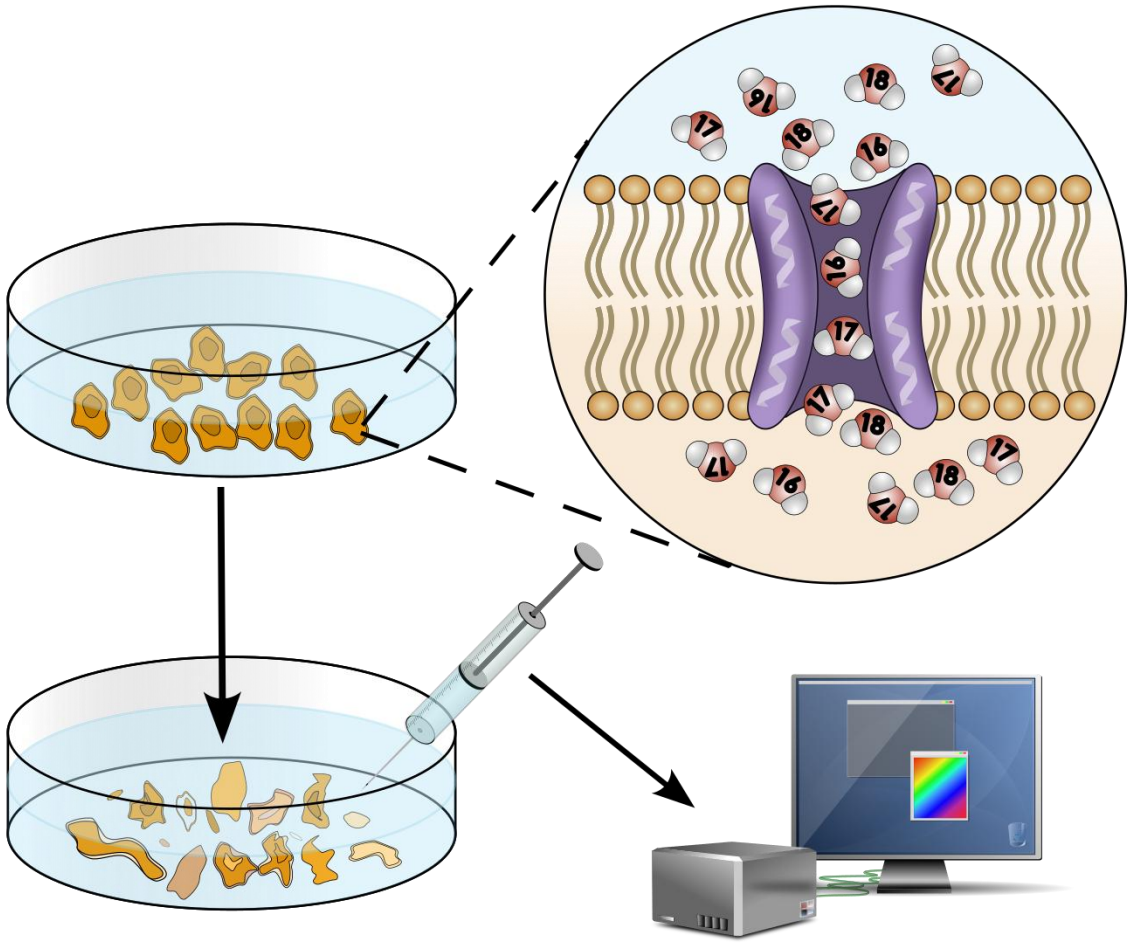
Water trasport into living cells- ISOTOPES



Aquaporins – water channels



Experimental Design

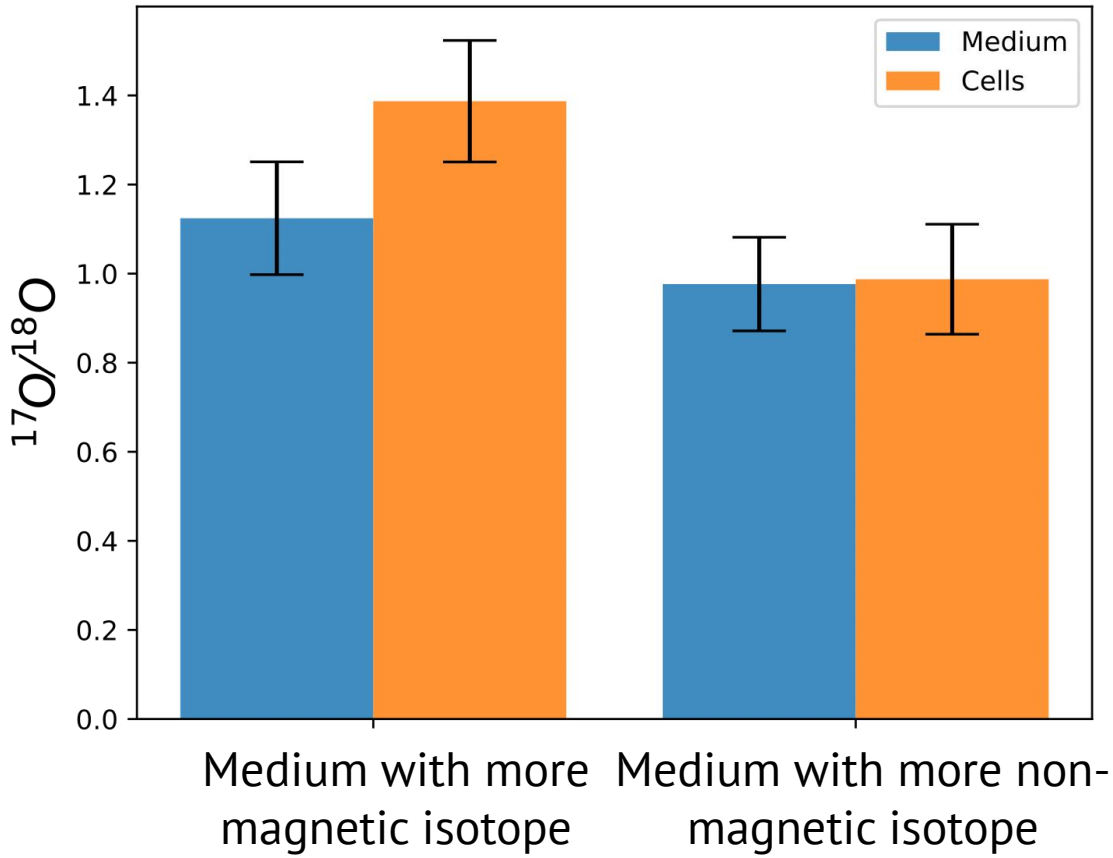


Yuval Kolodny , HUJI
Amijai Saragovi, HUJI
Nir Galili, WIS
Prof. Itay Halevy , WIS

Dr. Yuval Kolodny

Ofek Vardi , Naama Maroudas-Sklare , yuval kolodny ,et al. , ”Nuclear Spin Effects in Biological Processes”, PNAS (2023)

Results



Nir Galili, WIS
Prof. Itay Halevy , WIS
Yonatan Goldsmith, HUJI

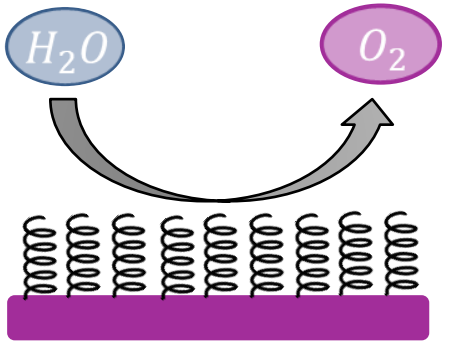
Naama Maroudas, HUJI
Ofek Vardi, HUJI

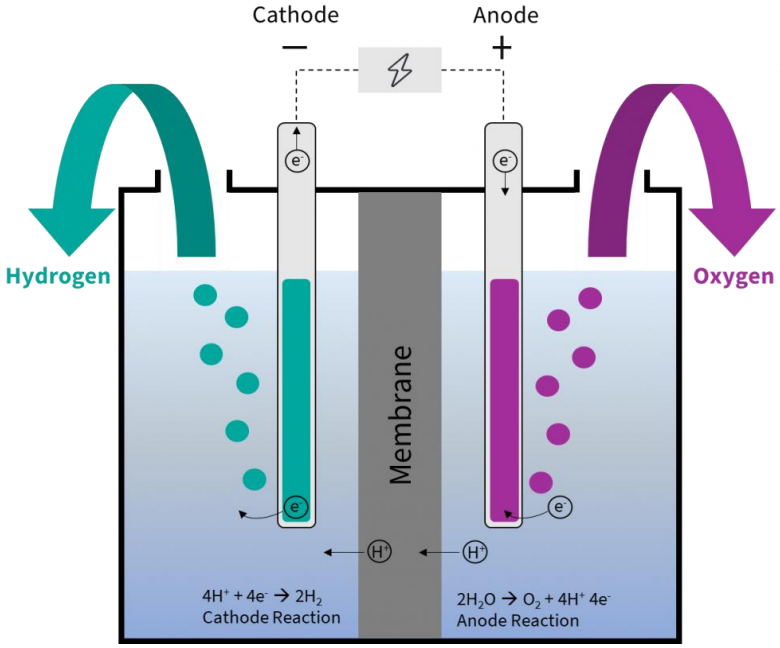
Electrolysis Experiments

$$2H_2O_{(l)} \rightarrow 2H_{2(g)} + O_{2(g)}$$

Nir Yuran, HUJI
Stav Ferrera, HUJI
Hagit Affek, HUJI
Prof. Boaz Luz, HUJI

Chiral coated anode enhaces the efficiency of the hydrolysis

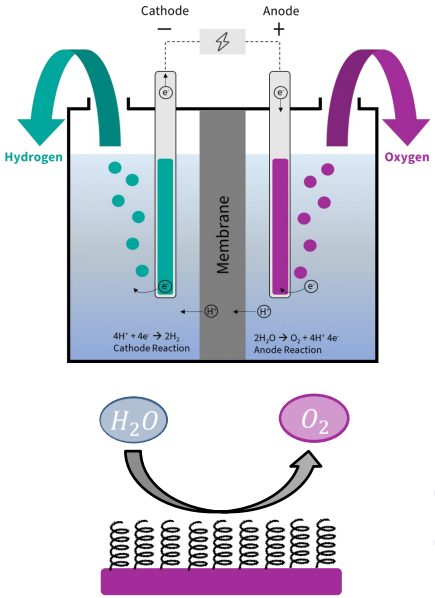




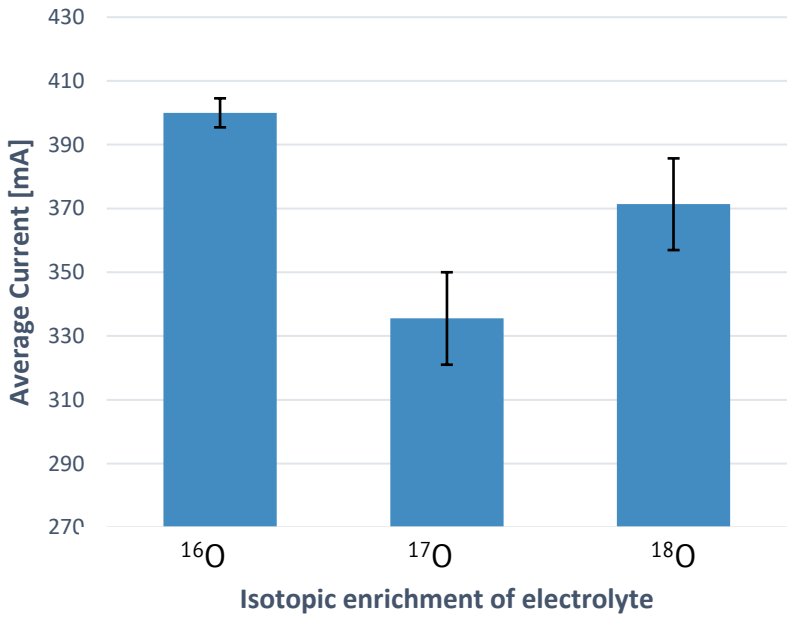
W. Mtangi et al. Role of the Electron Spin Polarization in Water Splitting, *The Journal of Physical Chemistry Letters* **2015** *6* (24), 4916-4922 DOI:10.1021/acs.jpclett.5b02419
W. Mtangi *et al.*, "Control of Electrons' Spin Eliminates Hydrogen Peroxide Formation during Water Splitting," *Journal of the American Chemical Society*, vol. 139, no. 7 doi: 10.1021/jacs.6b12971

