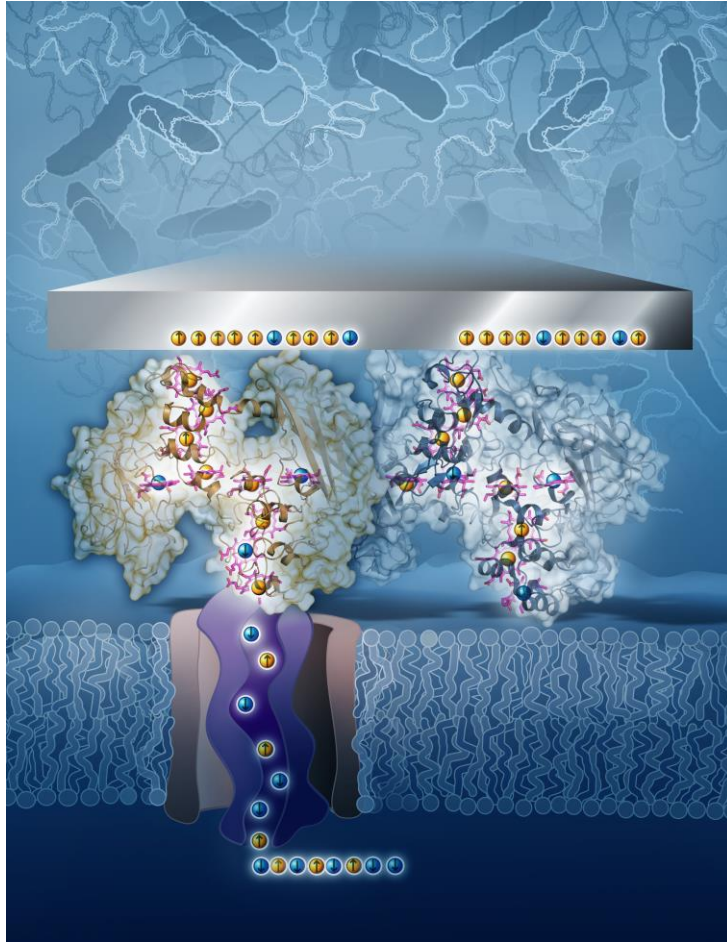


The Mechanisms and Implications of Chiral Induced Spin Selectivity in Biological systems



Moh El-Naggar

Christina Niman, Nir Sukenik, Marko Chavez, Sukram Yadav, Cole Harris, Tram Dang, Joshua Atkinson, Grace Chong, Yunke Zhao, Fengjie Zhao, James Boedicker, Jeff Gralnick, Yossi Paltiel, Tomasz Baczewski, Ron Naaman, Fabien Pinaud, Steve Finkel



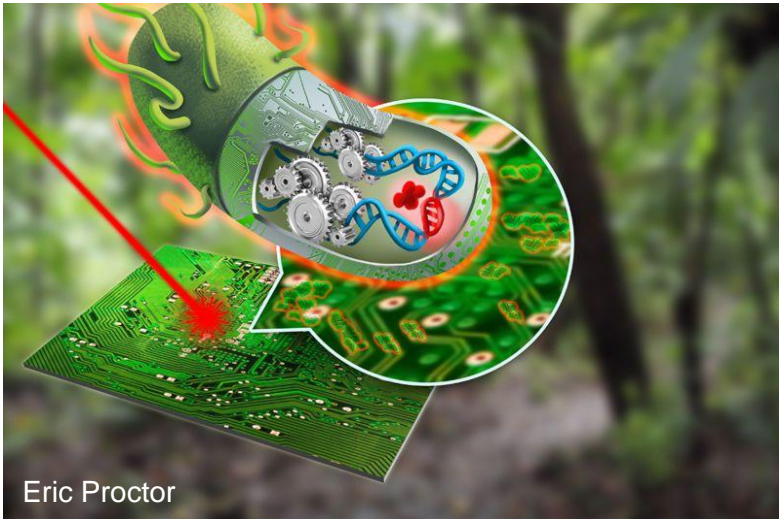
USC University of
Southern California

Department of Physics and Astronomy
Department of Biological Sciences
Department of Chemistry

www.elnaggarlab.org

Biotic-Abiotic Electron Exchange

Towards Understanding & Controlling Living Cells that Directly Integrate and Communicate (Electron Transfer) with Electrodes

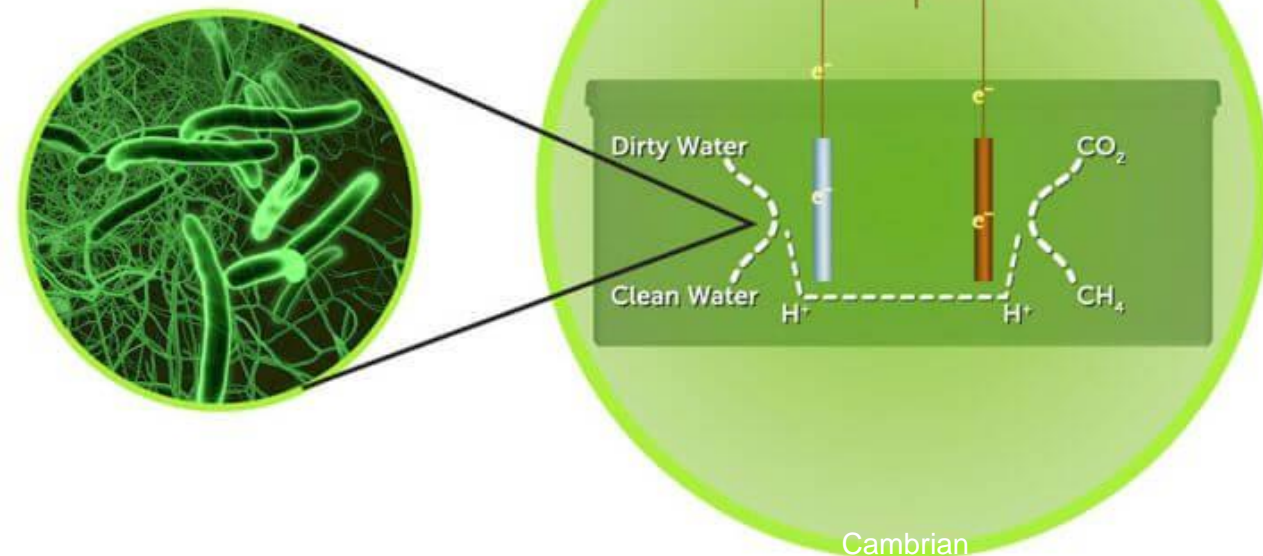


Living Electronics

- Cell-Electronics Interfaces
- Biosensors
- Biocomputing
- Information Storage

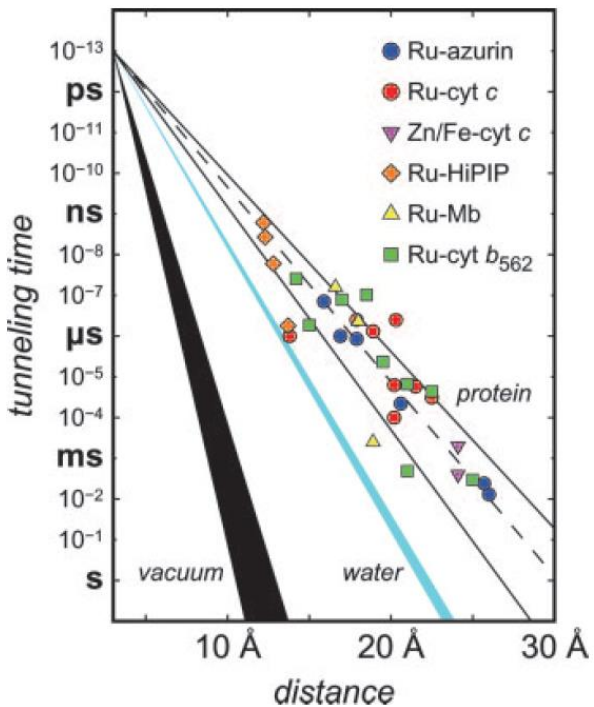


Energy-Water-Waste Nexus



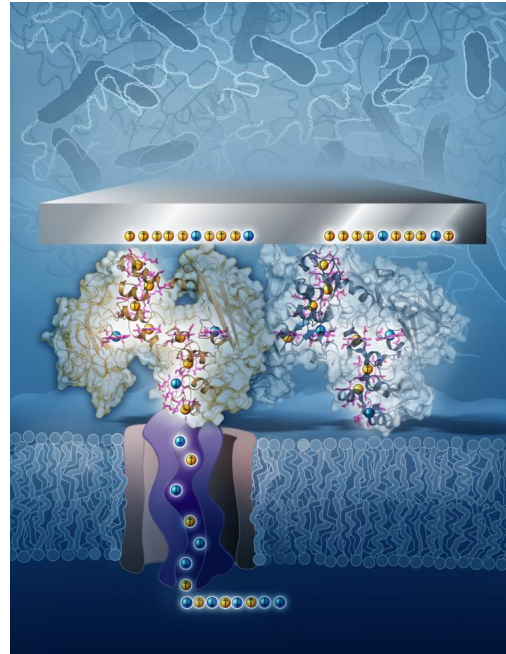
Microbes host electron transport networks that span cells and across the biotic-abiotic interface

