Assessing Phase Coherence in the Chiral Induced Spin Selectivity Effect: Review of Theoretical Approaches

Aisha Kermiche

University of California - Los Angeles, Department of Electrical Engineering, Quantum Biology Tech (QuBiT) Lab

Outline

1. Introducing the CISS Effect
2. Potential applications
3. Literature review: ambiguities in experimental results
4. Current work: reproduction of charge transport models
5. Future directions

Objectives (in progress)

Recreate and compare theoretical models proposed in literature
Propose novel simulation approach to determine coherence of electron transport in chiral molecules

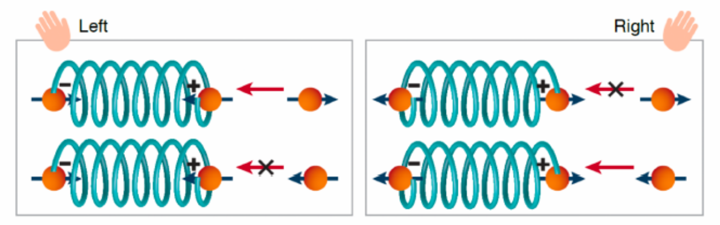
Overview of chiral induced spin selectivity effect

Unlike in man-made electronic devices, where electron transport is facilitated through metals and semimetals, biological systems rely on electron transport through diamagnetic, insulating molecules with minimum heat dissipation.

Chiral molecules can produce spin polarized electrons without the need for ferromagnetism, meaning they are promising as a new class to topological materials.

Characteristics of the CISS effect

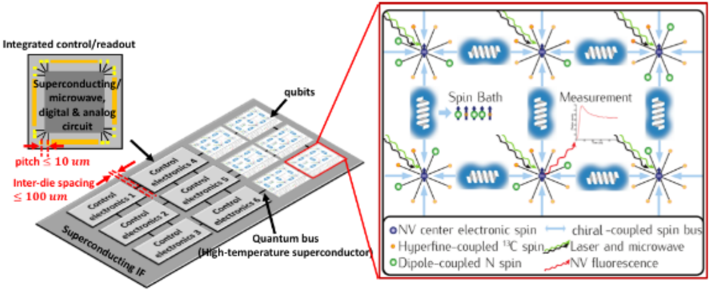
1. non-equilibrium effect, requiring electron transfer through chiral molecules
2. requires large spin-orbit coupling (SOC) enhancement
3. flipping the chirality of the molecule flips the polarization
4. as of current evidence, polarization increases with increasing length of the chiral molecule.



S. Mishra et al., "Spin Filtering Along Chiral Polymers," Angewandte Chemie, vol. 132, no. 34, pp. 14779–14784, 2020, doi: 10.1002/ange.202006570.

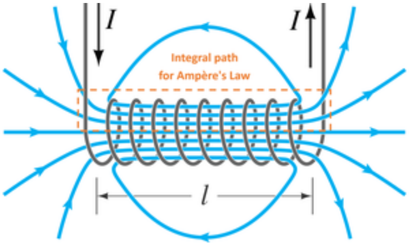
Potential applications

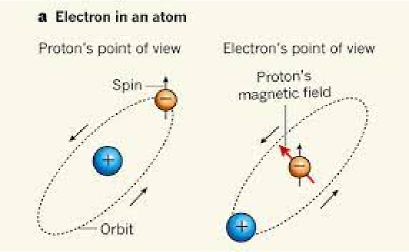
- This ability to manipulate and control spin through charge transfer processes at room temperature with minimum heating can be exploited in the development of spintronic devices, with implications for the transfer and storage of information in quantum computing applications.
- In order to be useful, charge transfer must be coherent in these interconnects.



C. Aiello, "Towards a Room-Temperature Hierarchical Interconnect System for Quantum Information Processing." (accessed Dec. 09, 2021)

Classical intuition





- Theoretical approaches so far have assumed a close connection between chirality and spin-orbit interaction.
- So perhaps it could be the quantum version of the solenoid field, chiral induced spin orbit coupling, could explain it, but still **the order of magnitude is far too small**.

Experimental results

Language of spin-flipping, spin-filtering is ambiguous

- If the chiral molecule is truly “spin-filtering”, that means that the wave function collapses as it is transmitted, rendering the effect useless for qubit transport (though it is still applicable for qubit preparation)
- Weizmann Institute group (original investigators of the effect) claim that experiments support the effect as spin filtering rather than spin flipping, and that their current model **does not require the charge transport to be coherent**.