Electrolysis Experiments

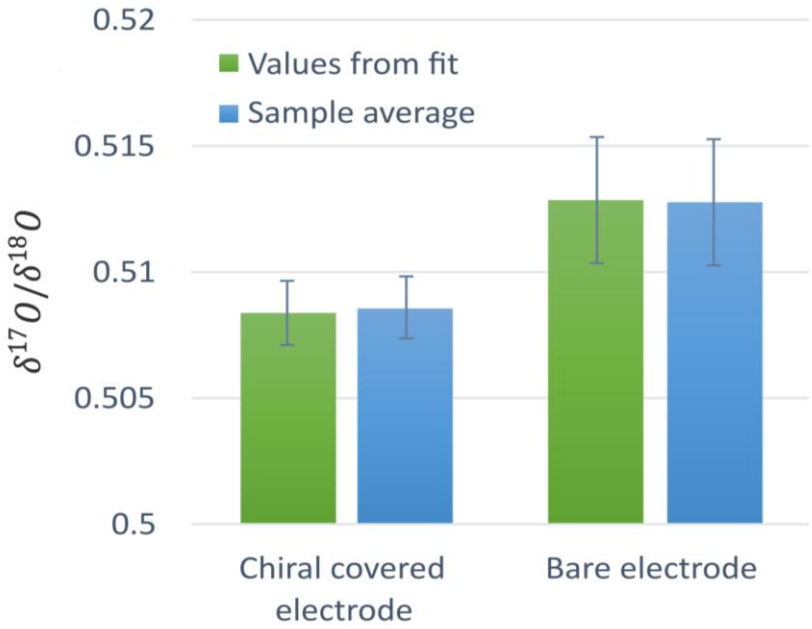
Nir Yuran, HUJI
Stav Ferrera, HUJI
Hagit P. Affek , HUJI
Boaz Luz, HUJI



Current produced:
bias against ^{17}O



$O_{2(g)}$ produced:
bias against ^{17}O

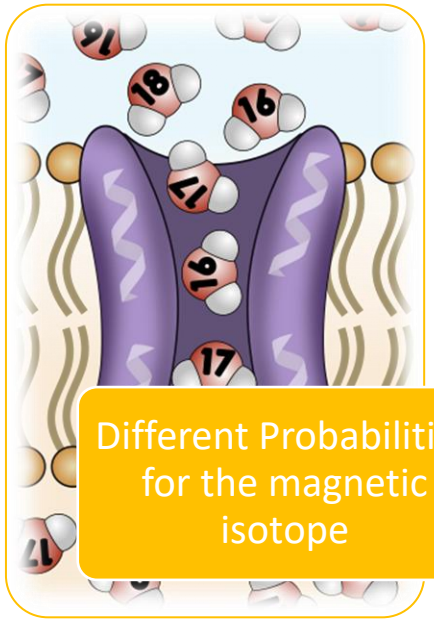


Deviation from expected mass dependency

The Magnetic Isotope is Different!

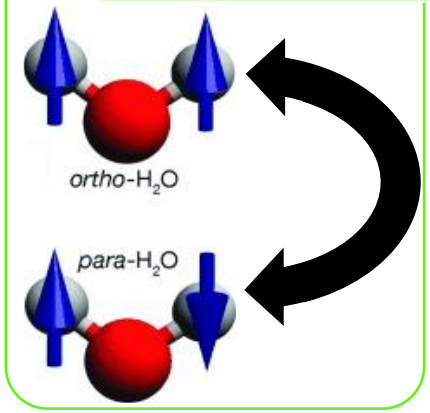
Theoretical Models
(nuclear spin motion couples to electronic spin)

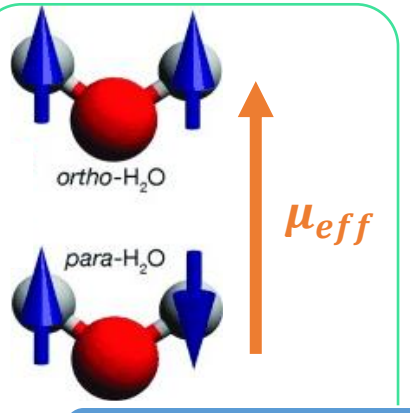
Prof. Mikhail Lemeshko,ISTA
Dr. Areg Ghazaryan, ISTA
Dr. Artem Volosniev, ISTA



Different Probabilities for the magnetic isotope

Nuclear spin can prompt spin conversion





Ortho – Para states have different effective dipole moments

Different response to electric field

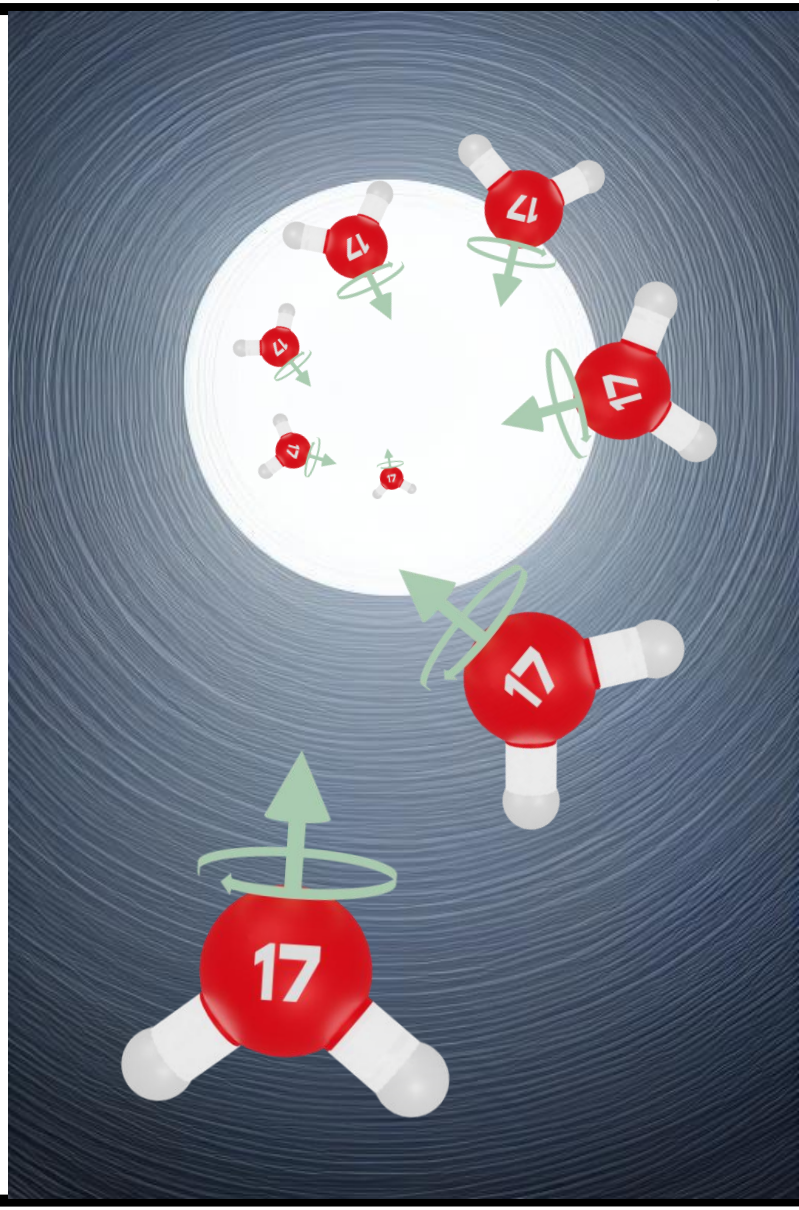
- Suggesting different rates for moving through the AQP
- Larger dipole moment → will be easier to rotate and break their hydrogen bonds

- B. Meier et al. (2018) , Spin-Isomer Conversion of Water at Room Temperature and Quantum-Rotor-Induced Nuclear Polarization in the Water-Endofullerene H2 O@ C60
- Horke et al. (2014), Separating *Para* and *Ortho* Water. Angew. Chem. Int. Ed., 53: 11965-11968.

What can we learn

- We observed and modeled new nuclear spin interactions in chemical and biological environments.
- Electrical polarization as a result of CISS generates angular momentum transferred from electron spin to nuclear spin –non direct method

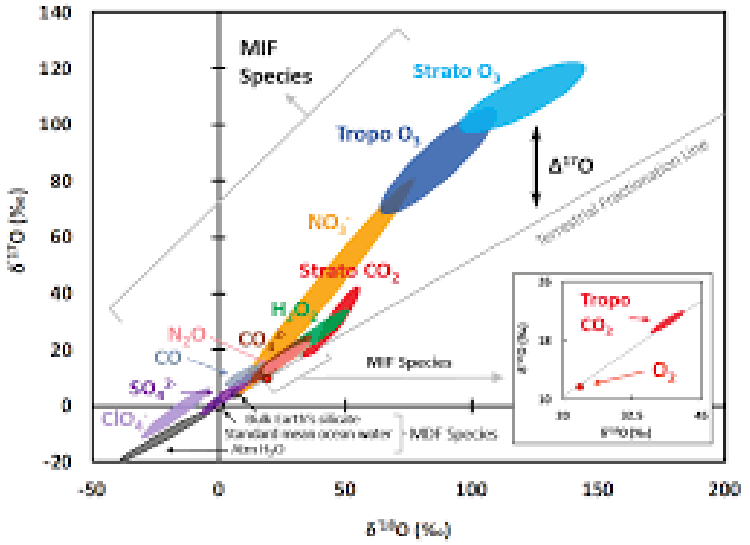
We showed a possible method for ^{17}O enrichment
(possible applications in MRI)



Can We Explain the Bias Towards the Magnetic Isotope?

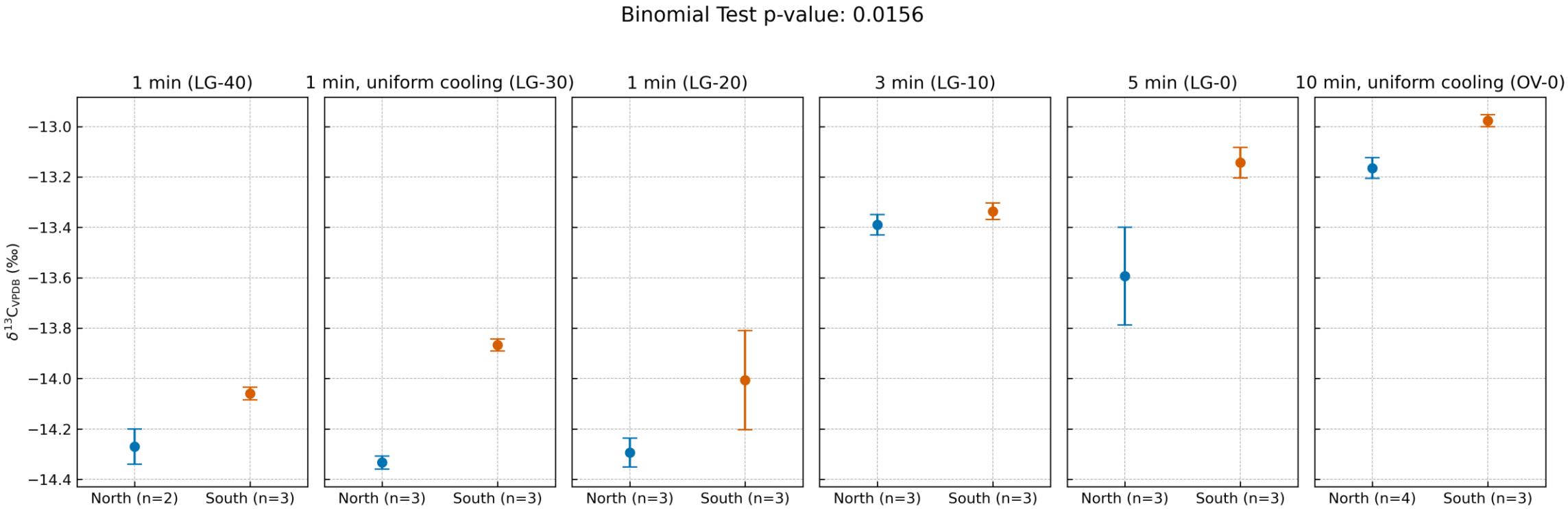
Isotope effect in life

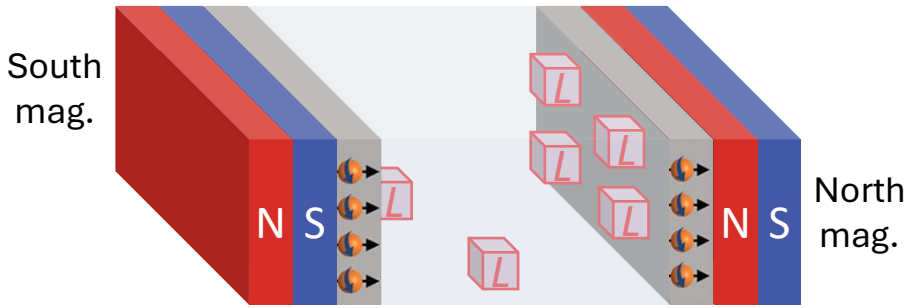
Since the discovery of a chemically produced mass-independent isotope effect by Thiemens and Heidenreich (1983), it has been demonstrated that there exists an extensive range of applications and observations in nature.