ET Proteins



Gray and Winkler, *PNAS* 2005

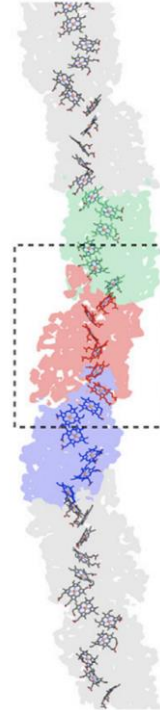
Extracellular Electron Transfer



Mishra and Pirbadian
JACS 2020

~10 nm

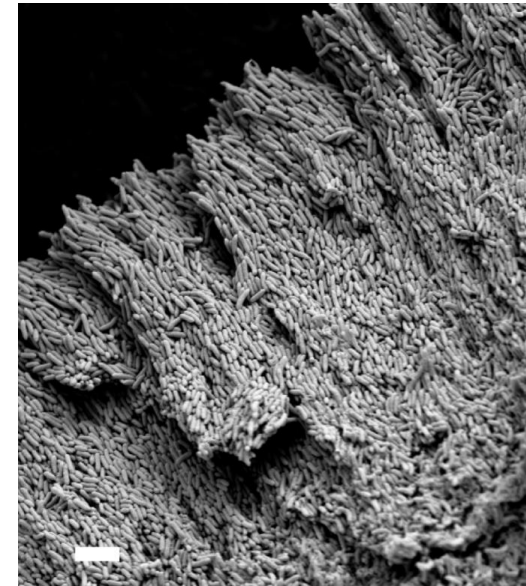
Bacterial Nanowires



Wang *et al.*, *Cell* 2019

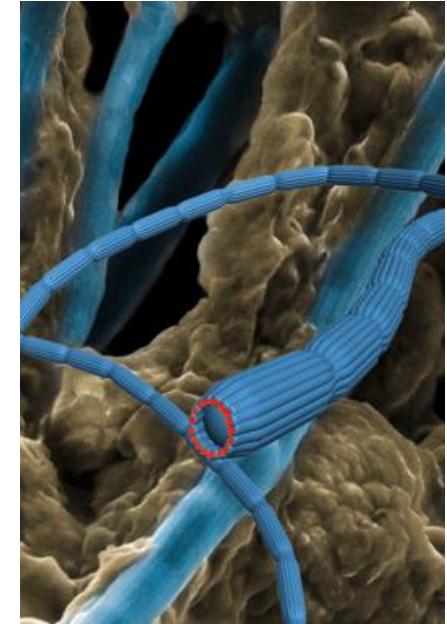
~10 μ m

Conductive Biofilms



~100 μ m

Cable Bacteria



Pfeffer *et al.* *Nature*, 2012
Yang *et al.* *eLife* 2024

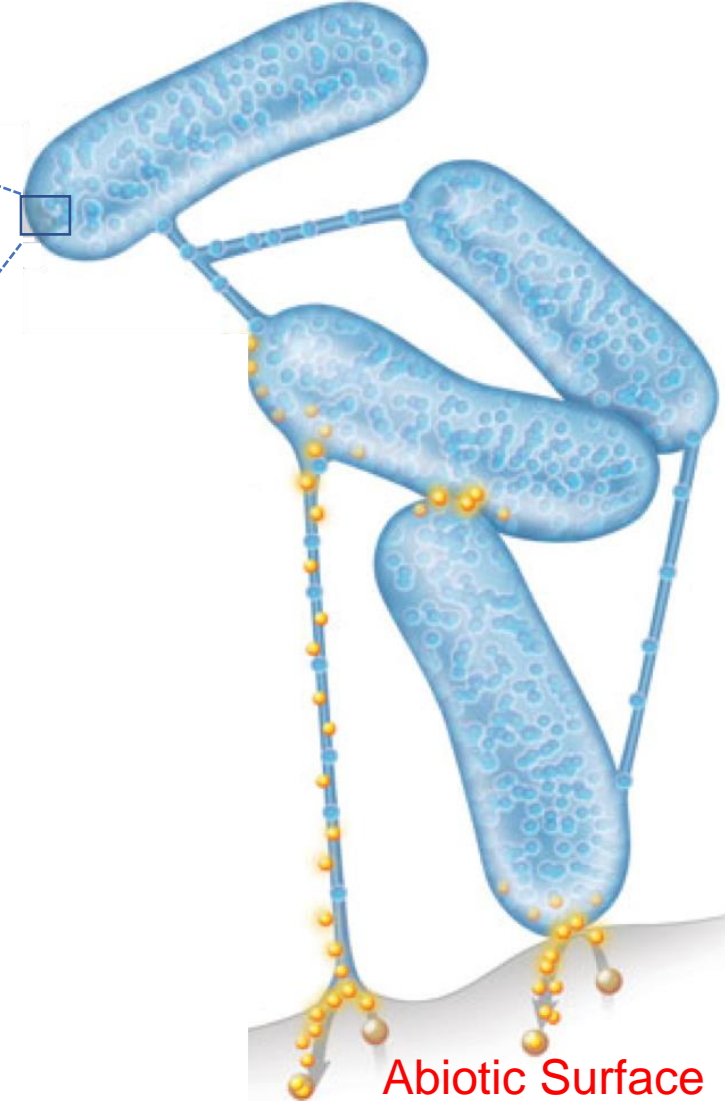
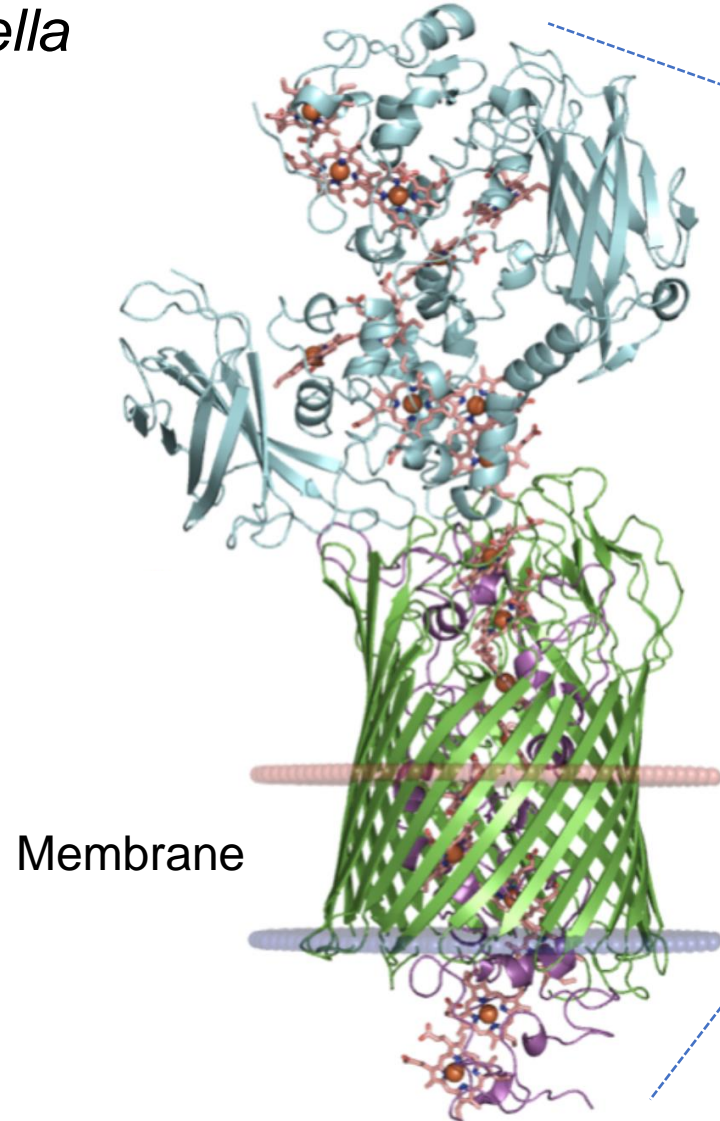
~ mm – cm (!)

nm

MtrABC: The Extracellular Electron Conduit in *Shewanella*

El-Naggar & Finkel. **Live Wires: Electrical Signaling Between Bacteria**, The Scientist, 27, 2013

Chong, Karbelkar, El-Naggar, **Nature's conductors: what can microbial multi-heme cytochromes teach us about electron transport and biological energy conversion?** Current Opinion in Chemical Biology, 47, 2018



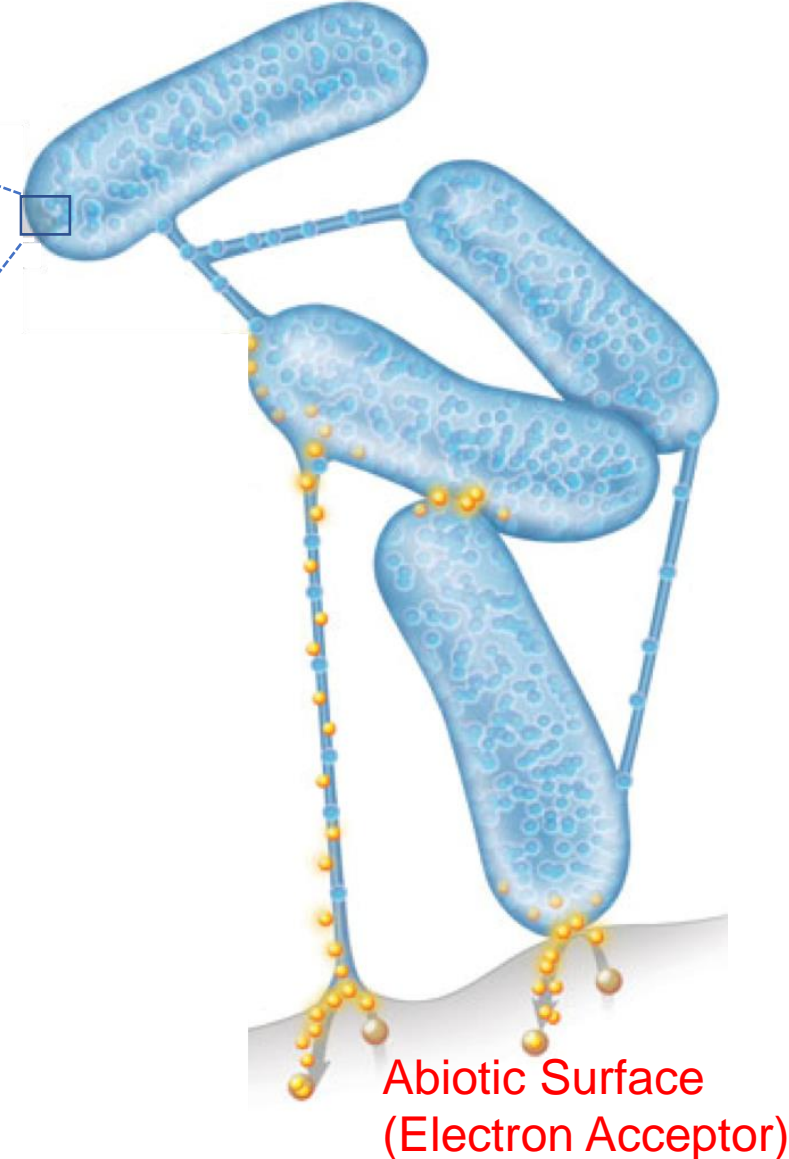
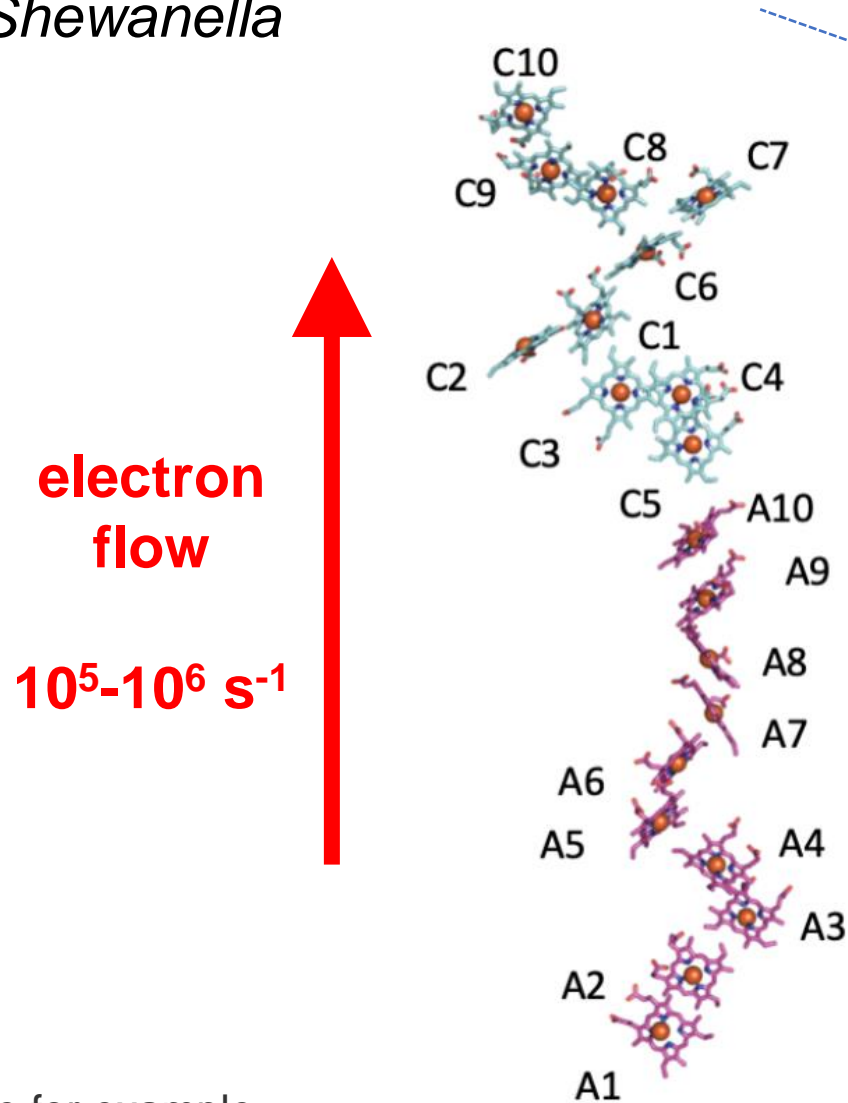
Abiotic Surface
(Electron Acceptor)

Structure from:
Edwards *et al.* 181 Cell, 2020

MtrABC: The Extracellular Electron Conduit in *Shewanella*

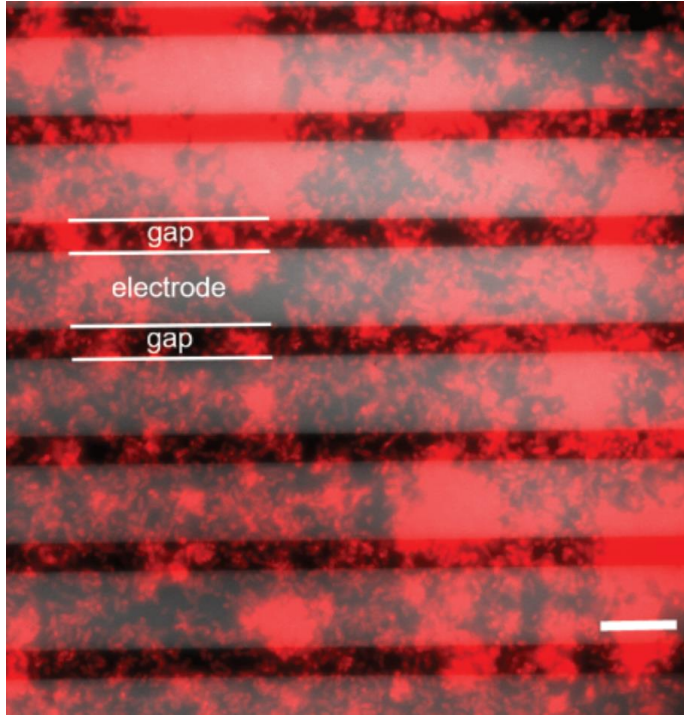
El-Naggar & Finkel. **Live Wires: Electrical Signaling Between Bacteria**, The Scientist, 27, 2013

Chong, Karbelkar, El-Naggar, **Nature's conductors: what can microbial multi-heme cytochromes teach us about electron transport and biological energy conversion?** Current Opinion in Chemical Biology, 47, 2018