Spin Filtering Along Chiral Polymers

Suryakant Mishra, Amit Kumar Mondal, Eilam Z. B. Smolinsky, Ron Naaman, Katsuhiro Maeda,* Tatsuya Nishimura,* Tsuyoshi Taniguchi, Takumu Yoshida, Kokoro Takayama und Eiji Yashima*

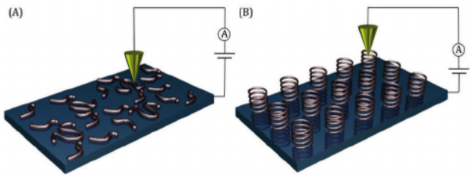
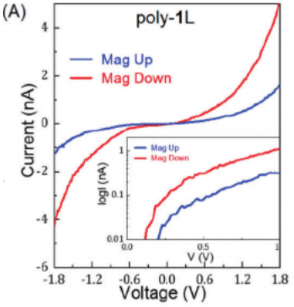


Figure 1: Experimental set up



){wi

Weizmann group conclusions

- The nonlinear I-V curves suggests that **back-scattering is suppressed**
- Spin polarization scales proportional to the length of the molecule.
- **Because there is a different threshhold for each spin conduction this indicated no spin flipping**. The molecules are passive filters. They don't actively flip the spin, only reject unfavorable spins at a higher probability.
- Polarization is similar to that obtained with photoelectrons
- **The spin orbit coupling allows for long range electron transfer**. It allows for electron transfer in proteins and biological systems because back scattering is suppressed.

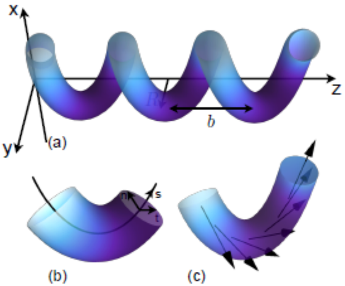
Broad range of modeling approaches exist

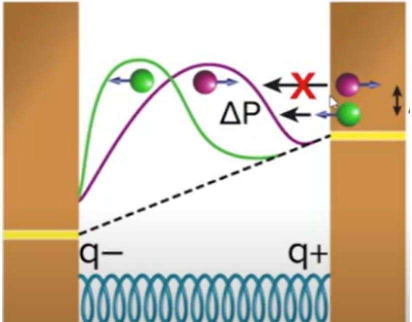
Theory of Chirality Induced Spin Selectivity: Progress and Challenges

Ferdinand Evers,[1,*] Amnon Aharony,[2] Nir Bar-Gill,[3] Ora Entin-Wohlman,[4] Per Hedegård,[5] Oded Hod,[6] Pavel Jelinek,[7] Grzegorz Kamieniarz,[8] Mikhail Lemeshko,[9] Karen Michaeli,[10] Vladimiro Mujica,[11] Ron Naaman,[12] Yossi Paltiel,[3] Sivan Refaely-Abramson,[13] Oren Tal,[12] Jos Thijssen,[14] Michael Thoss,[15] Jan M. van Ruitenbeek,[16] Latha Venkataraman,[17] David H. Waldeck,[18] Binghai Yan,[10] and Leeor Kronik[13,†]

At present, a unifying scheme that would allow one to interpret all experiments in terms of only a single microscopic effect – the "CISS effect" - has not yet been identified. While such a framework cannot be ruled out, chirality-induced spin selectivity may perhaps be thought of as a set of phenomena that have a unifying scheme only in the sense that they all derive from the interplay of spin-orbit interaction and chirality. For example, it has been

Analytical tight binding, time reversible model





Symmetry analysis

Insight into the Origin of Chiral-Induced Spin Selectivity from a Symmetry Analysis of Electronic Transmission

Martin Sebastian Zöllner, Solmar Varela, Ernesto Medina, Vladimiro Mujica, and Carmen Herrmann*

-Imaginary terms in the Hamiltonian are a result of spin orbit coupling, and they **preserve the Hermitian nature of the Hamiltonian - SOC is not related to the breaking of time reversal symmetry**. Obeys **Kramer's Degeneracy**