Work in progress with preliminary results with John M. Eiler

L-Glutamic acid experiments





*error bars = 1 SEM

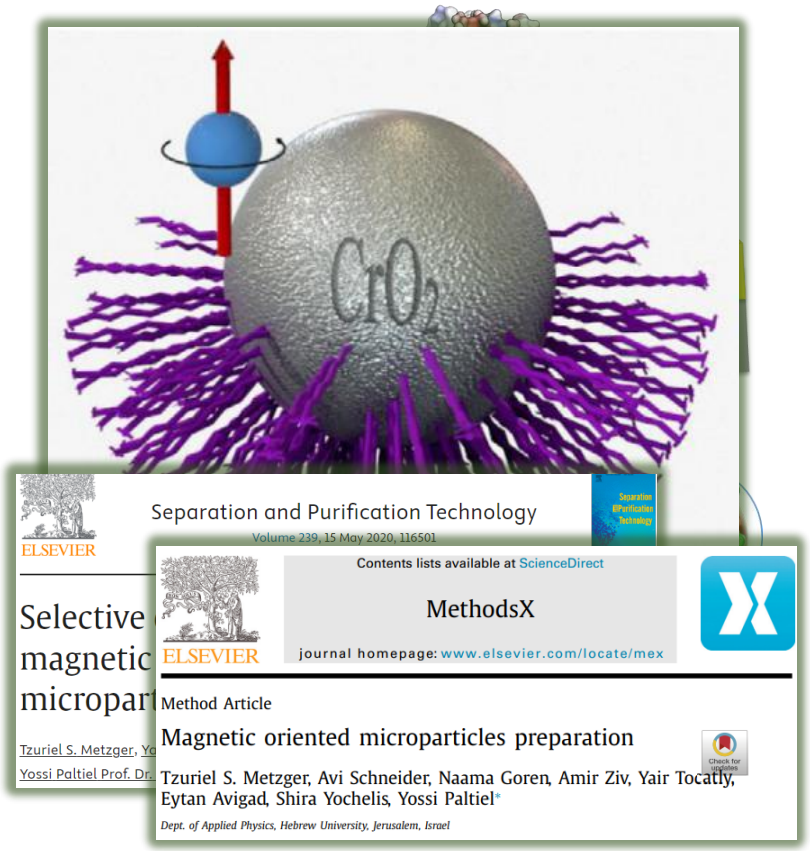
Janus particles

Establishing a simple platform for spin-controlled measurements in solution

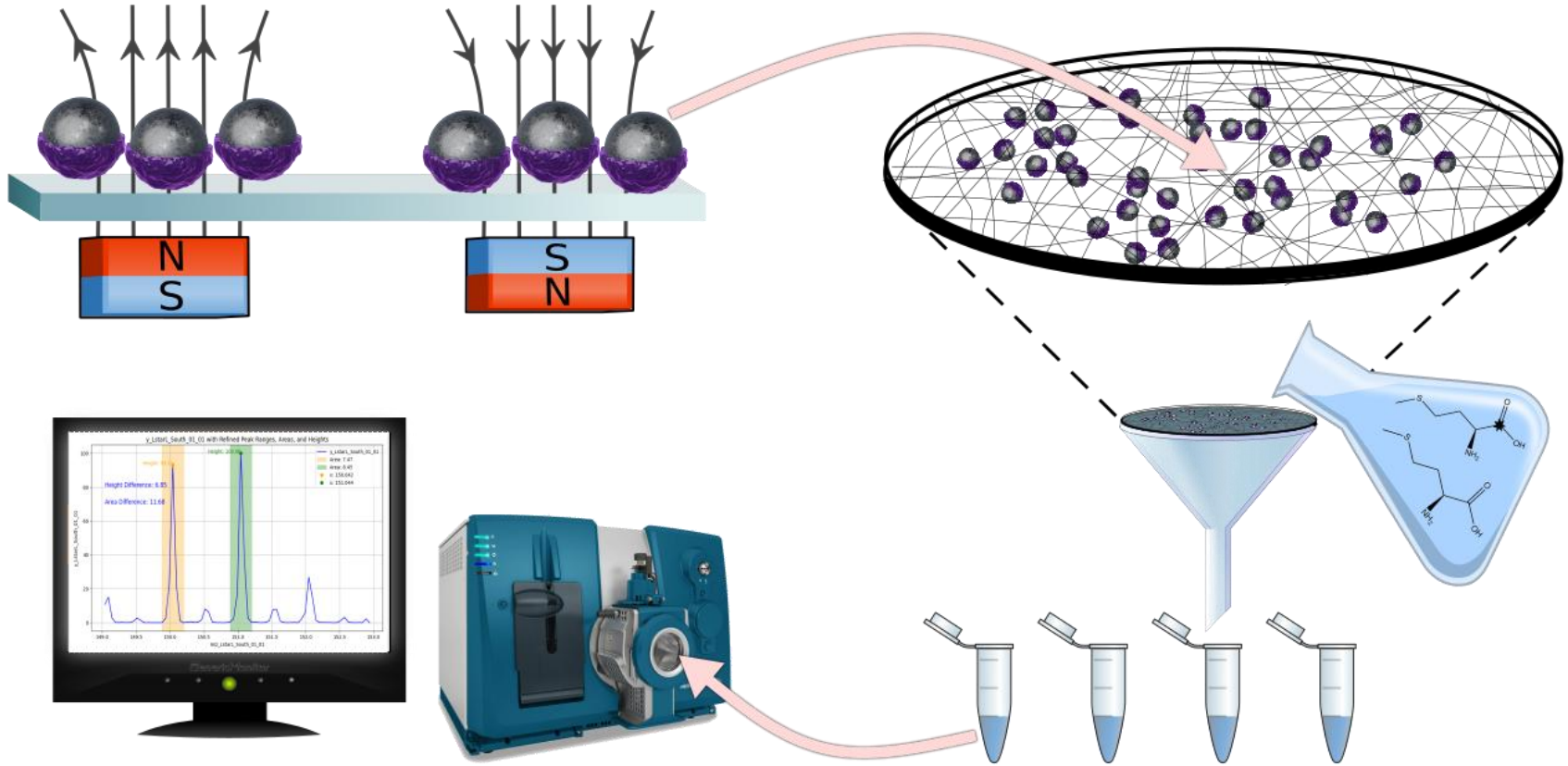
Janus-like magnetic particles

Developed for enantiomer separation

Goal – Implement as research tool



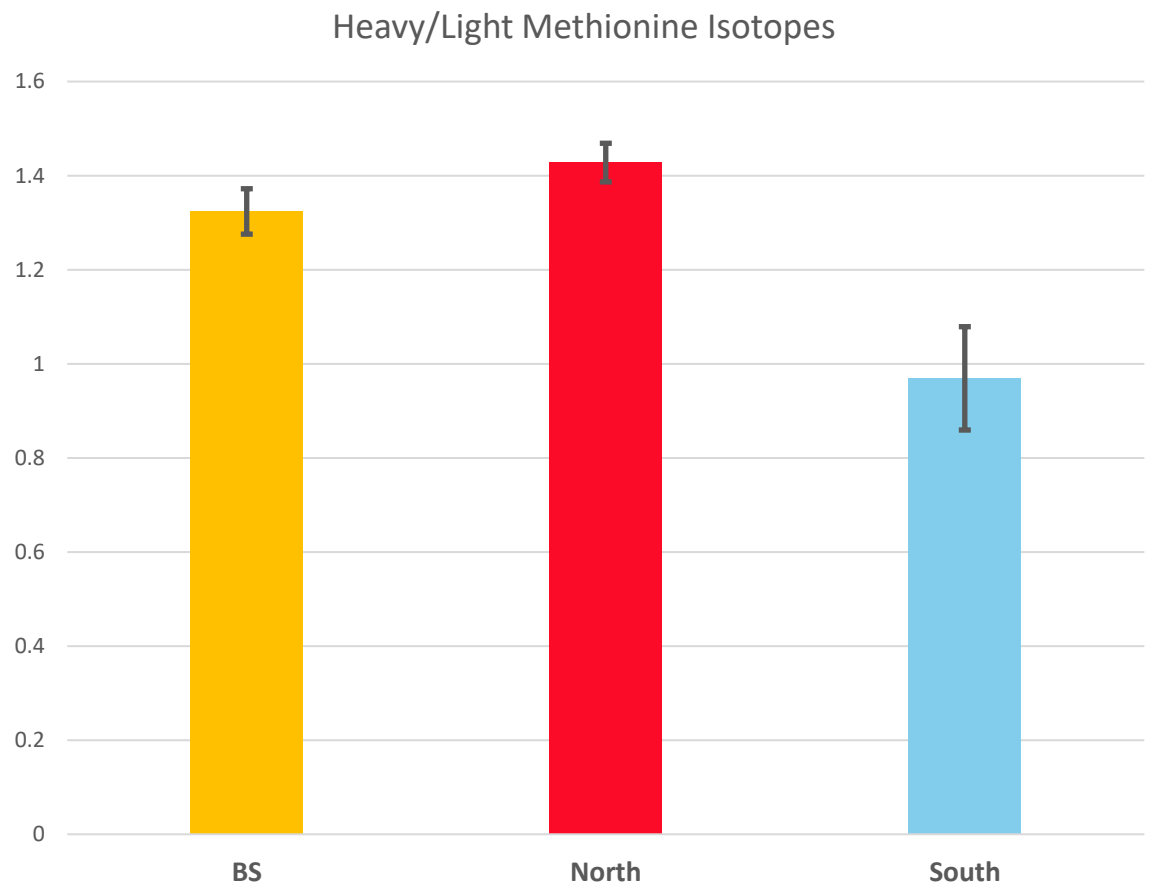
Experimental Setup



In collaboration with Prof. Michal Sharon (Weizmann)

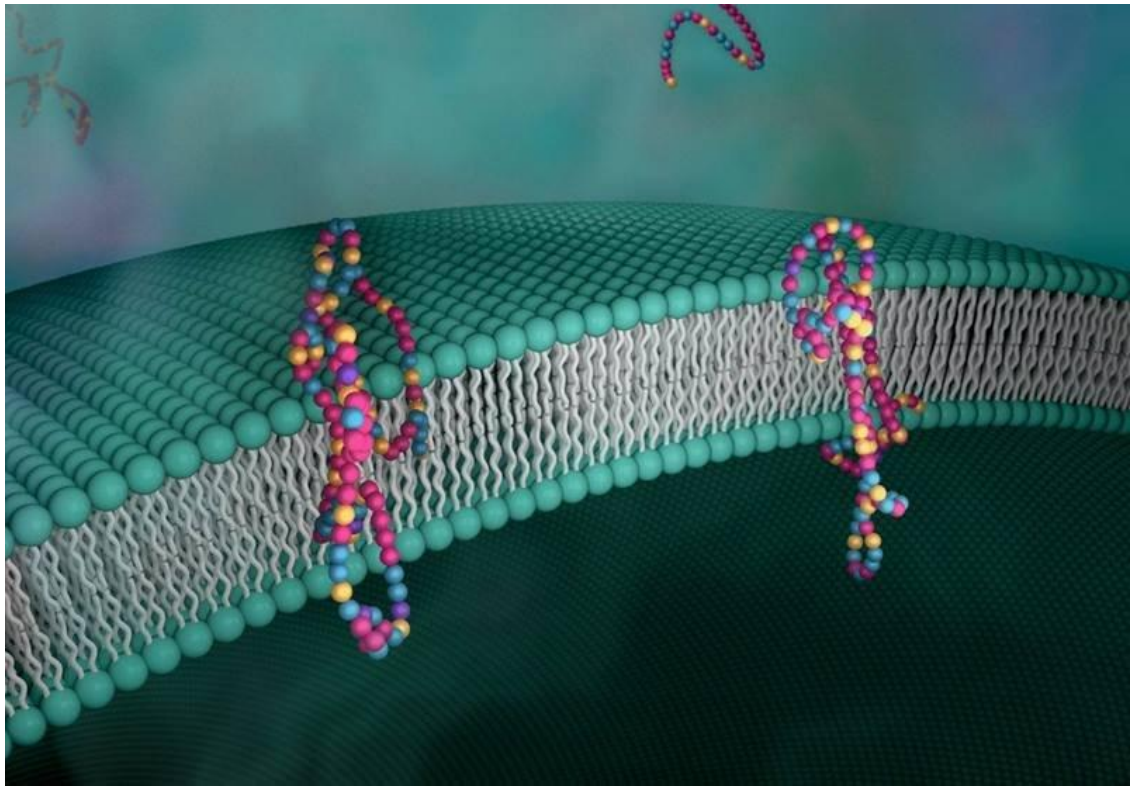
Isotopic Composition of Methionine in Early Filtrate Volume

First set up-
measured in Weizmann



Q-star (<1ml volume passed)-previous results

What about Proton transfer



One of the basic charge transfer mechanisms in life

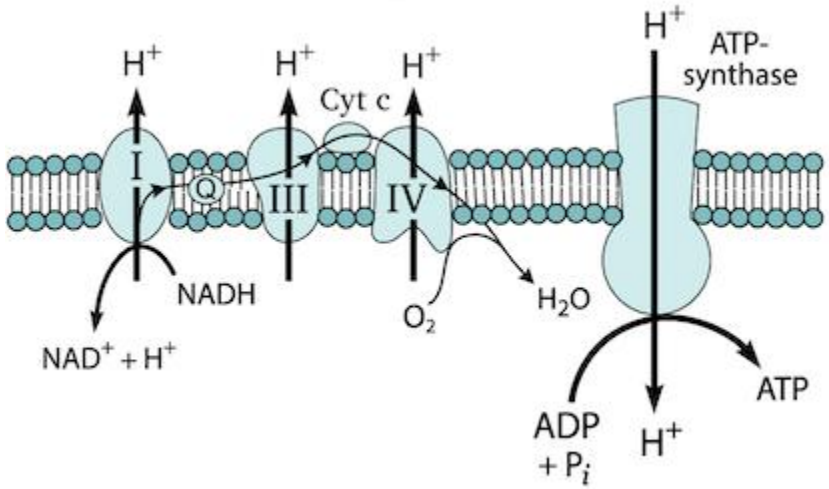


Image of a designer material that mimics biological cell membranes for proton transport.
Image courtesy of Oak Ridge National Laboratory

The Other Side of Chiral Transport

What else is affected by chiral transport?