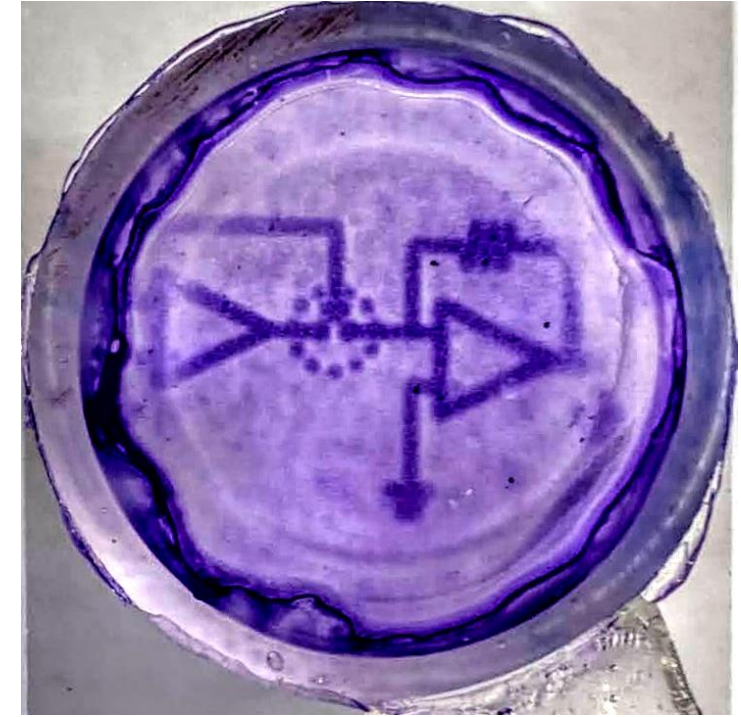
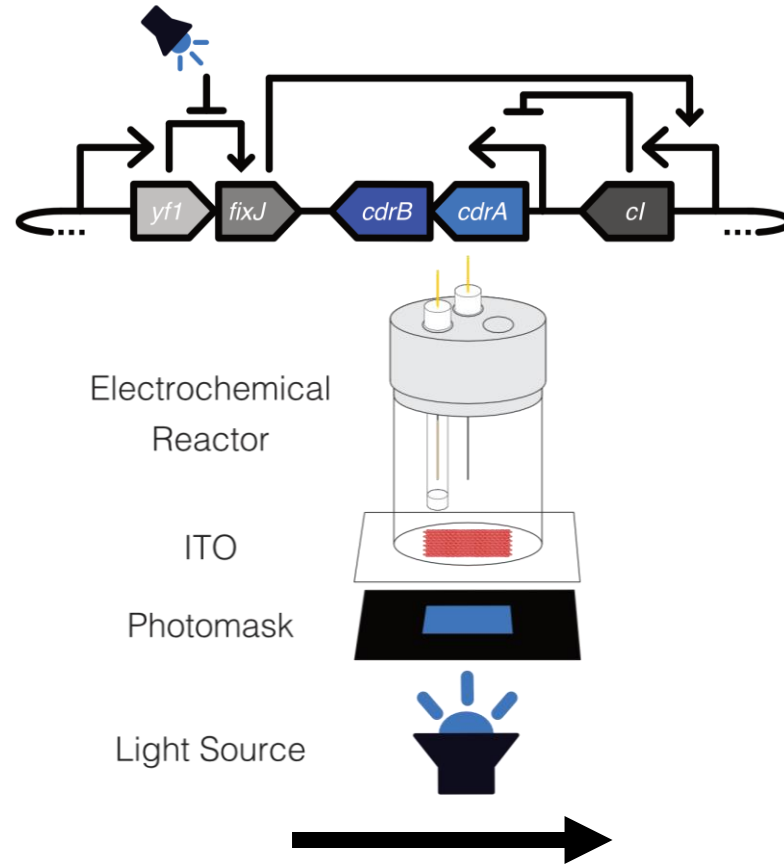


See for example:
Jiang *et al.* *PNAS* 116 (9), 2019
van Wonderen *et al.* *PNAS* 118 (39),

Turning biofilms into programmable living materials



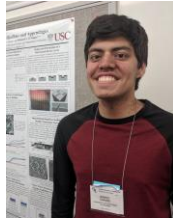
Xu S, *et al.*, *J. Am. Chem. Soc.* (2018)



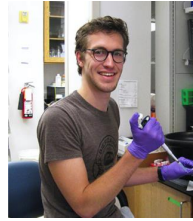
James
Boedicker



Fengjie
Zhao



Marko
Chavez



Josh
Atkinson



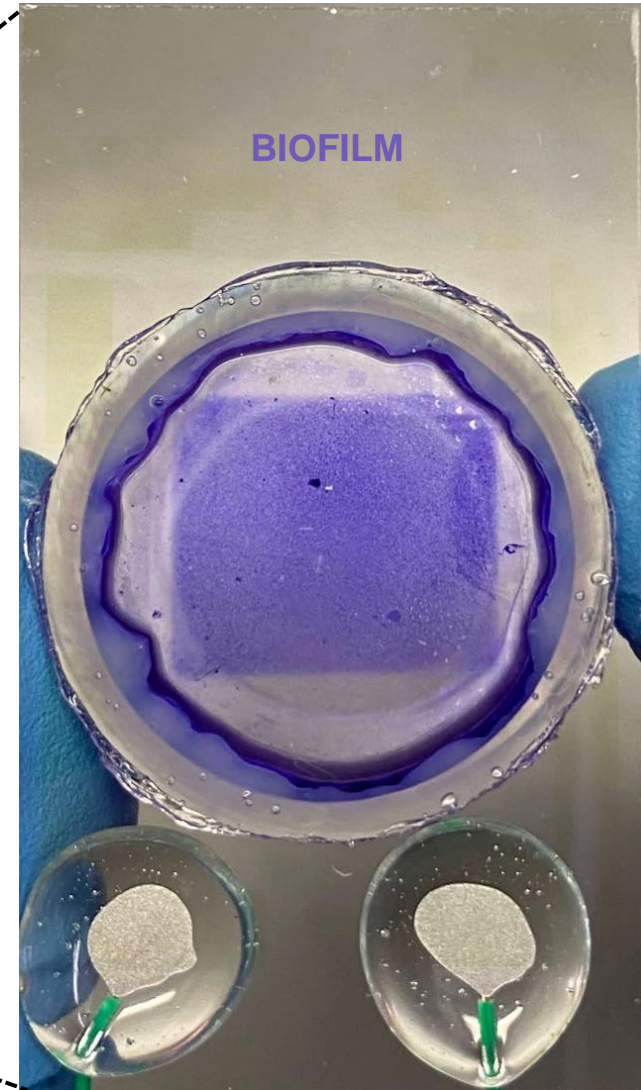
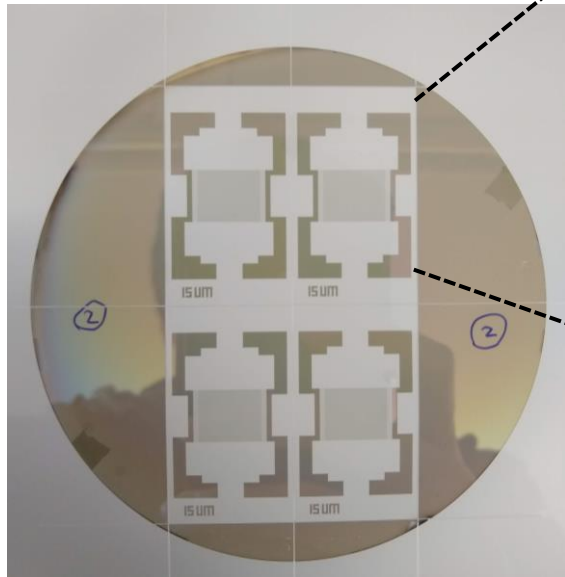
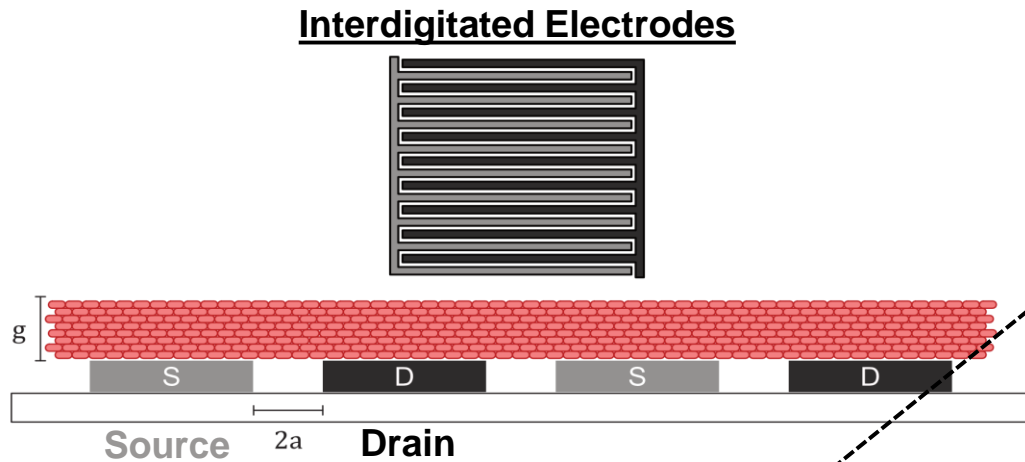
Christina
Niman



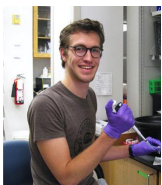
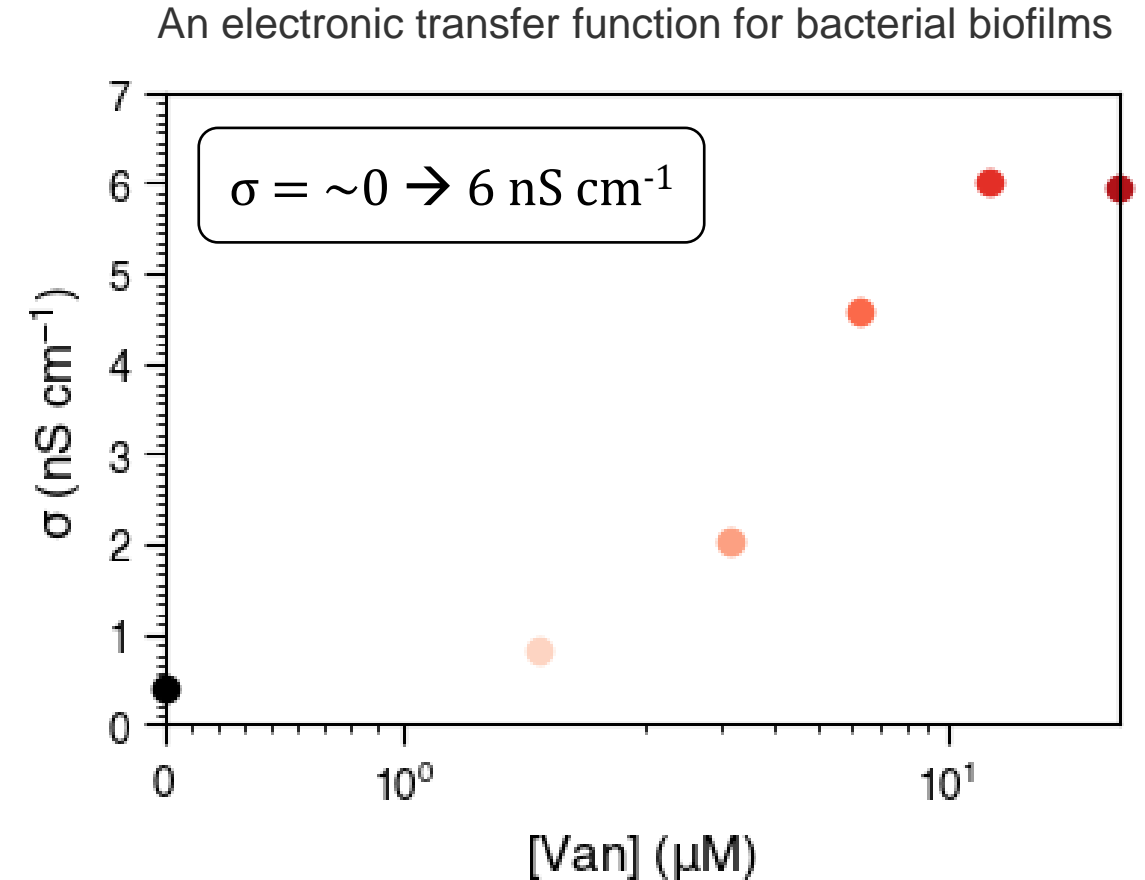
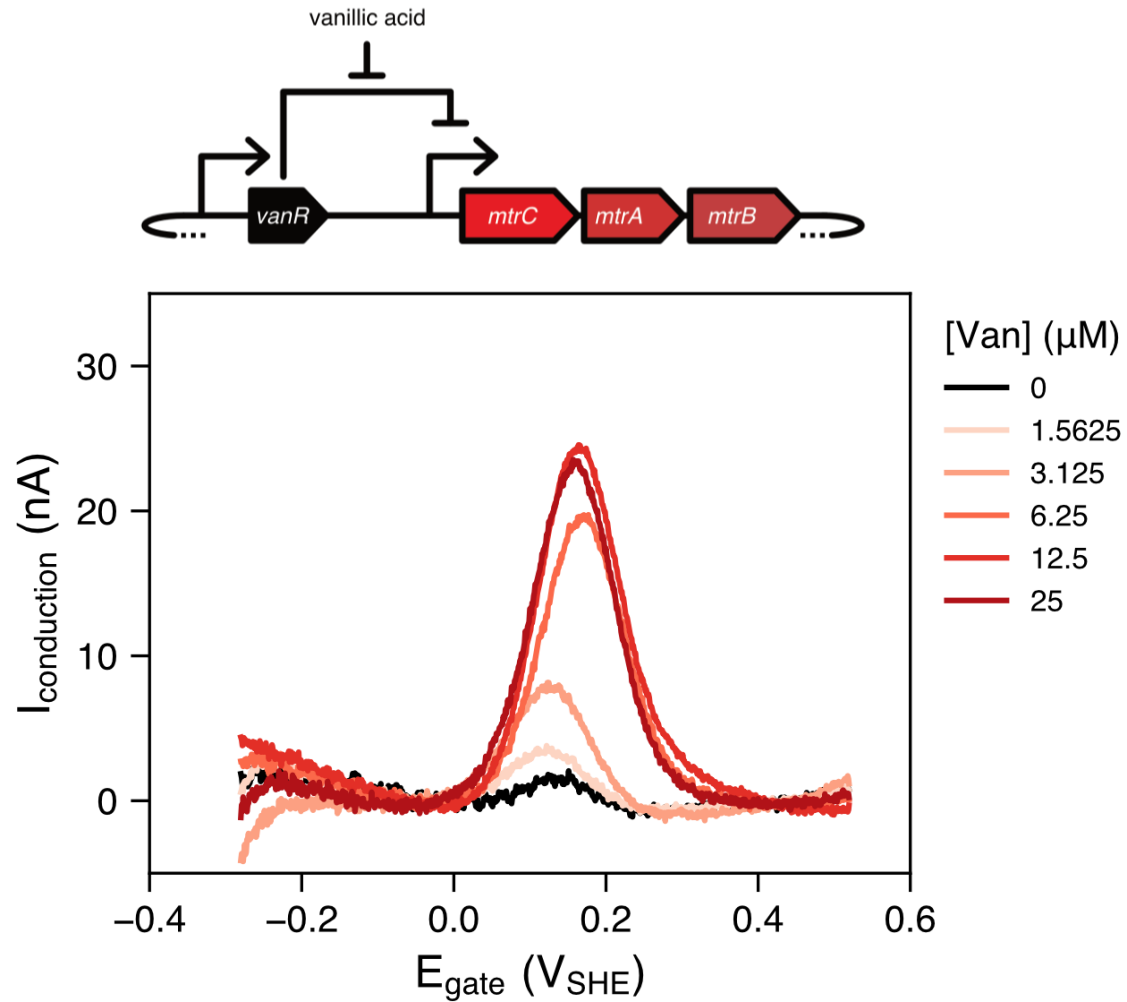
Jeff
Gralnick