Applying Landauer Formalism

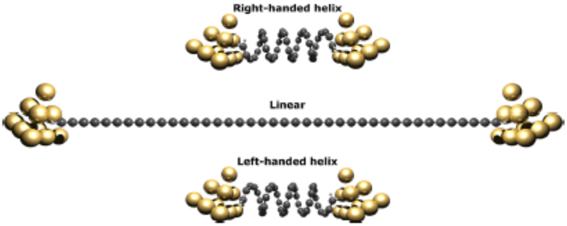
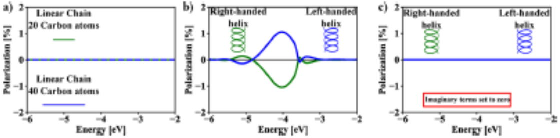


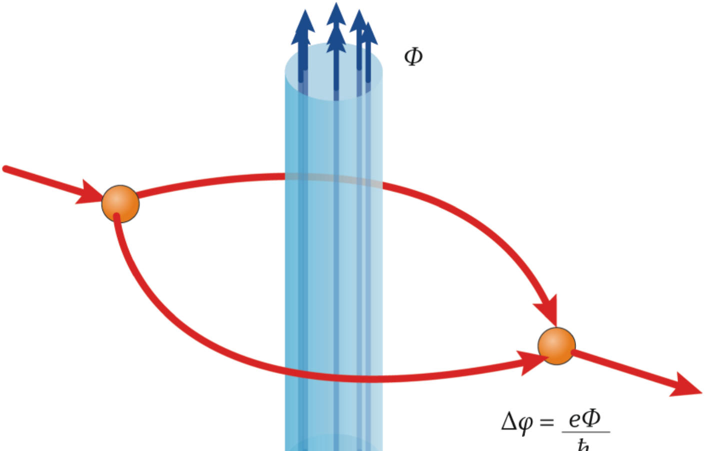
Figure 1. Gold−molecule−gold junctions as used in the DFT calculations consisting of a molecule placed between two 10-atomic gold clusters. Left-handed helix (lower system), right-handed helix (upper system), and the 40-atomic chain (middle system) are depicted.



Full Green's function characterization of a chiral molecular junction, DFT

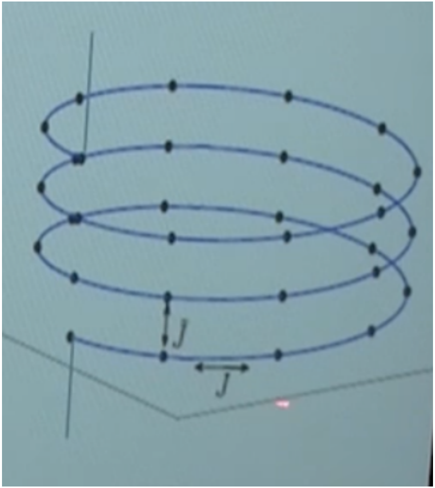
Aharonov-Bohm (AB) Effect

- An electron experiences a phase difference due to a magnetic field.
- The induced phase has to undergo a time irreversible transformation, which can be done by either
  - Introducing an external magnetic field
  - Introducing leakages



Spin-dependent transport through a chiral molecule in the presence of spin-orbit interaction and non-unitary effects

Shlomi Matityahu,[1,*] Yasuhiro Utsumi,[2] Amnon Aharony,[1,3,4] Ora Entin-Wohlman,[1,3,4] and Carlos A. Balseiro[5,6]



Tentative schedule of tasks in the coming months

1. NEGF single electron model of electron transport
2. Seeing how the parameterization of the electron trajectory
3. An examination of topological resonance when you change the pitch and frequency of the chiral molecule
4. A change in functional groups and how that affects the spin polarization and coherence
5. I want to be able to tie a thermodynamic account of information to the quantum mechanics of the CISS effect. The relevant textbooks include:

Main conclusions

- Destruction of unitary transformation, either through the destruction of time reversal or reflection symmetry, may be necessary to achieve charge polarization
- Interference pattern is obtainable, implying that a phase superposition is preserved
- Main theoretical considerations are
  - Symmetry (time parity)
  - Leakages
  - Non-equilibrium effects

Future work for the QuBiT lab

Introducing interferometry experiments into the investigation of the CISS effect

Relating CISS effect to spin-controlled reactions