Proton Transport

Naama Goren

PNAS RESEARCH ARTICLE | APPLIED PHYSICAL SCIENCES OPEN ACCESS Check for updates

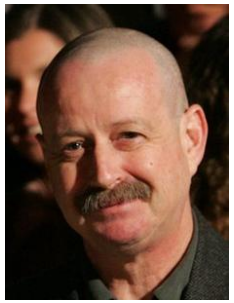
Coupling between electrons' spin and proton transfer in chiral biological crystals

Naama Goren[a], Perumal Pandurangan[b,1], Yael Eisenberg-Domovich[c], Shira Yochelis[a], Nir Keren[d], Jean-Philippe Ansermet[e], Ron Naaman[f,2], Oded Livnah[c], Nurit Ashkenasy[b,2], and Yossi Paltiel[a,2]

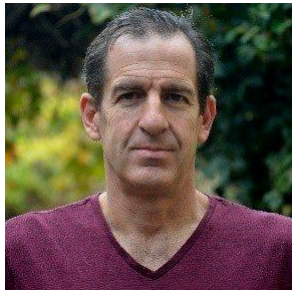
Affiliations are included on p. 7.

Edited by Monica Olvera de la Cruz, Northwestern University, Evanston, IL; received January 10, 2025; accepted April 3, 2025

Prof. Nurit Ashkenasy
BGU



Prof. Oded Livnah
HUJI

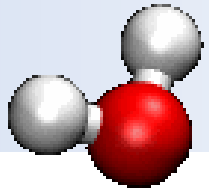
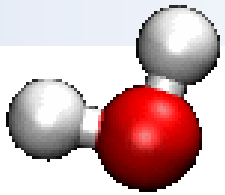
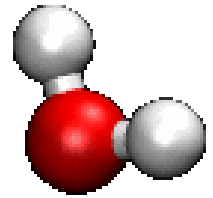
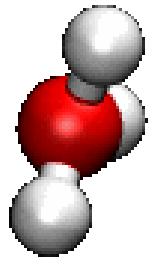


Prof. Nir keren
HUJI

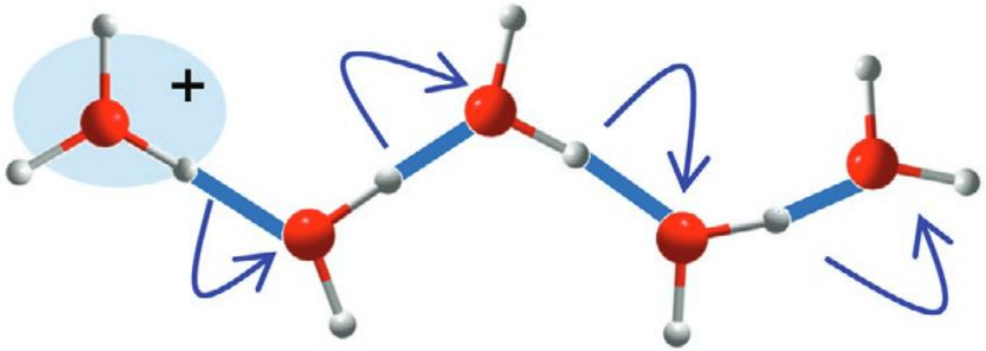
Prof. Ron Naaman
Weizmann

Prof. Jean-Philippe Ansermet
EPFL

Proton Transport Mechanisms

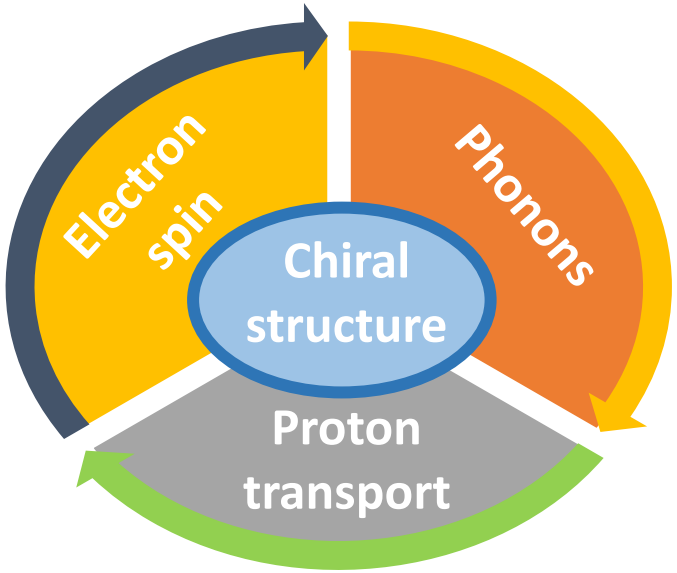
Grotthuss - Hopping



Vehicle

K. I. Otake et al., Small (2021)

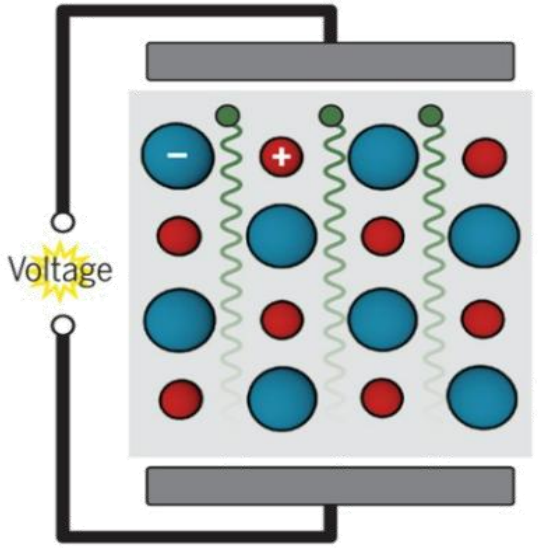
Proton-coupled electron transfer (PCET)

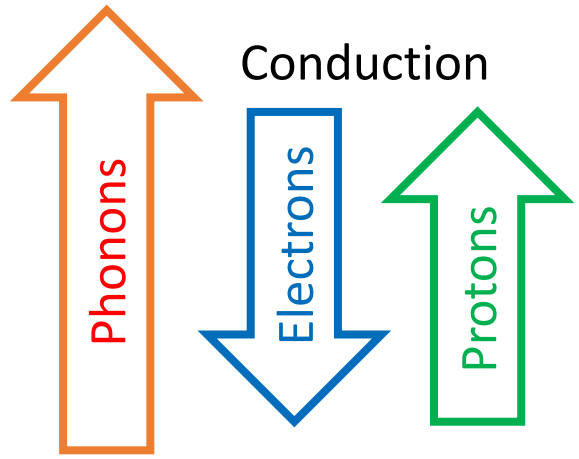


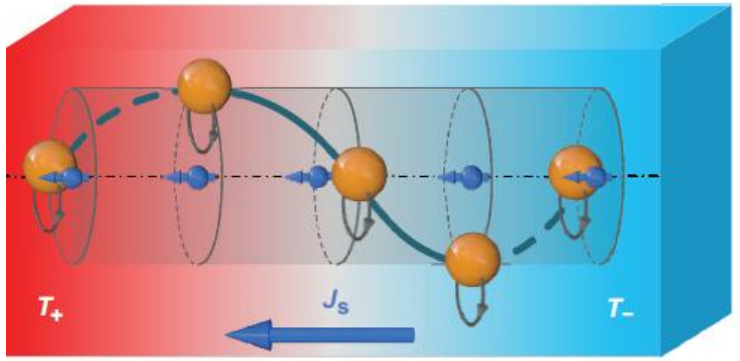
Phonons – (chiral phonons)

The Role of Phonons

- Influence conduction
- Chiral phonons
  - Preserve angular momentum
  - Enhance spin polarization





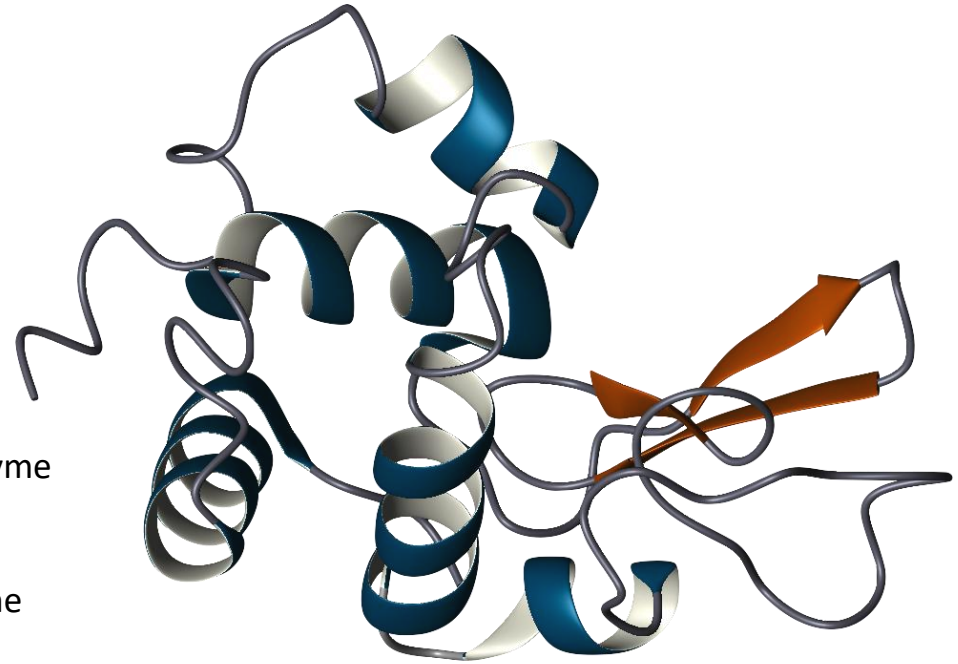


X. Li *et al.*, Sci. China-Phys. Mech. Astron. (2024)

Lysozyme Crystal – A Model System

Properties:

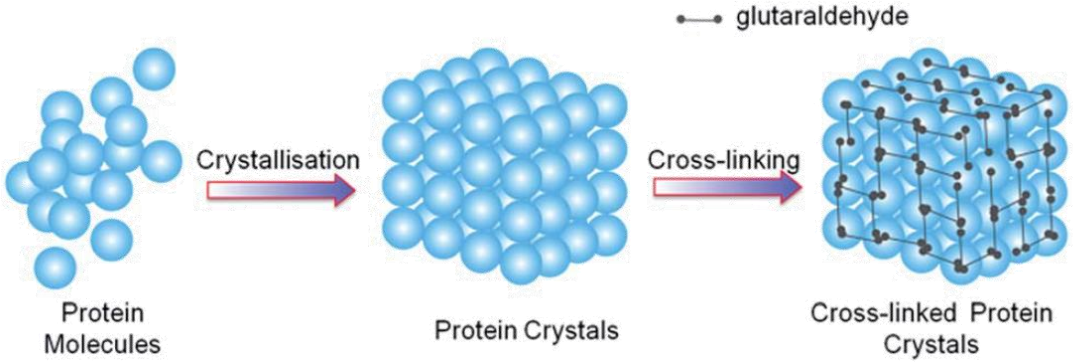
- Biological crystal
- Chiral structure
- Conduct protons



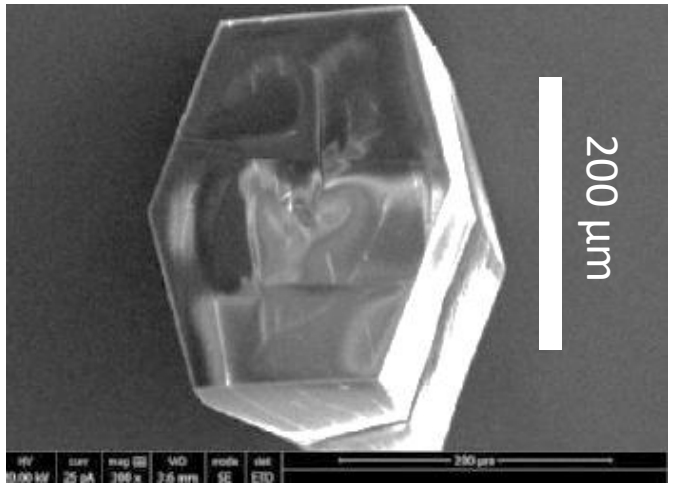
Dr. Yael Eisenberg-Domovich
Oded Livnah
Biology, HUJI

- The antibacterial property of hen egg white, due to the lysozyme it contains, was first observed by Laschtschenko in 1909.
- The bacteria-killing activity was demonstrated in 1922 by Alexander Fleming, the discoverer of penicillin, who coined the term "lysozyme".