Zhao, Chavez *et al.* *ACS SynBio*, 2024
Atkinson, Chavez *et al.* unpublished

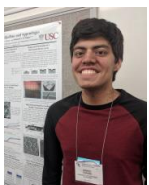
Photopatterning and Electronic Control of Biofilms



Biofilm doping: Control of carrier (cytochrome) density



Josh Atkinson

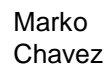
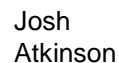
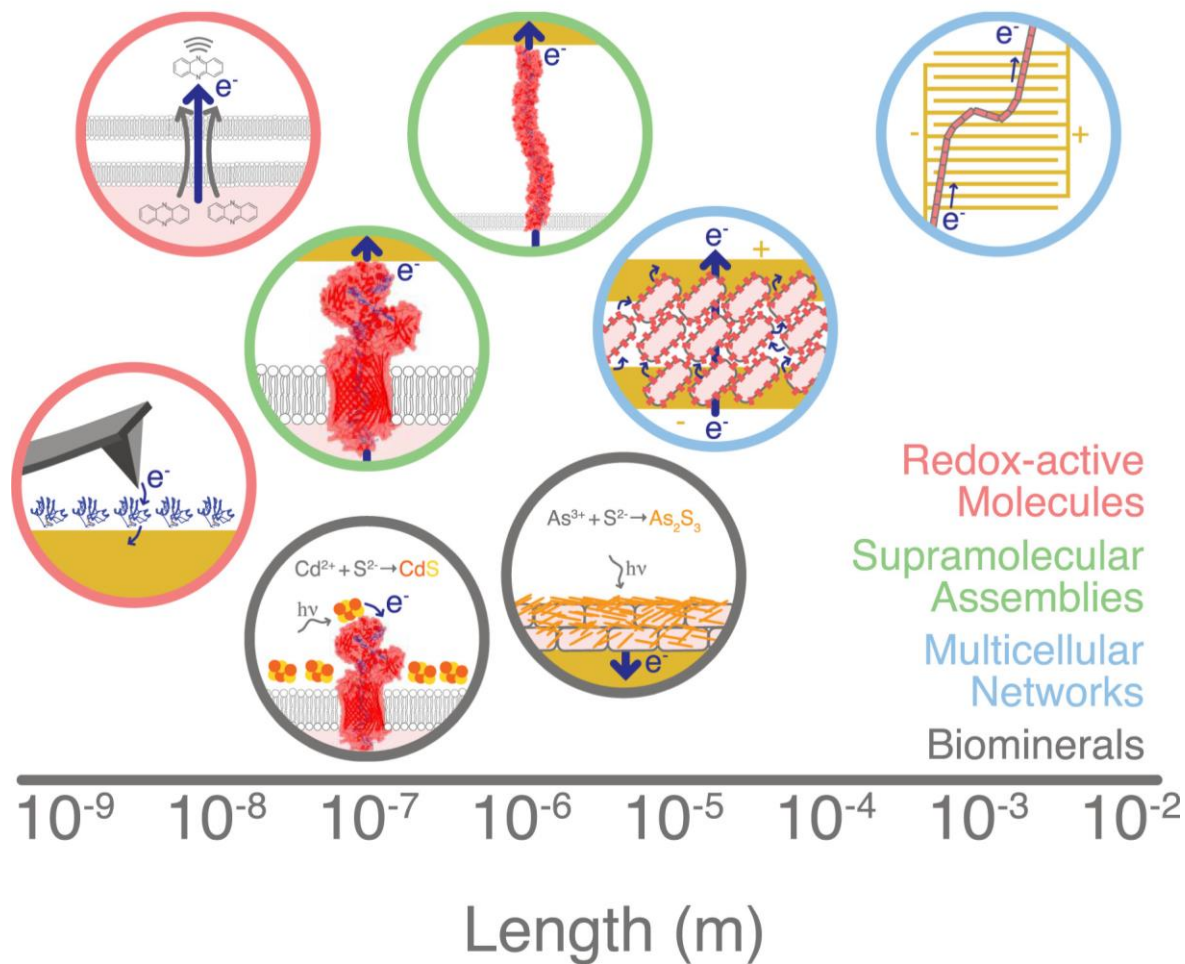


Marko Chavez

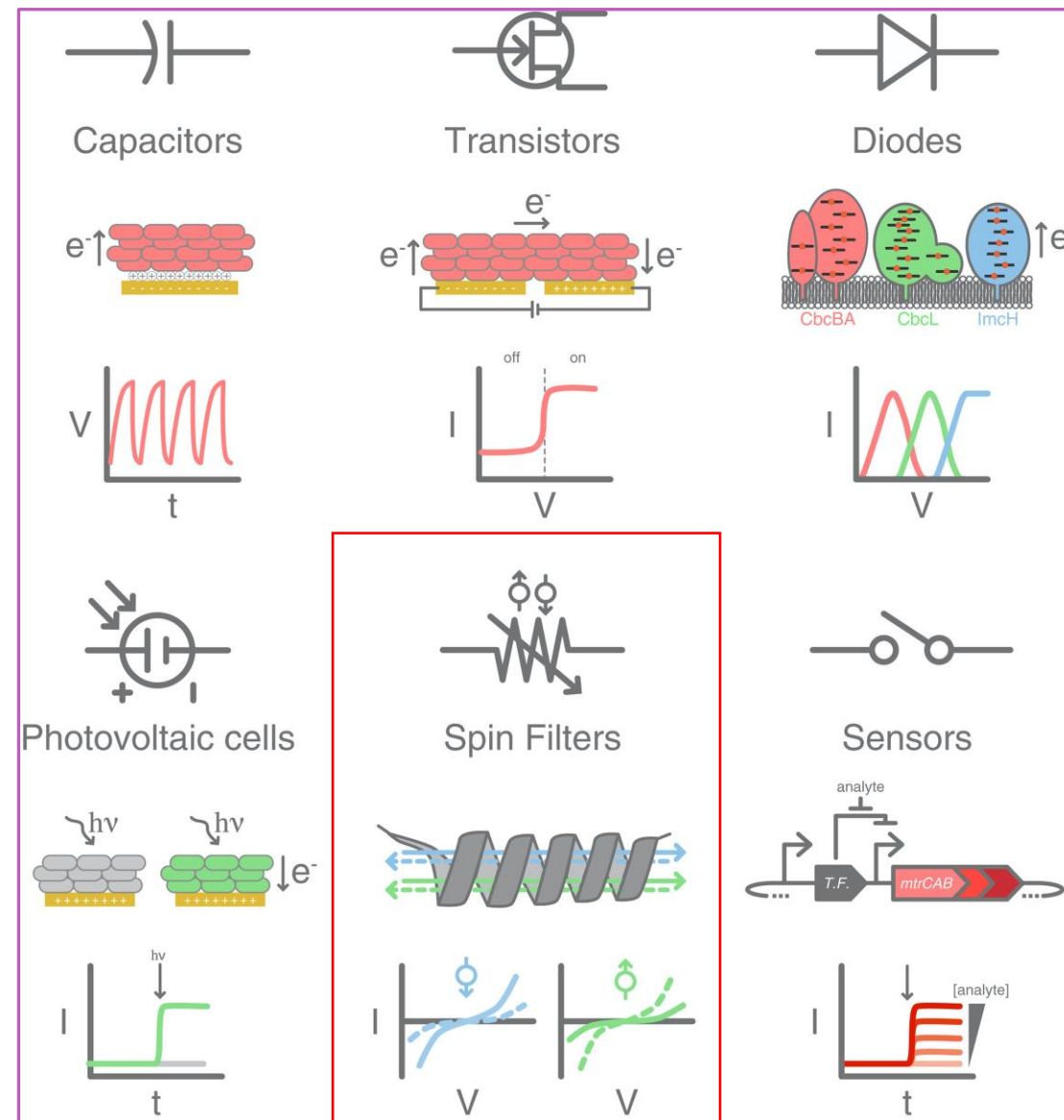


Christina Niman

Atkinson, Chavez, Niman, *et al.*, in prep (2024)



J.T. Atkinson, M.S. Chavez, C.M. Niman, M.Y. El-Naggar.
**Living electronics: A catalogue of engineered living
electronic components**, 16, Microbial Biotechnology, 2023

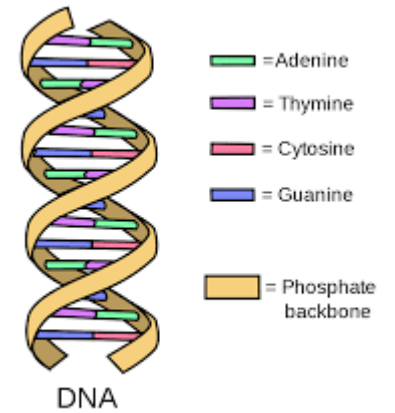
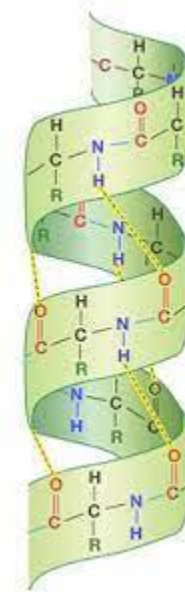
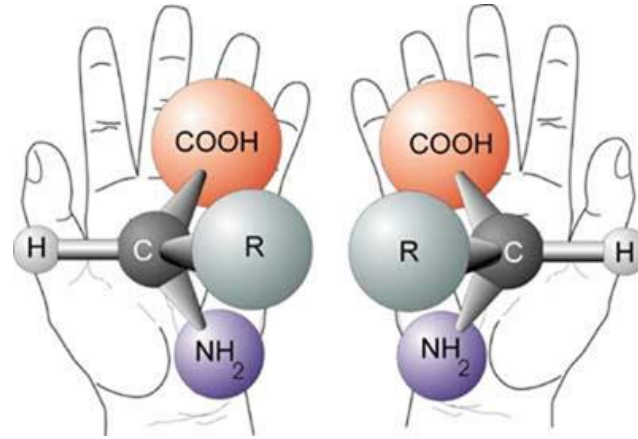


So what does any of this have to do with spin? Enter **Chiral Induced Spin Selectivity**

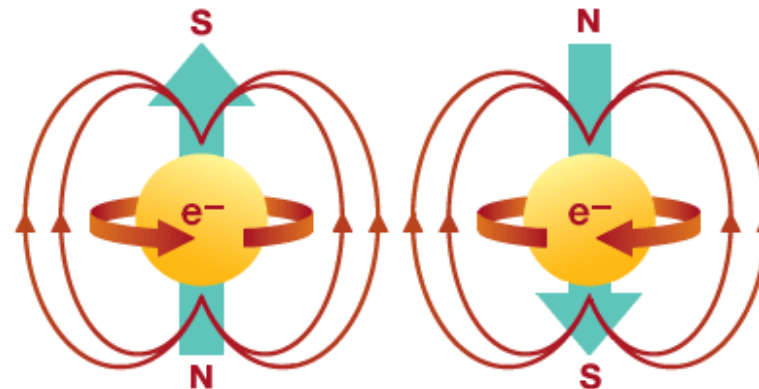
There are two players in the effect:

Chiral Molecules

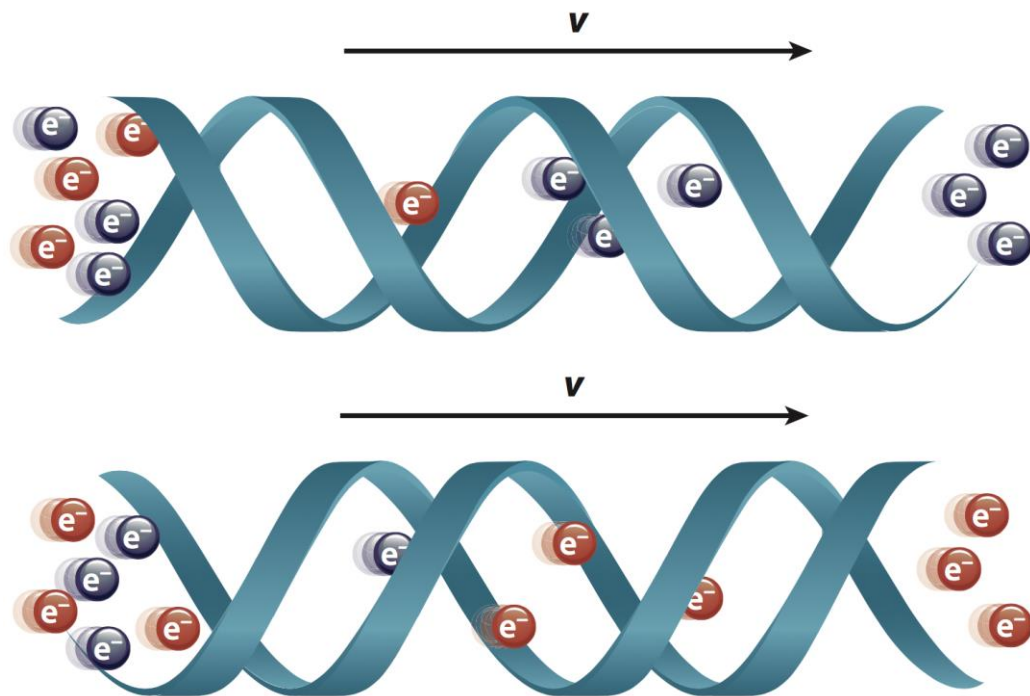
An object “has chirality if its image in a plane mirror, ideally realized, cannot be brought to coincide with itself.” Lord Kelvin, 1893



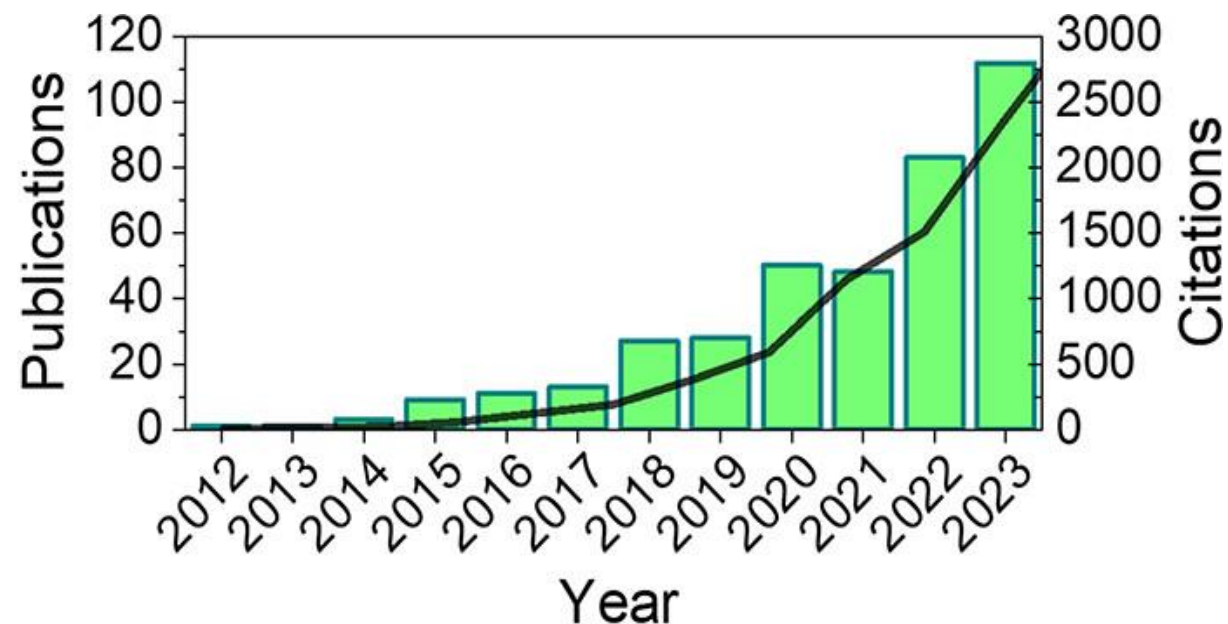
Electron Spin



Chiral Induced Spin Selectivity (CISS)



Confirmed with photoelectron spectroscopy, magnetic controlled fluorescence, single molecule conduction, spin-specific electrochemistry on oligopeptides, DNA, etc



Bloom, Paltiel, Naaman, Waldeck, *Chiral Induced Spin Selectivity, Chemical Reviews* 2024

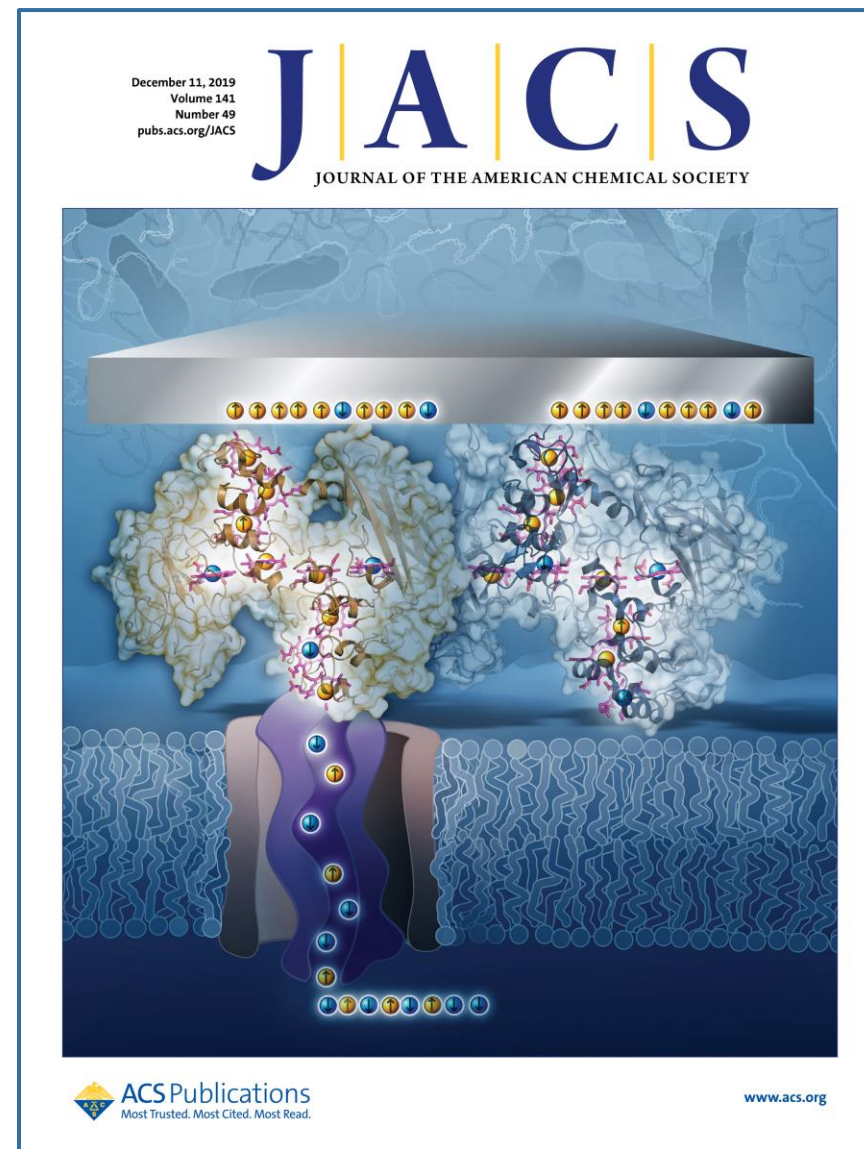


Collaboration with Ron Naaman
(WIS, Israel)

Ray et al. Science, 1999
Goehler et al. Science 2011
Mondal et al. ACS Nano 2015
Kumar et al. PNAS 2017
Banerjee-Ghosh et al. Science 2018
Naaman, Nature Reviews Chemistry, 2019

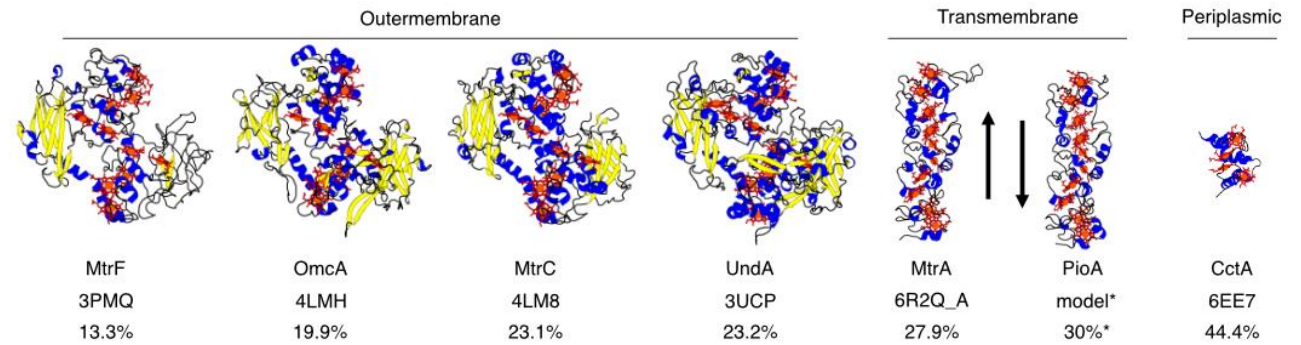
What do the multiheme cytochromes of extracellular respiration offer CISS studies?

- ‘Actual’ biological wires with electron transmission that impacts bioenergetics
- Naturally evolved to interface to surfaces/electrodes
- Gives us an opportunity to test the impact of CISS on physiology (e.g. respiration rates)

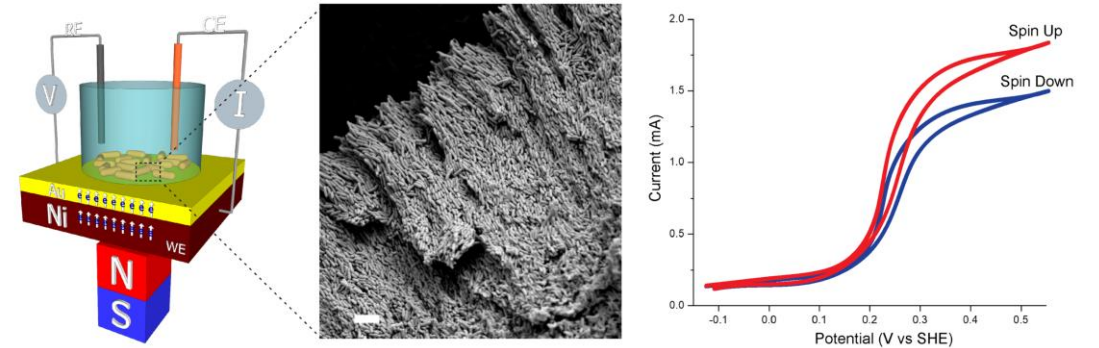


The Mechanisms and Implications of Chiral Induced Spin Selectivity in Biological Systems

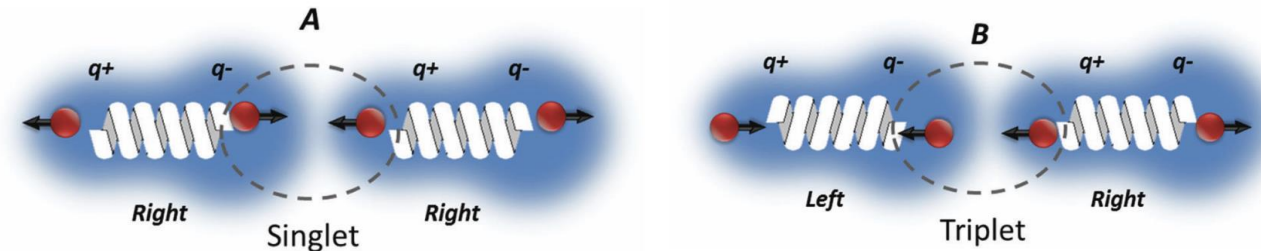
1. Discover the structural determinants (protein secondary structure and organization of redox centers) of spin selectivity in multiheme cytochromes and biological wires.



