In Silico Investigation into the Origin of the Chiral Induced Spin Selectivity Effect

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Introduction to the Chiral Induced Spin-Selectivity Effect

[[Overview]]

Unlike in man-made electronic devices where electron transport is facilitated through metals and semimetals, biological systems rely on electron transport through insulating molecules with minimum heat dissipation.[1]

The chiral induced spin selectivity effect (CISS) is a phenomenon in which electron spin polarization is produced as a result of chiral electrode molecule transfer processes. This is usually done through the transmission of electrons through a chiral environment. [2]

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[1] [[@michaeli_origin_2019#^c49063]]

[2] [[@aiello_chirality-based_nodate#^7f12c8]]

Characteristics of CISS

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.

Illustration of spin polarization[3] Fig. 1-1: Illustration of spin polarization-induced enantioselective reaction mechanism.

Two important experimental questions arise from this[4]: 1. Why is the transmission through helical molecules larger than expected? 2. What causes then robust CISS?

Links

1. [[Biological Homochirality remains a mystery]] #### References

[3] [[@aiello_chirality-based_nodate#^7f12c8]]
[4] [[@michaeli_origin_2019#^c49063]]

Objectives

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