Cross-linked crystals

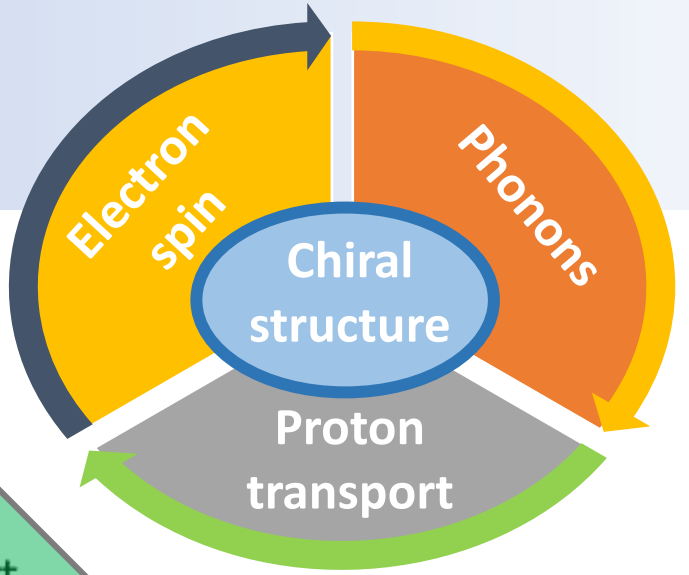


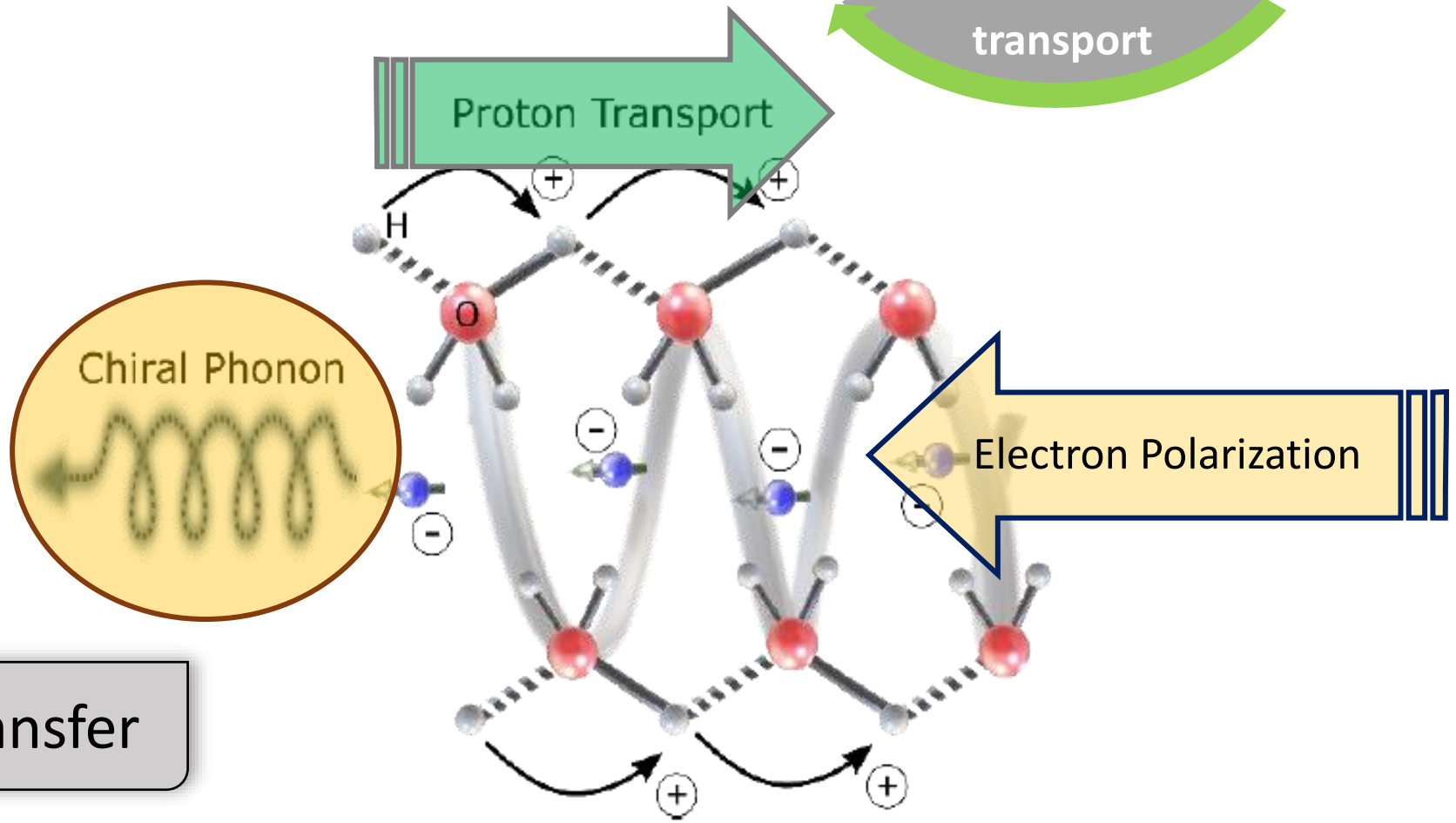
E. k. Yan et al., RSC Adv., 2015



Model

- Lysozyme –
  - ❑ **Chiral biological crystal**
  - ❑ Proton conduction
    - ❖ Electron transfer
    - ❖ **Phonons**
- CISS



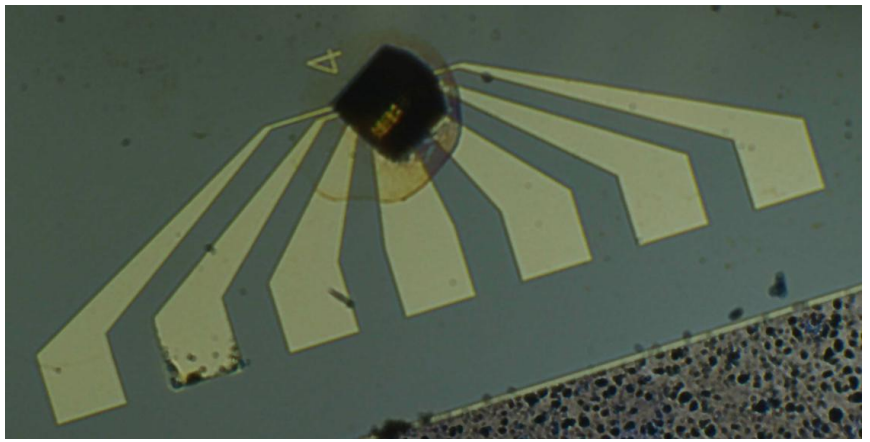


Spin-selective proton transfer

Experimental Setup

Device:

- Au-Ni electrodes

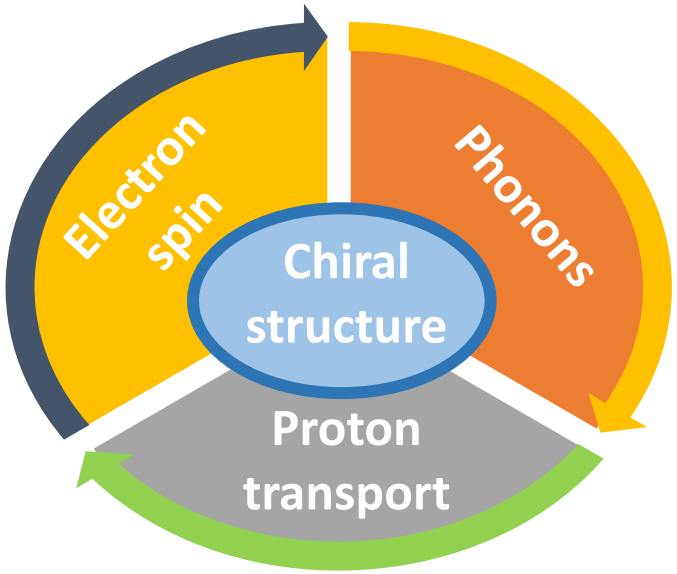


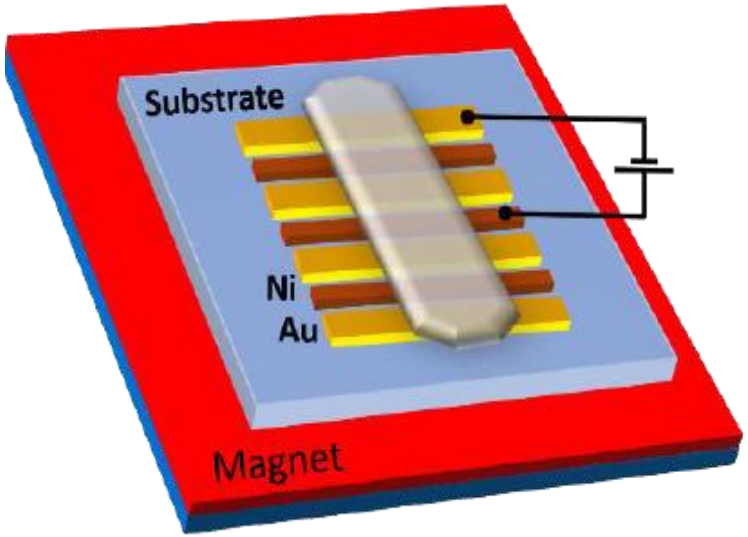
Measurements:

- IV (DC)
- Impedance spectroscopy (IS) (AC)
- 2nd Harmonic (AC)

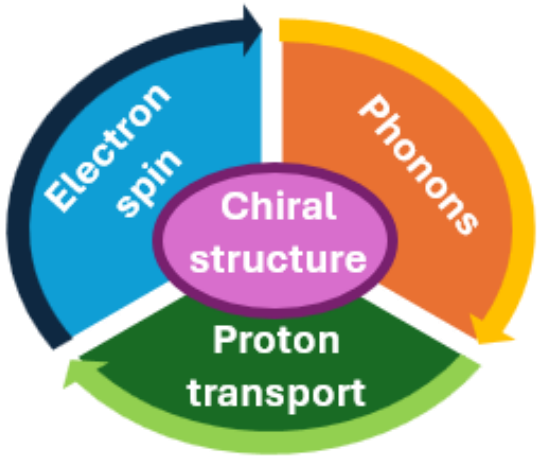
Parameters:

- Humidity level & source
- Contacts materials
- Temperature
- Magnetic field



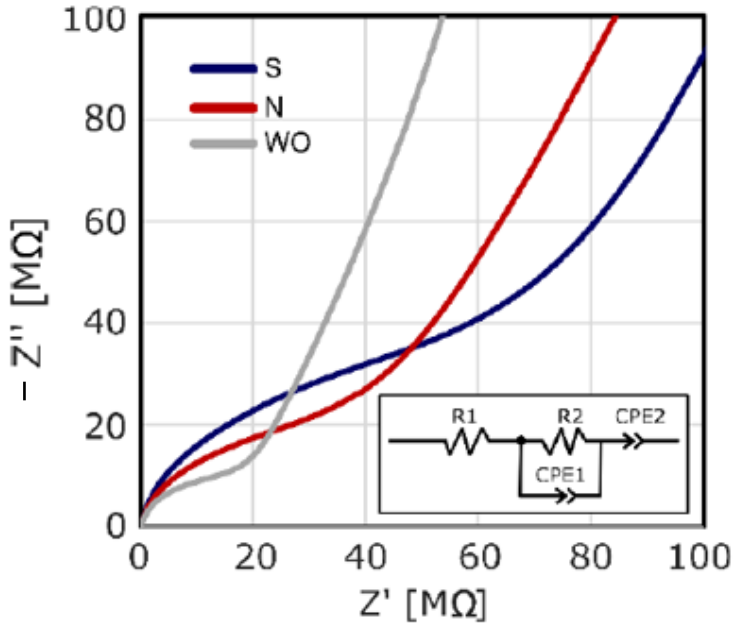


Methods



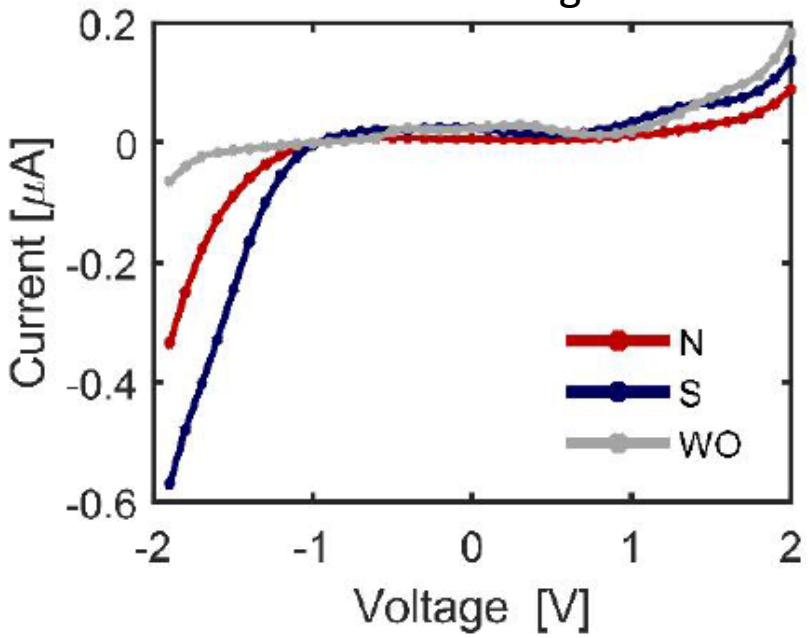
IS

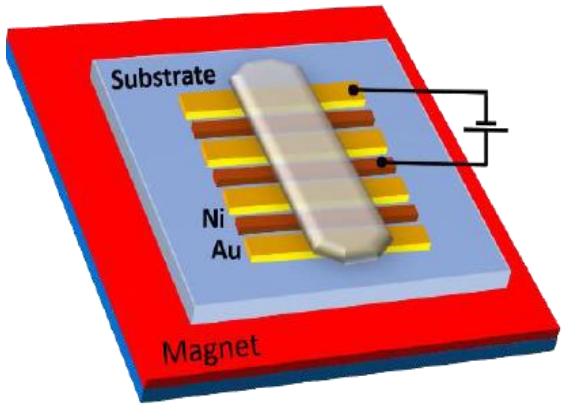
Impedance Spectroscopy



IV

Current-Voltage



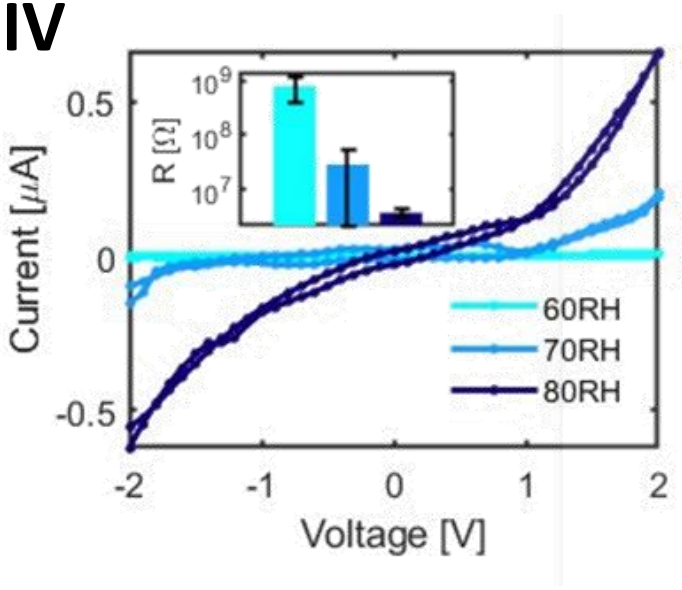


$$\%CISS = 100 * \frac{R_N - R_S}{R_S + R_N}$$

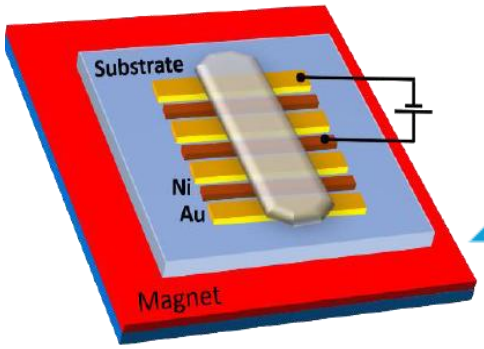
$\%CISS \neq 0$ ⇒ Spin preference

Results - Humidity Level – **Proton Conduction**

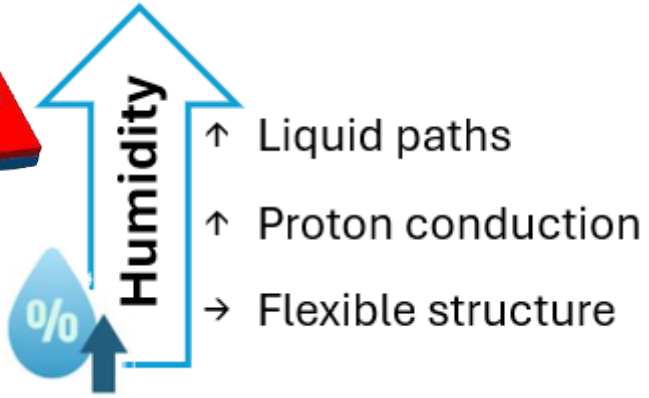
IV

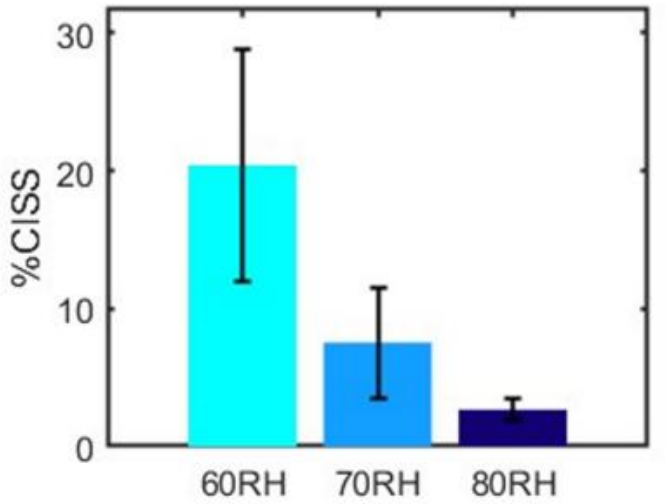


Humidity improve Conductance



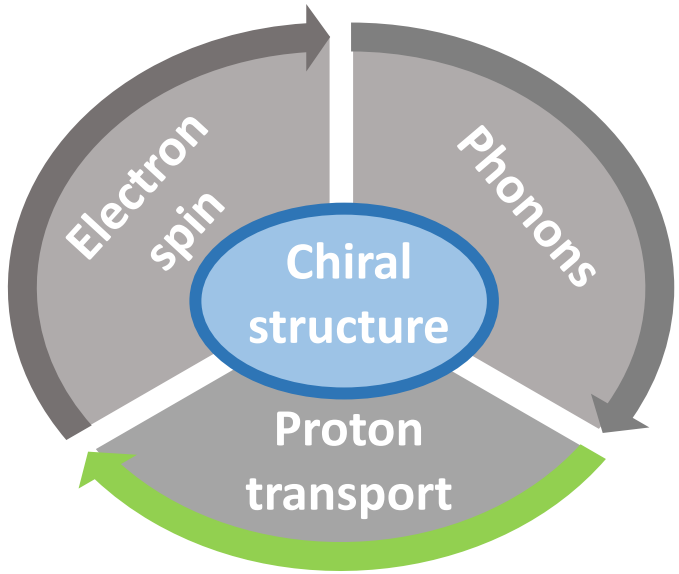
$$\%CISS = 100 * \frac{R_N - R_S}{R_S + R_N}$$





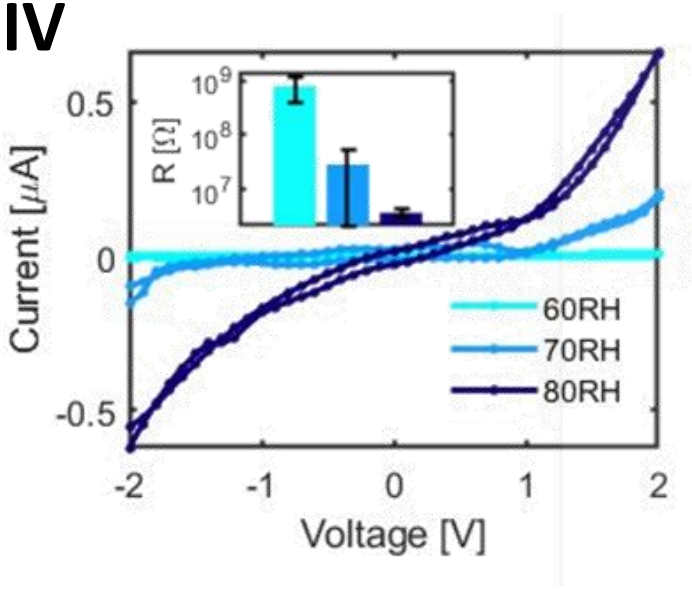
CISS is more dominant in lower humidity

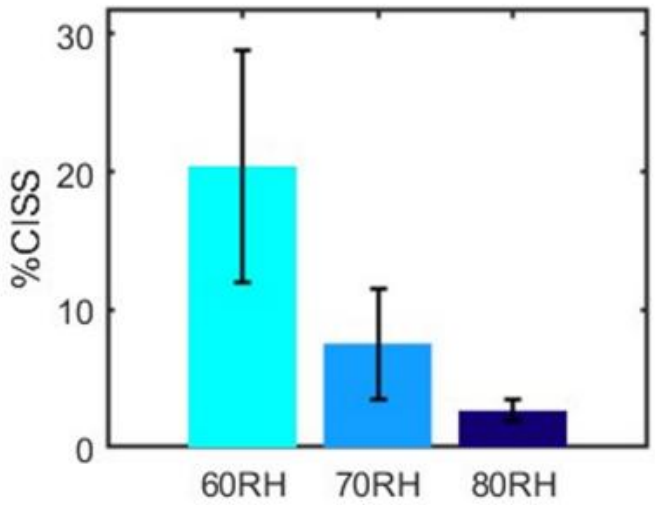
Protons are Less restricted to chiral structure.

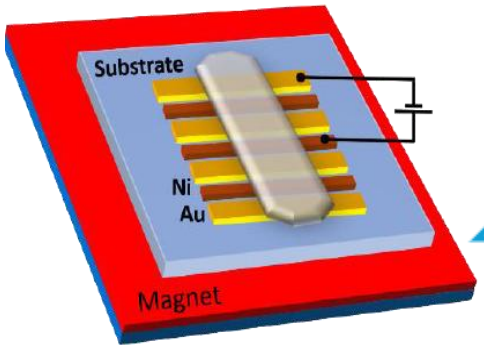


Results - Humidity Level – **Proton Conduction**

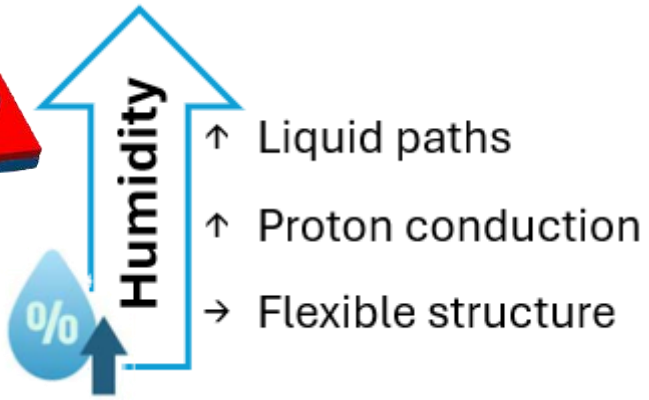
IV



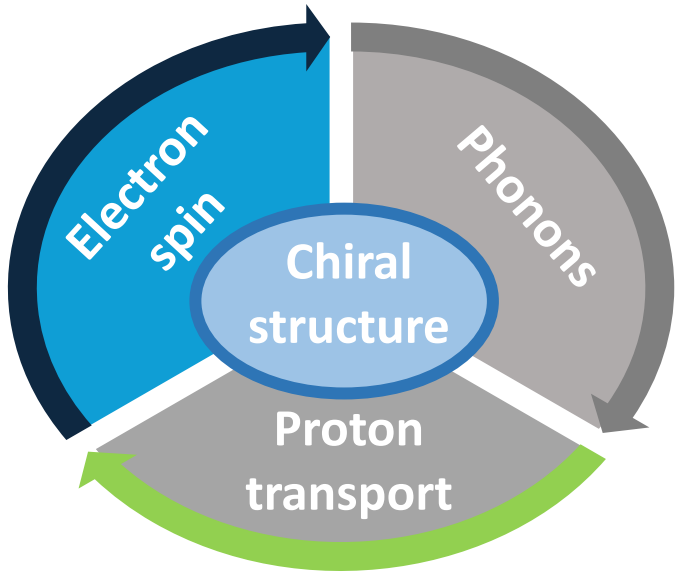




$$\%CISS = 100 * \frac{R_N - R_S}{R_S + R_N}$$

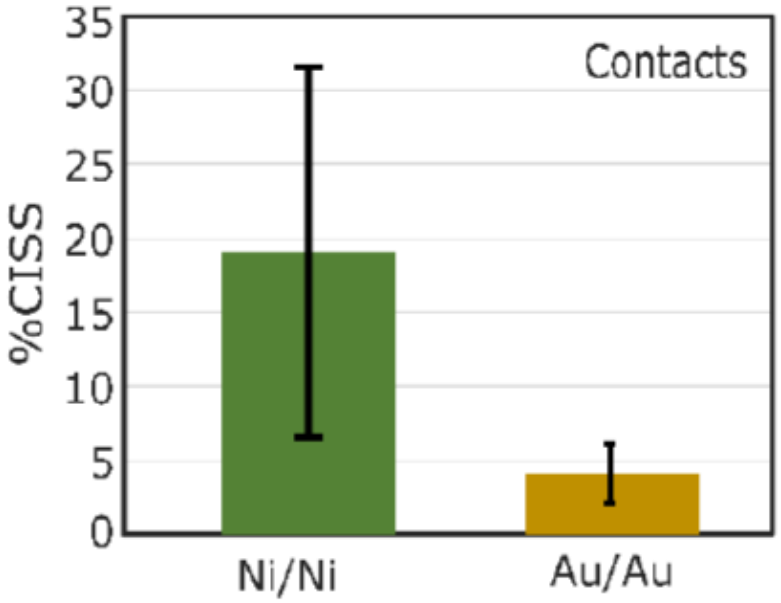


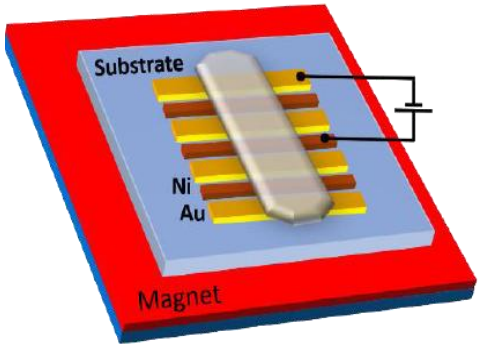
Proton transfer coupled to electron spin