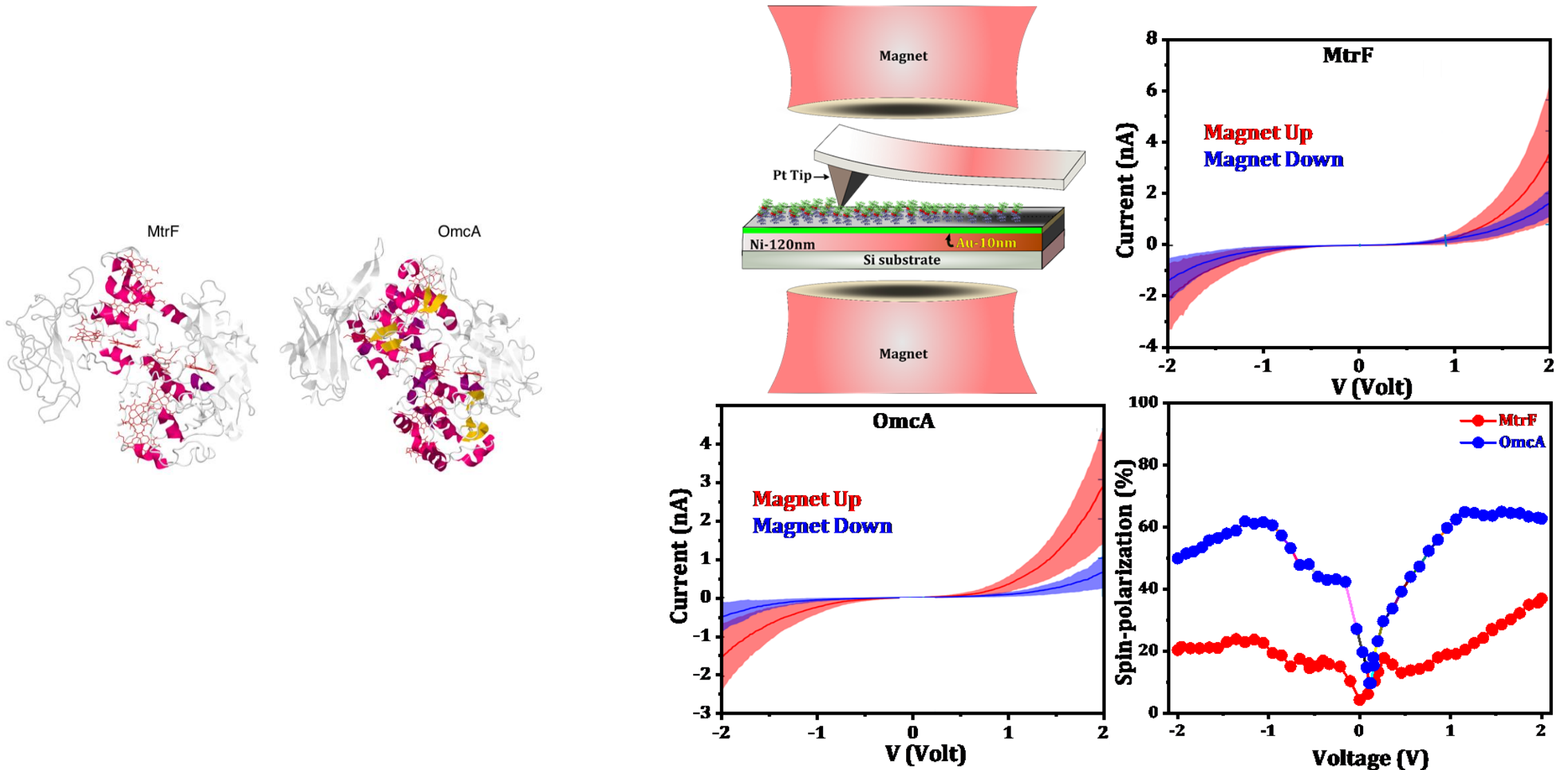
2. Identify whether spin selective electron transport affects extracellular respiration *in vivo*.

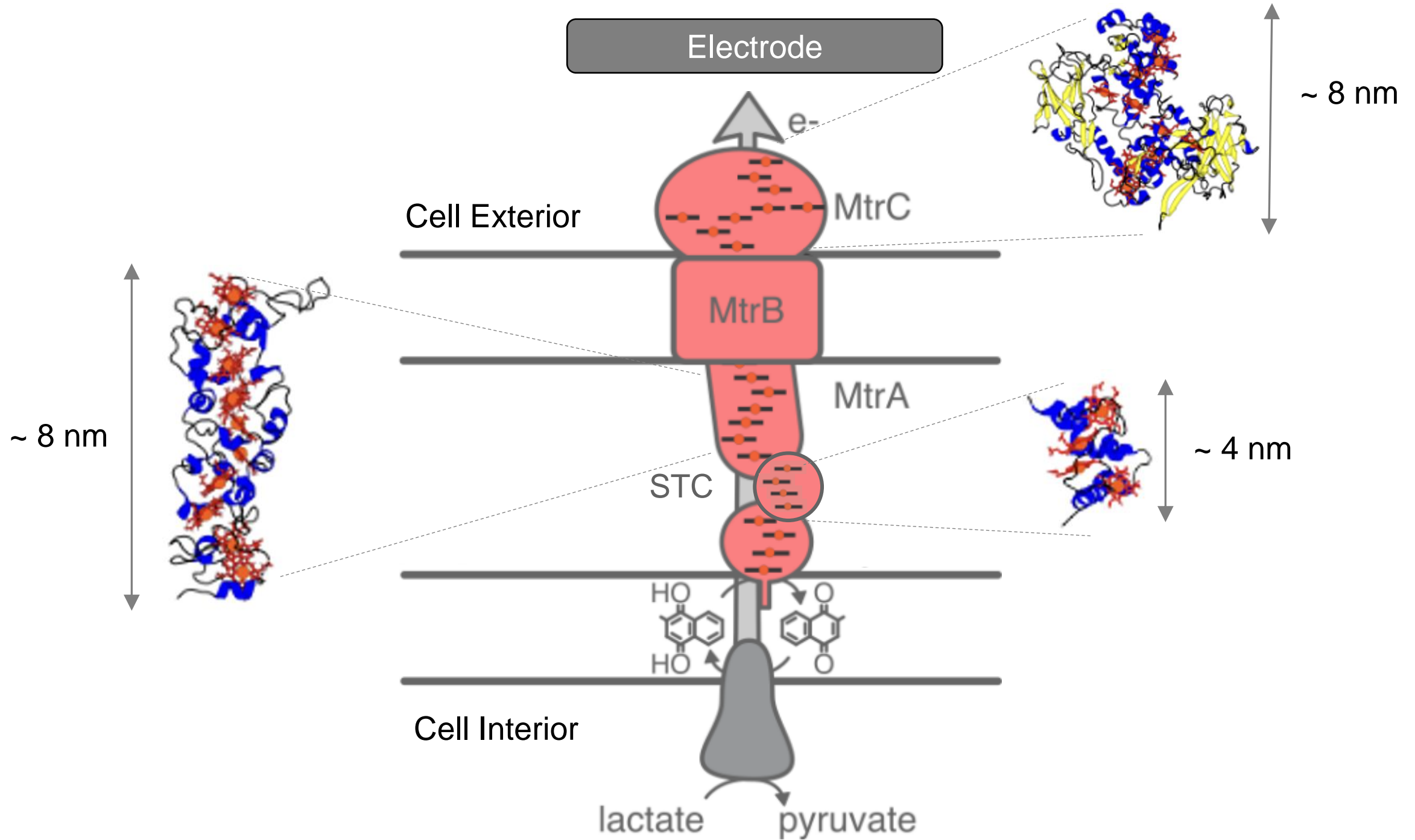


3. Identify the role of chiral induced spin selectivity in controlling the interaction between proteins and damaged DNA, and regulating protein-protein recognition through a novel spin-dependent charge reorganization allosteric effect.



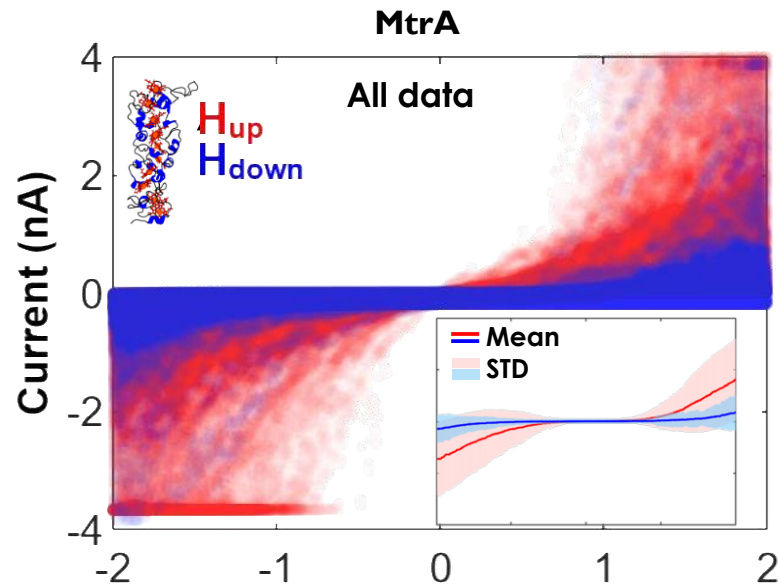
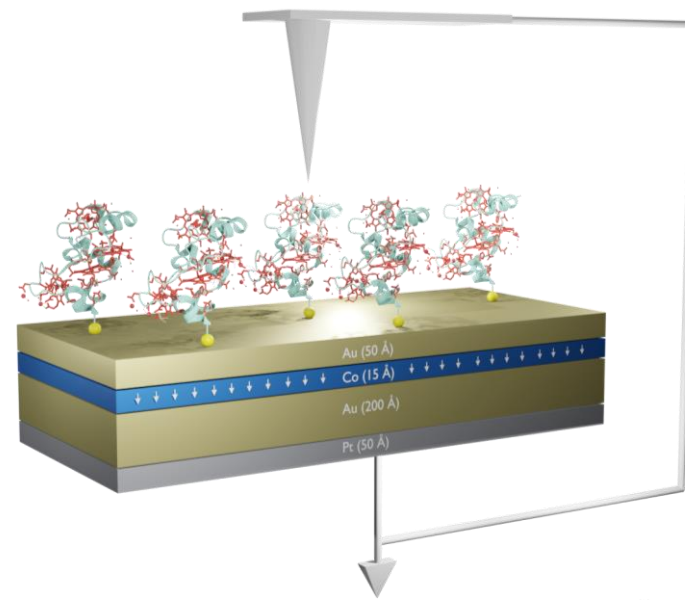
Magnetic Conducting Probe Atomic Force Microscopy





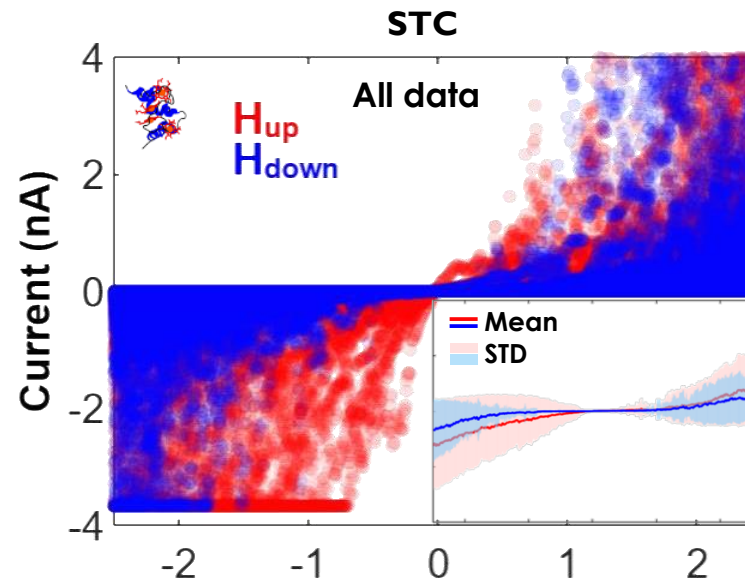
Cysteine-tagged cytochrome monolayers

Al₂O₃(0001)/Pt 5 nm/Au 20 nm/Co 1.5 nm/Au 5 nm substrate with out-of-plane magnetization easy axis



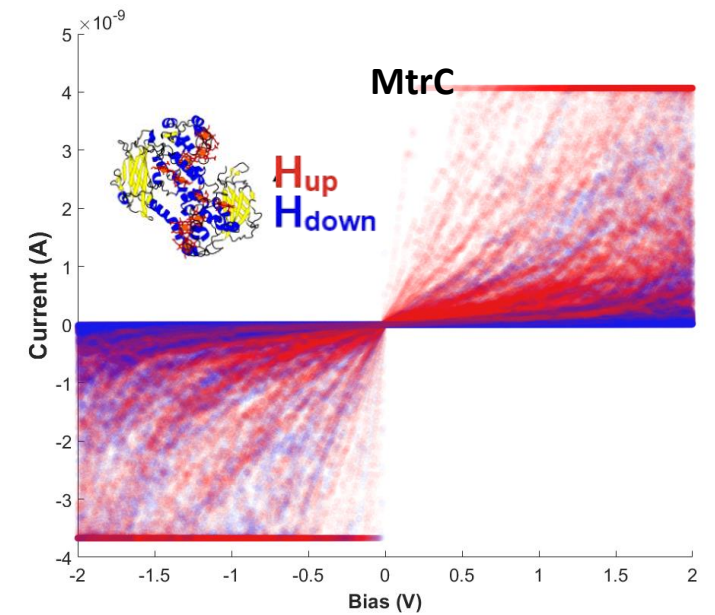
$$\frac{|I_{up} - I_{do}|}{I_{up} + I_{do}}$$

$77 \pm 3 \%$



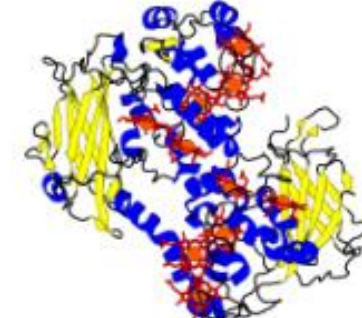
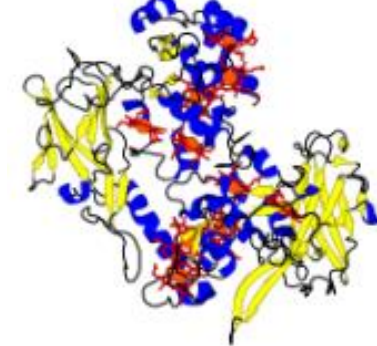
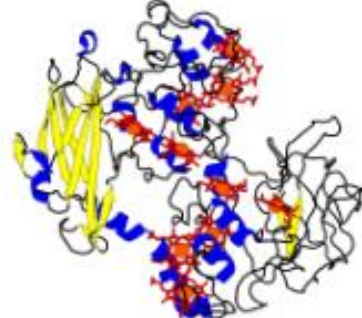
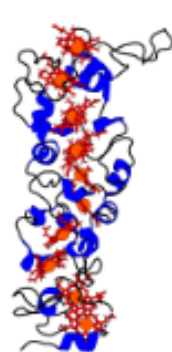
$$\frac{|I_{up} - I_{do}|}{I_{up} + I_{do}}$$

$35 \pm 18 \%$



$$\frac{|I_{up} - I_{do}|}{I_{up} + I_{do}}$$

$65 \pm 4 \%.^{**}$



Protein	CctA	MtrA	MtrF	OmcA	MtrC
PDB	6EE7	6R2Q_A	3PMQ	4LMH	4LM8
Helical Content	44.4%	27.9%	13.3%	19.9%	23.1%
Spin Polarization	$35 \pm 18 \% ^2$	$77 \pm 3 \% ^2$	$37 \pm 3 \% . ^1$	$63 \pm 2 \% . ^1$	$65 \pm 4 \% . ^3$

1. Mishra, Pirbadian *et al.* *JACS* (2020)

2. Niman, Sukenik *et al.* *Journal of Chemical Physics* (2023)

3. Sukenik, Yadav, Dang *et al.* *unpublished* (2024)

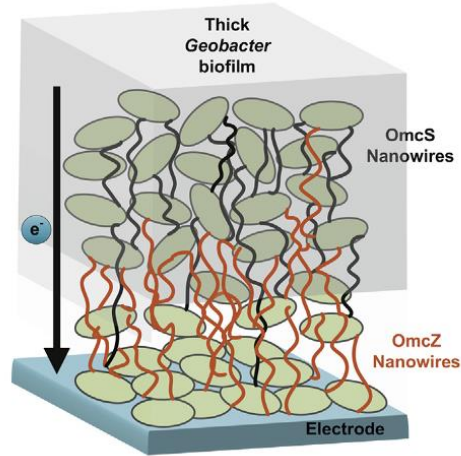
Lessons

CISS in multiheme cytochromes is size-dependent. Longer electron transport path → Higher spin polarization

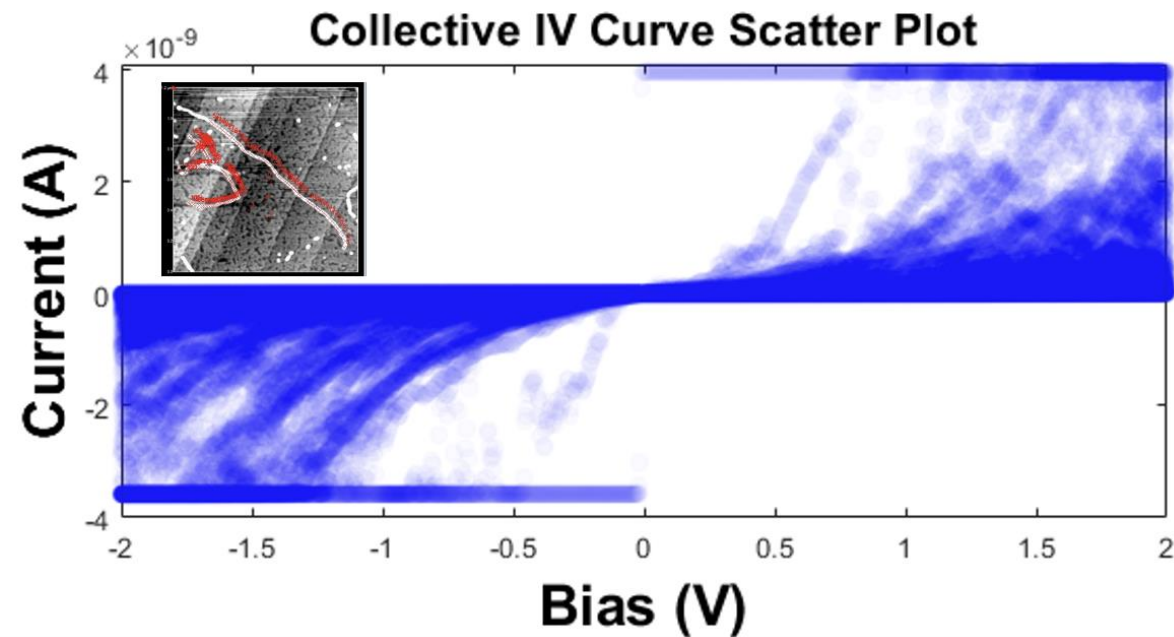
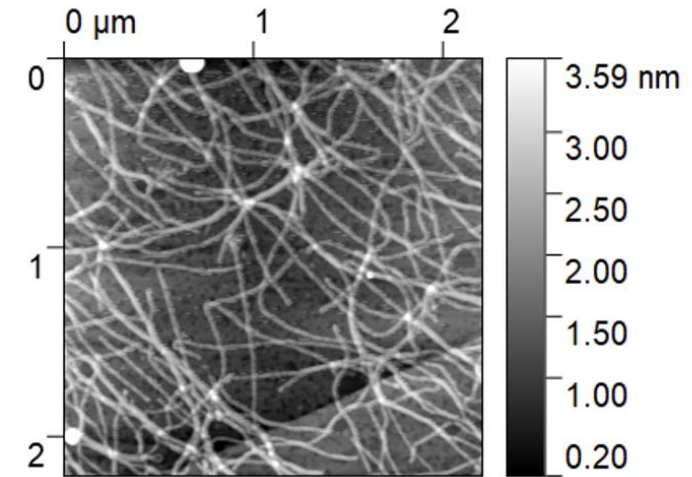
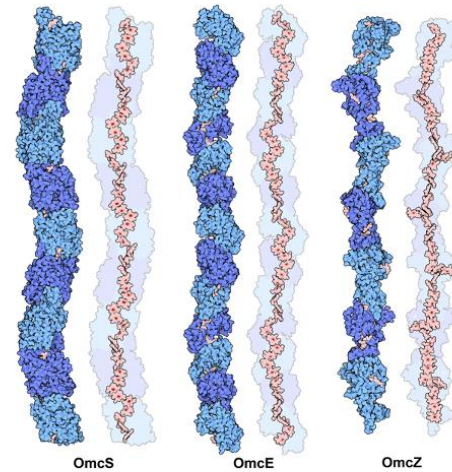
For similar size multiheme proteins, secondary structure (likely helicity) plays a role

All the components of the extracellular electron transport pathway are spin selective

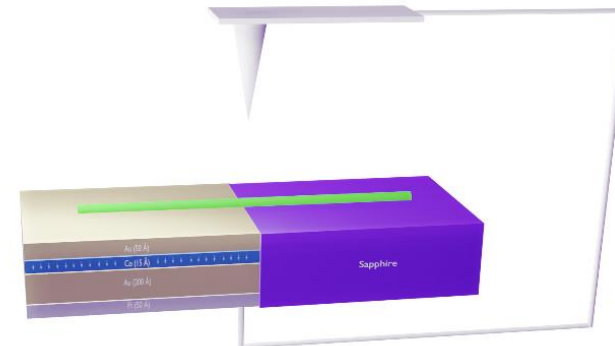
Is this sustained over larger length scales? (ongoing)



Yalcin & Malvankar, *COCB*, 2020



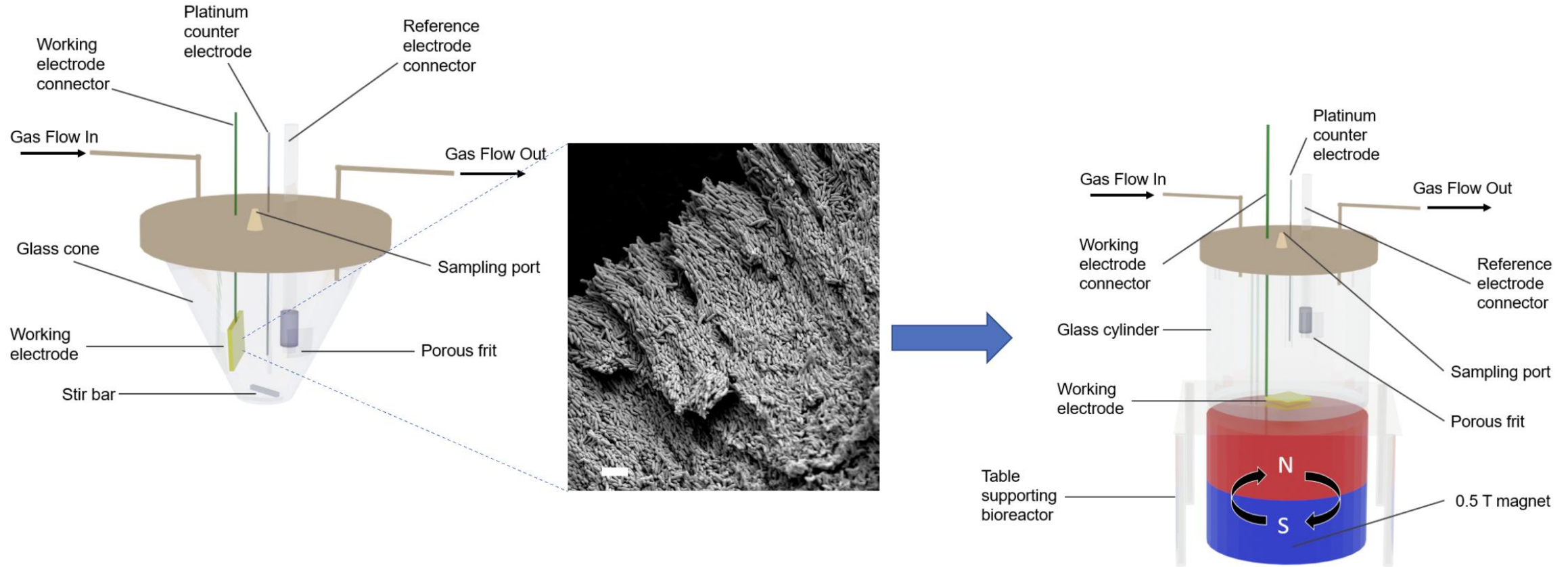
Next: spin polarization measurements



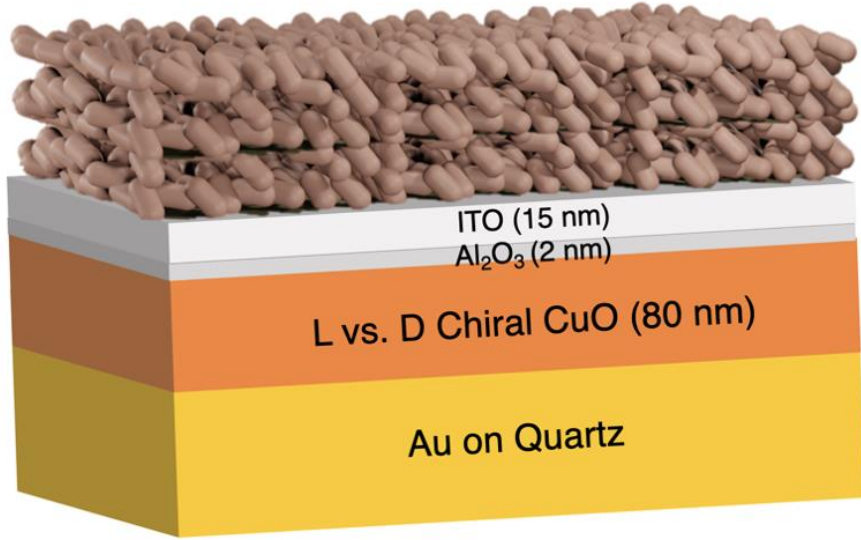
Cole Harris

Does CISS impact physiology?