Results - Contact Material – **Electron Spin**

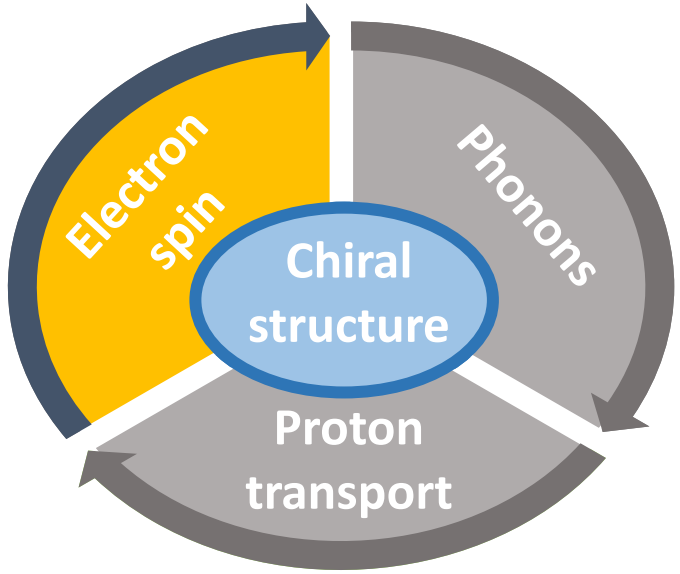
IS





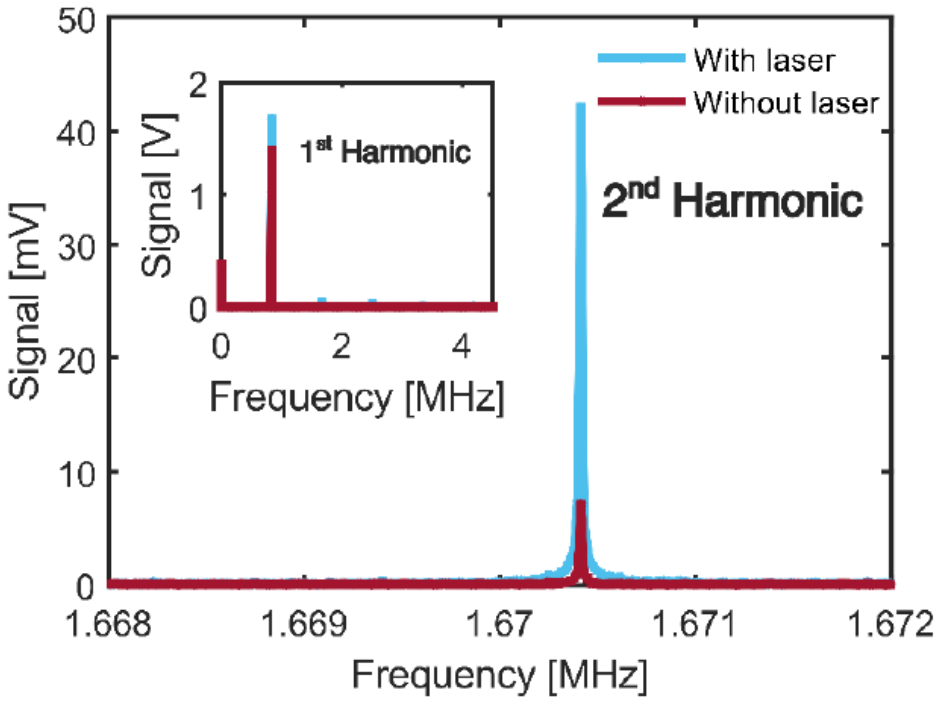
$$\%CISS = 100 * \frac{R_N - R_S}{R_S + R_N}$$

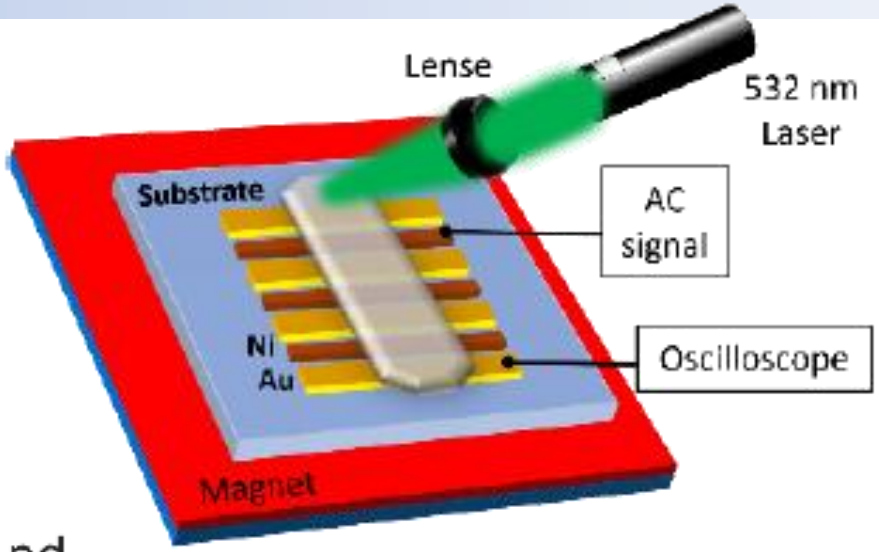
Proton transfer coupled to electron spin

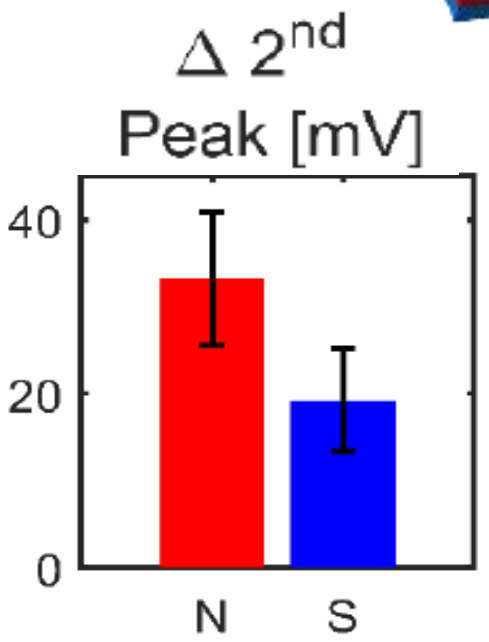


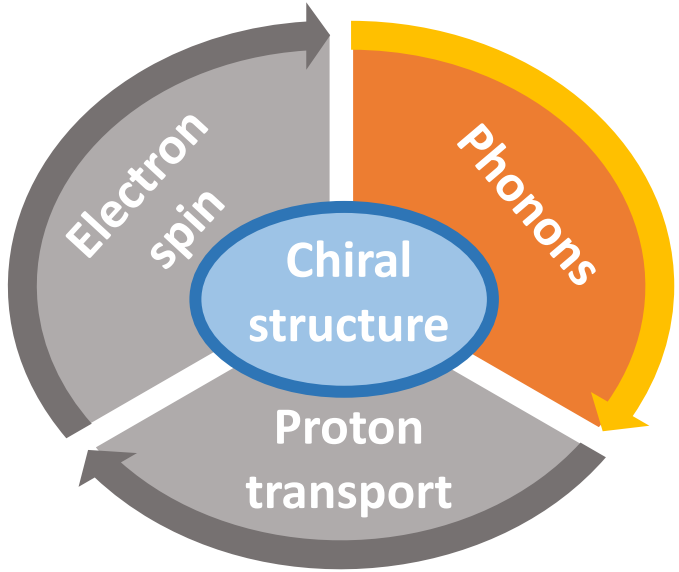
Results – Temperature – **Phonons**

2nd Harmonic



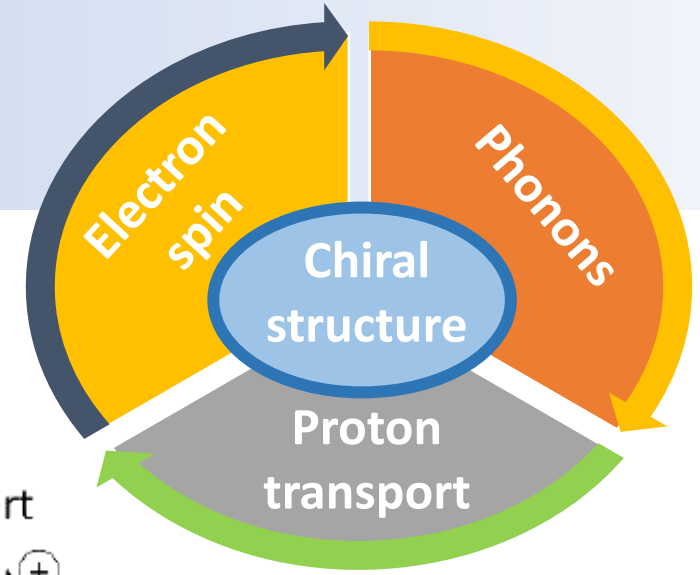




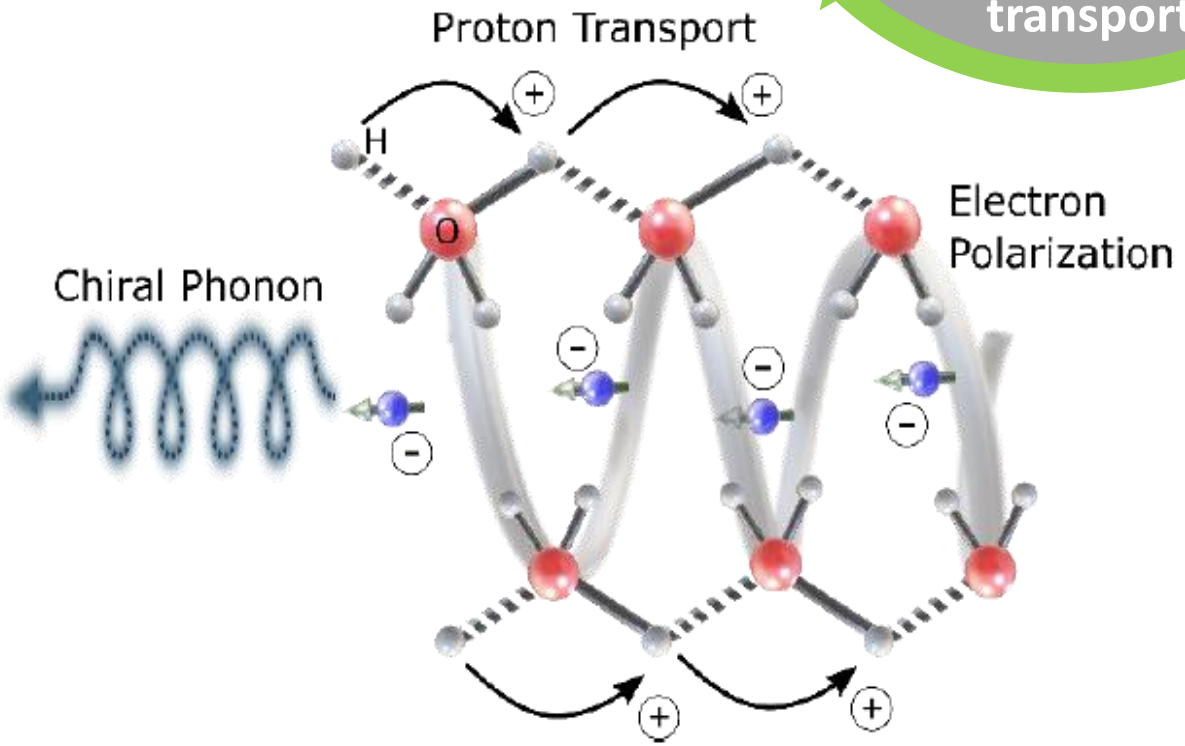


Proton transfer coupled with phonons & electron spin

Summary – Spin-Proton Coupling



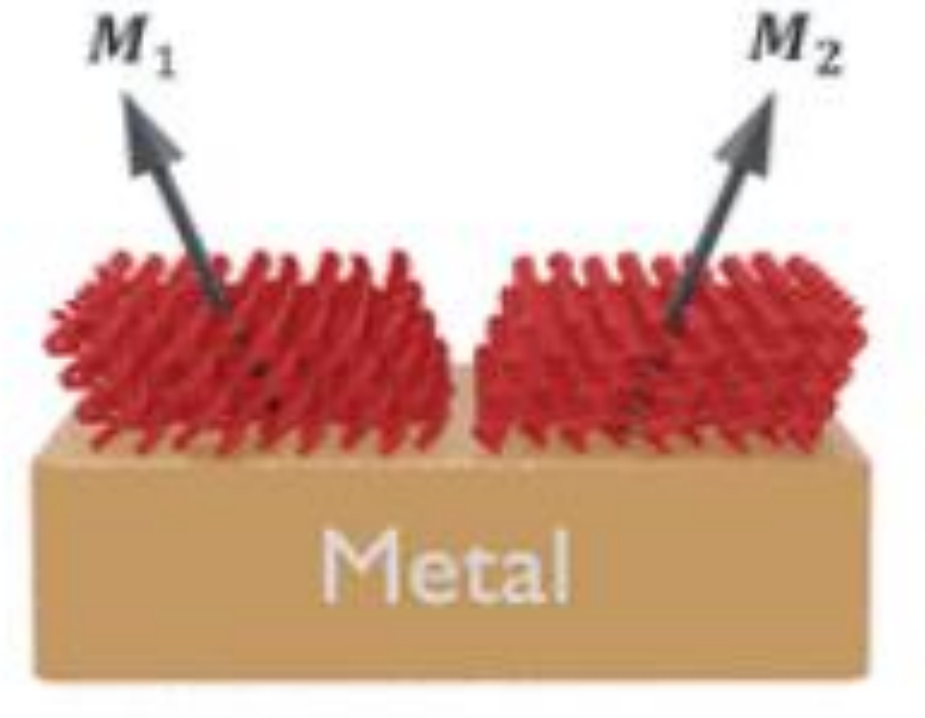
- → Apply Bias
- → Inject Polarized Electrons
- → Spin Preservation - CISS
- → Proton Transport
- → Electron Redistribution
- → Chiral Phonons
- → Enhanced Proton Transport



Protons transport coupled with phonons & electron spin

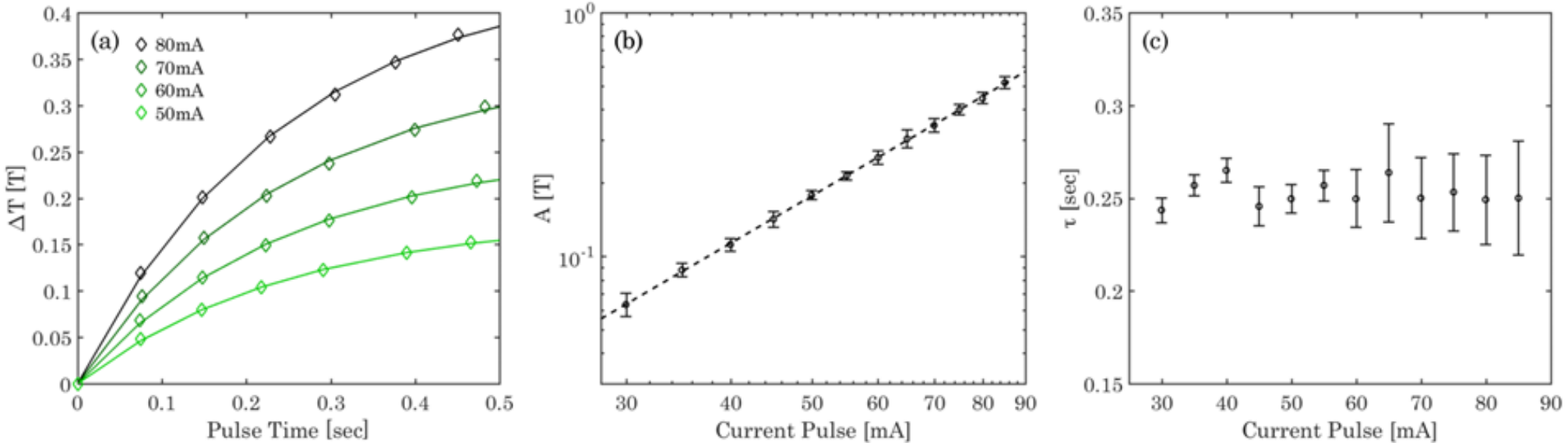
What about the chiral phonons heat conduction efficiency?

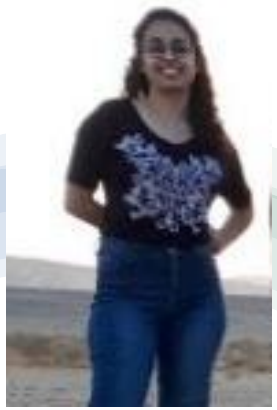
Chirality-Induced Selectivity of Phonon Angular Momenta in Chiral Quartz Crystals
Kazuki Ohe[1], Hiroaki Shishido[1,2], Masaki Kato[3], Shoyo Utsumi[2], Hiroyasu Matsuura[3], and Yoshihiko Togawa[1,2,4,*]
Phys. Rev. Lett. **132**, 056302 **(2024).**



- 50nm Au
- Measure heat conductance (at dif T)
- Adsorb a monolayer of molecules
- Measure heat conductance (at dif T)

Specific heat measurements

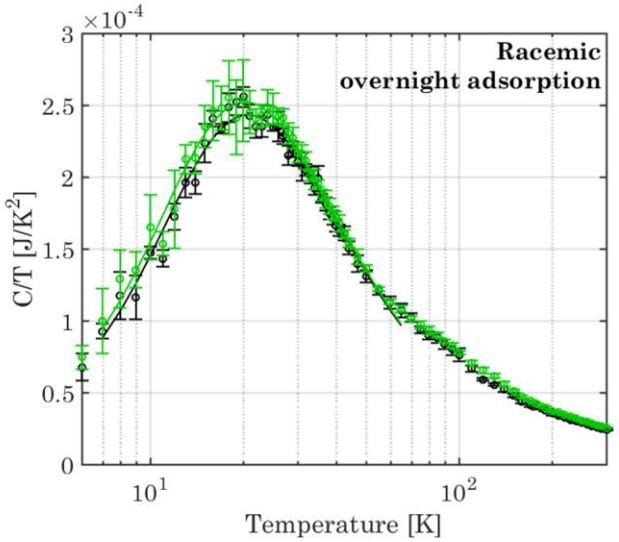


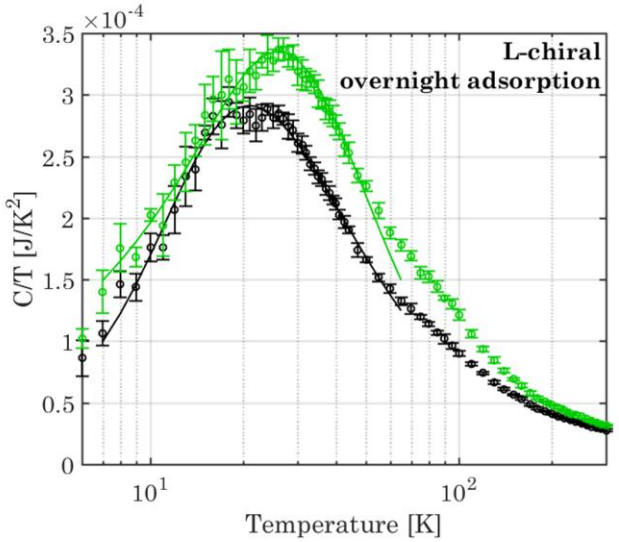


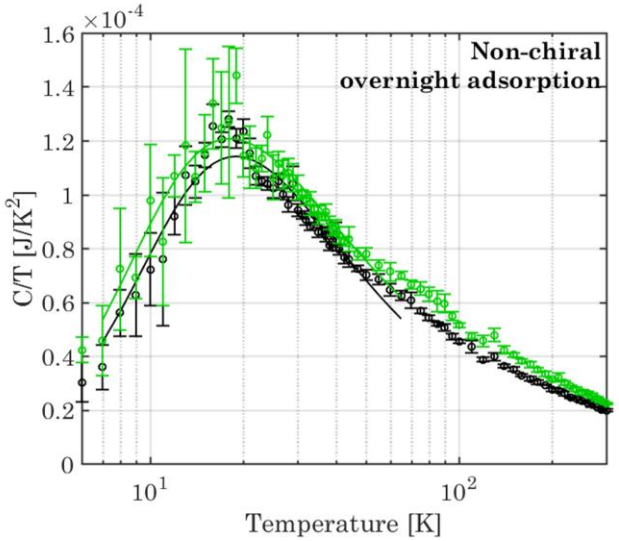
Influence of Chirality and Order on Phonon Dynamics in Molecularly Modified Gold Films

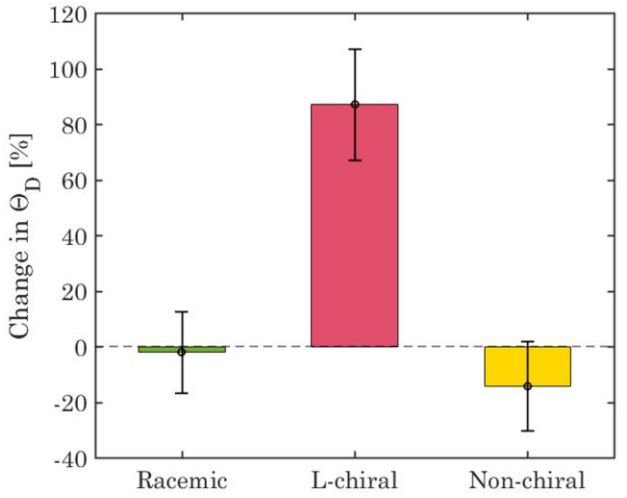
(a) Temperature evolution at T_0=150K. (b) Extracted prefactor A plotted against the current amplitude on a log-log scale. (c) Characteristic time τ extracted from temperature evolutions at different current amplitudes

C/T vs T data before (black) and after (green) surface treatment









Gold thin films (50nm thick) were deposited onto silicon wafers coated with a 1-μm-thick layer of thermally grown silicon dioxide.

The uniform chiral molecules arrangement of enantiopure molecules leads to suppress phonon scattering at the metal surface.

Conclusions

We observed and modeled new nuclear spin interactions in chemical and biological environments (may explain isotope effect in life)

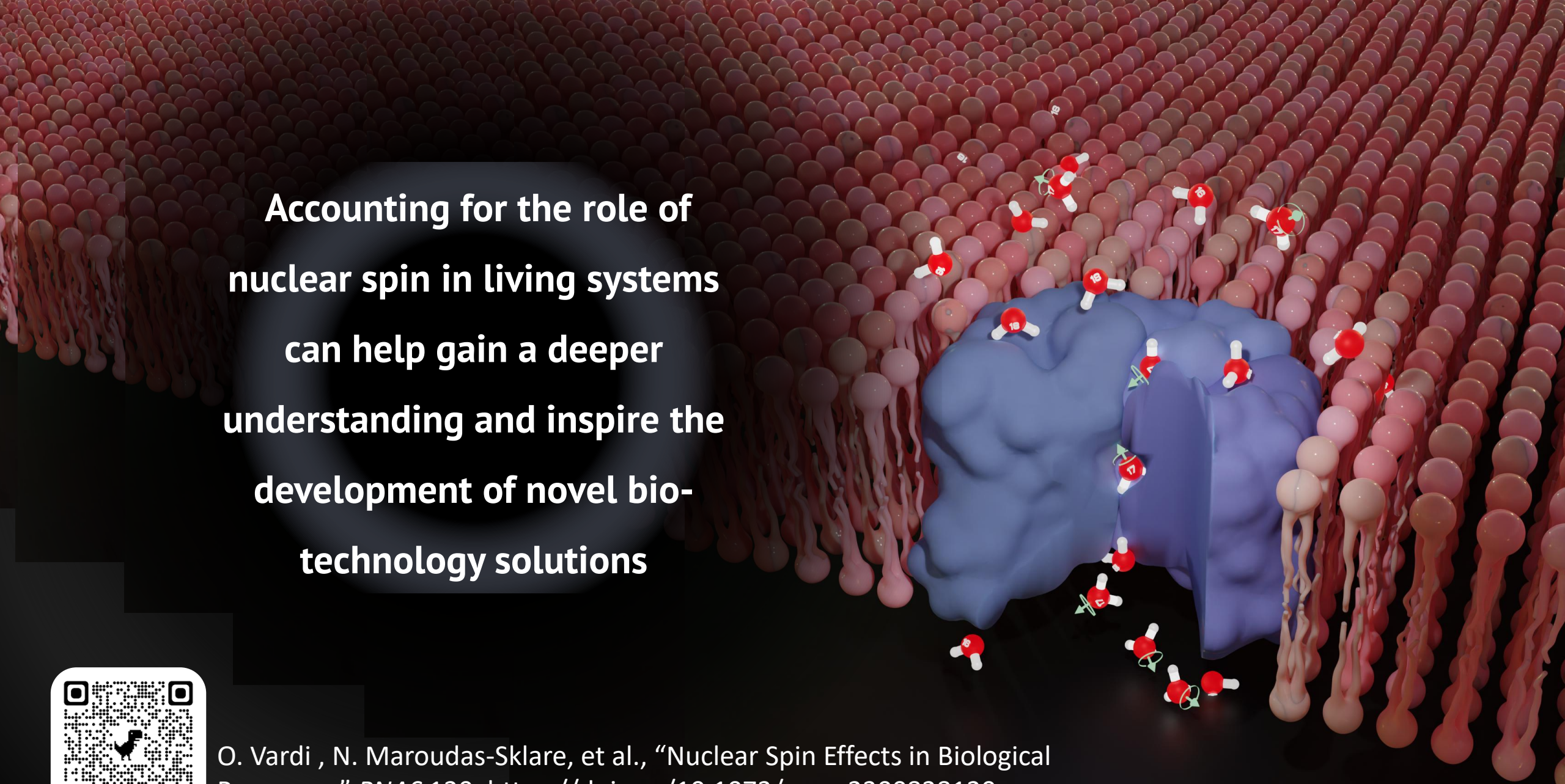
In both cases the nuclear interacts with the chiral environment creating a 2nd order CISS effect generated by polarization and long-lived phonons

In chiral crystals we can measure nuclear spin with magnetic electrodes

Angular momentum is conserved

Electron spin - > Chiral phonons-> Nuclear spin

Accounting for the role of nuclear spin in living systems can help gain a deeper understanding and inspire the development of novel bio-technology solutions



O. Vardi , N. Maroudas-Sklare, et al., “Nuclear Spin Effects in Biological Processes,” *PNAS* 120, https://doi.org/10.1073/pnas.2300828120.