Magneto-electrochemical Measurements of Extracellular Respiration in **Living** *Geobacter* Biofilms

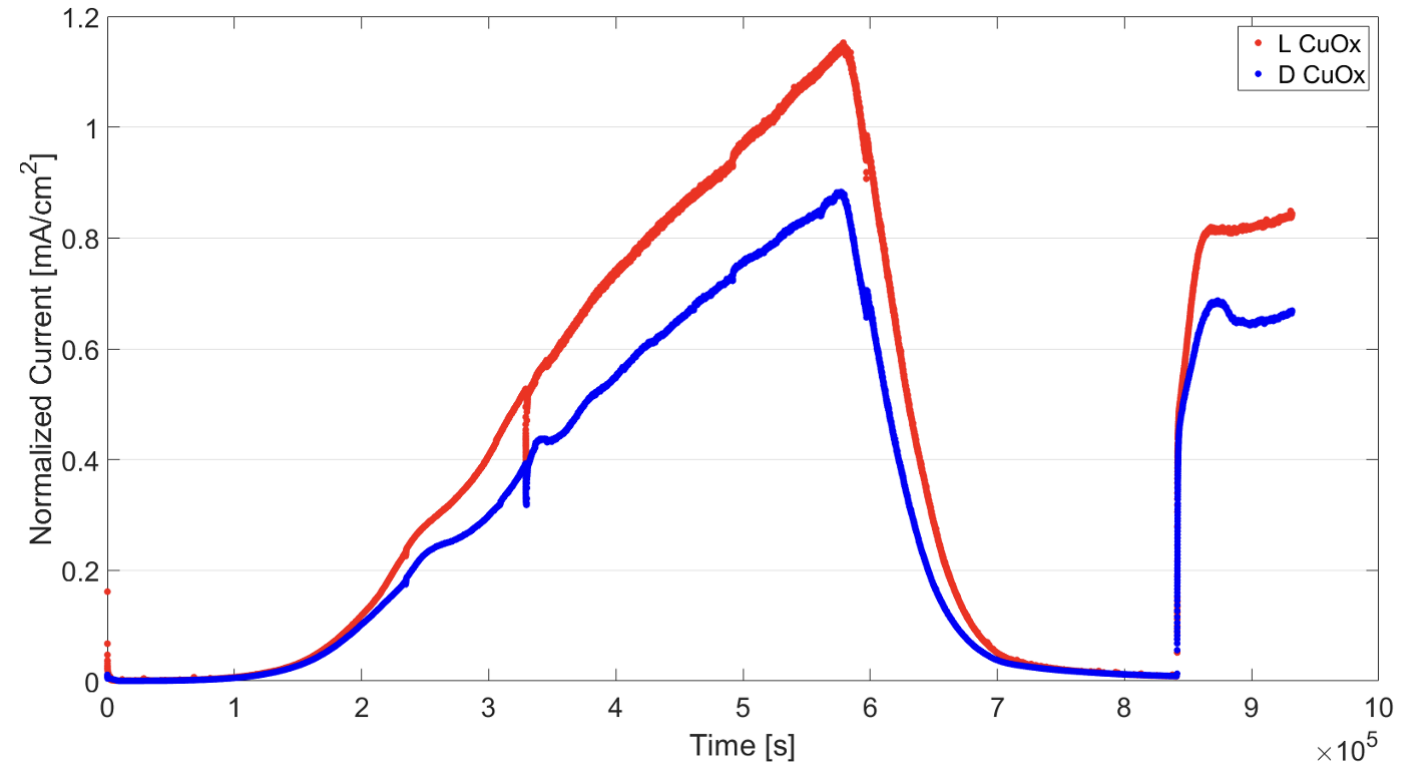


Measurements of Extracellular Respiration by **Living** *Geobacter* Biofilms on **Chiral** substrates



Chiral CuO electrodes provided by
Waldeck group (Pitt)

MURI Collaboration



Preliminary results



Dave Waldeck



Brian Bloom



Nazifa Tabbasum



Nir Sukenik

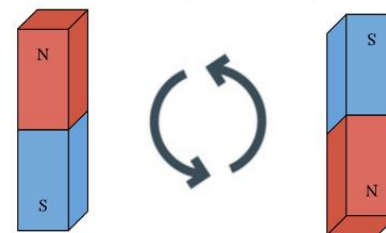
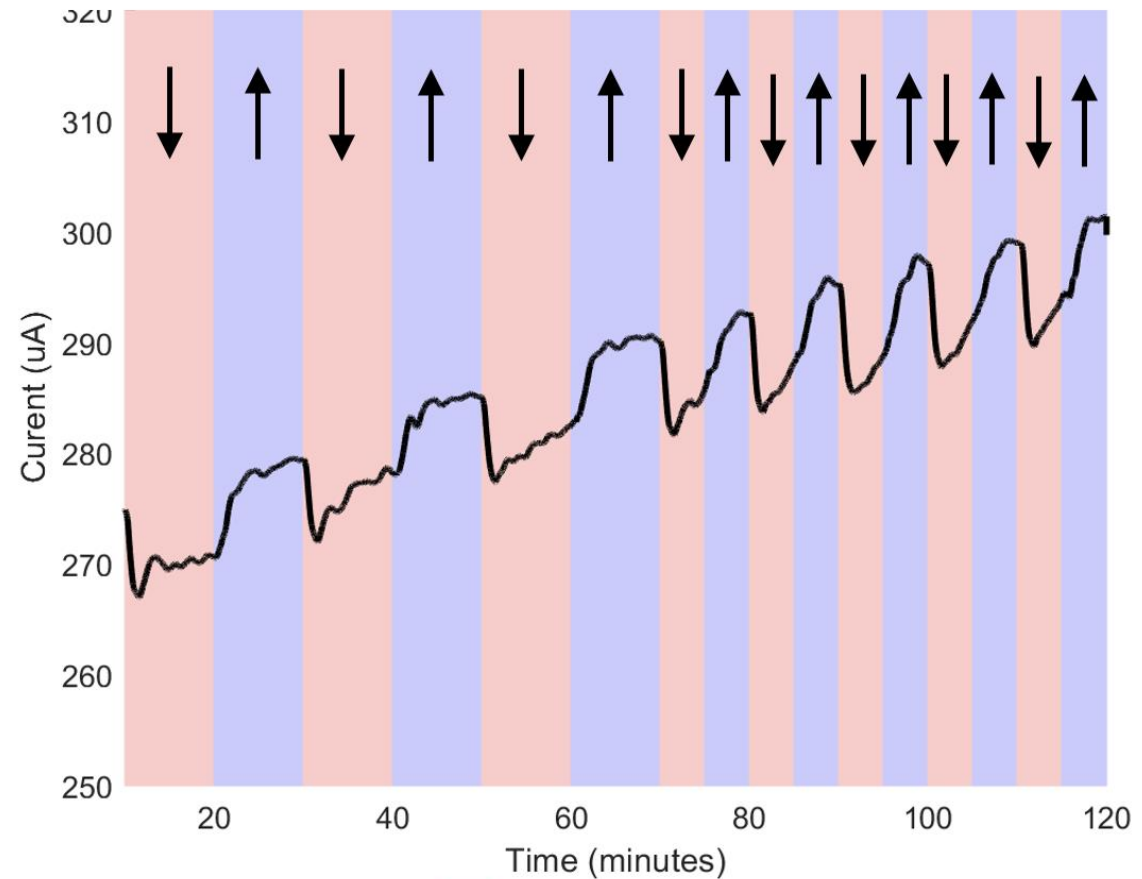
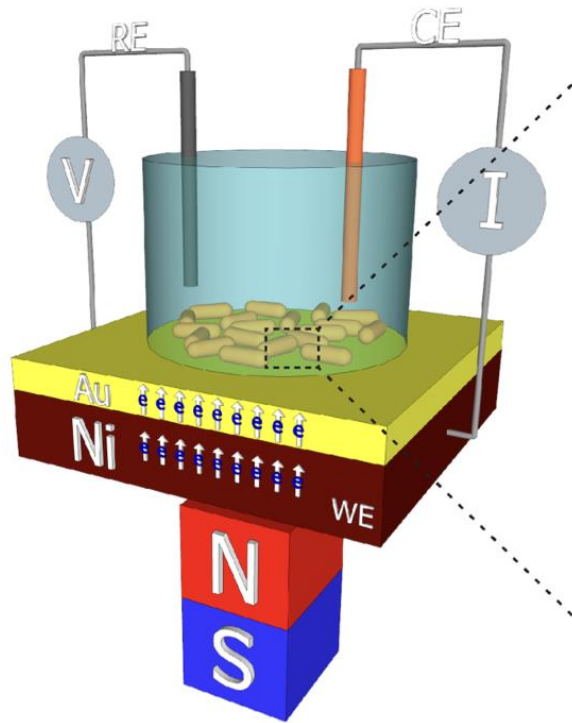


Sukram Yadav



Cole Harris

Magneto-electrochemical Measurements of Extracellular Respiration in **Living** *Geobacter* Biofilms



AFOSR-enabled Publications 2022-2024

T.K. Das, R. Naaman, J. Fransson, Insights into the Mechanism of Chiral-Induced Spin Selectivity: The Effect of Magnetic Field Direction and Temperature, *Advanced Materials*, 36, 29, 2024

N. Preeyanka, Q. Zhu, T.K. Das, R. Naaman, The Importance of Spin-Polarized Charge Reorganization in the Catalytic Activity of D-Glucose Oxidase, 25, 10, 2024

Bloom, Paltiel, Naaman, Waldeck, Chiral Induced Spin Selectivity, *Chem. Rev.* 124, 4, 2024

C.M Niman, N. Sukenik, T. Dang, J. Nwachukwu, M.A. Thirumurthy, A.K. Jones, R. Naaman, K. Santra, T.K. Das, Y. Paltiel, L.T. Baczewski, M.Y. El-Naggar, Bacterial extracellular electron transfer components are spin selective, *Journal of Chemical Physics*, 159, 14, 2023

A. Gupta, Y. Sang, C. Fontanesi, L. Turin, R. Naaman, Effect of Anesthesia Gases on the Oxygen Reduction Reaction, 4, 7, 2023

J.T Atkinson, M.S. Chavez, C.M. Niman, M.Y El-Naggar, Living electronics: A catalogue of engineered living electronic components, *Microbial Biotechnology* 16, 3. 2023

Q. Zhu,....., R. Naaman, The Role of Electrons Spin in DNA Oxidative Damage Recognition, *Cell Reports Physical Science*, 3, 12, 2022

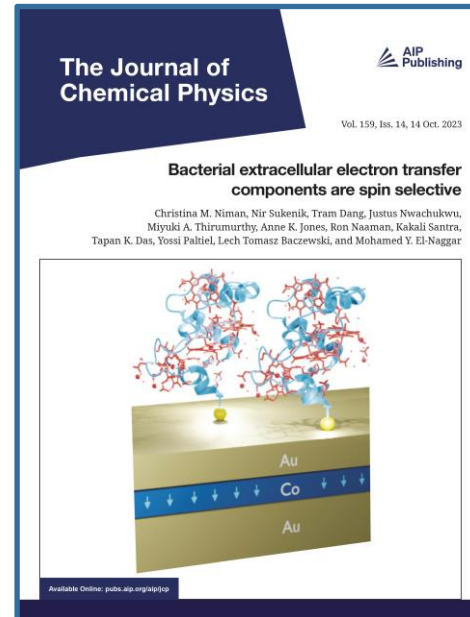
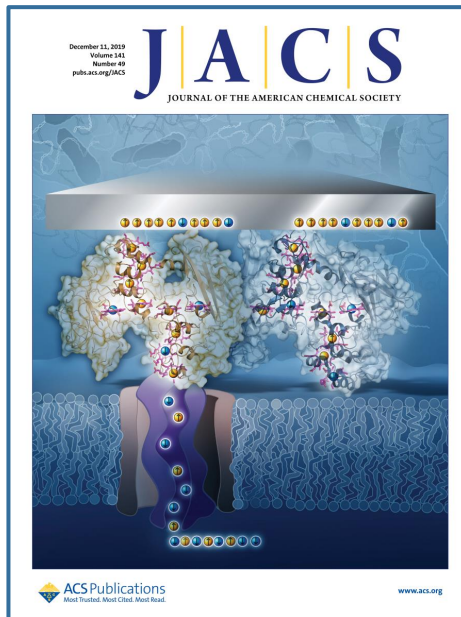
F. Zhao*, M.S. Chavez*, K. L Naughton, C. M Niman, J.T. Atkinson, J.A Gralnick, M.Y El-Naggar, J.Q Boedicker. Light-induced patterning of electroactive bacterial biofilms, *ACS Synthetic Biology*, 11 (7), 2327-2338, 2022

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, *Proceedings of the National Academy of Sciences of the United States of America*, 119, 2022

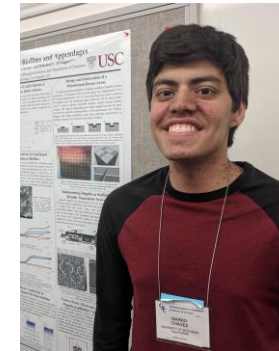
G.W. Chong, S. Pirbadian*, Y. Zhao, L.A. Zacharoff, F. Pinaud, M.Y. El-Naggar. Single molecule tracking of bacterial cell surface cytochromes reveals dynamics that impact long-distance electron transport, *Proceedings of the National Academy of Sciences of the United States of America*, 119 (19), e2119964119, 2022



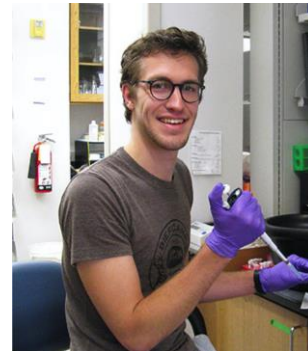
Podcast: New Spin on Electrons: How They Change Life and Power our Lives



Christina Niman:
PhD defense



Marko Chavez:
Rice Academy
Postdoctoral Fellow



Josh Atkinson:
Faculty position.
(Princeton 2024)



Ron
Naaman



Dave
Waldeck



Steve
Finkel



Ken
Nealson



James
Boedicker



Jeff
Gralnick

