Tentative Results from a Meta-Study of the CISS Literature

Jichen Feng, Joseph E. Subotnik, Abraham Nitzan
University of Pennsylvania

Question:

Can we learn anything new from the chirality induced spin-selectivity literatures, by reading and extracting data from the existing studies (experimental papers, especially) and study the correlations within and between these results?

Answer:

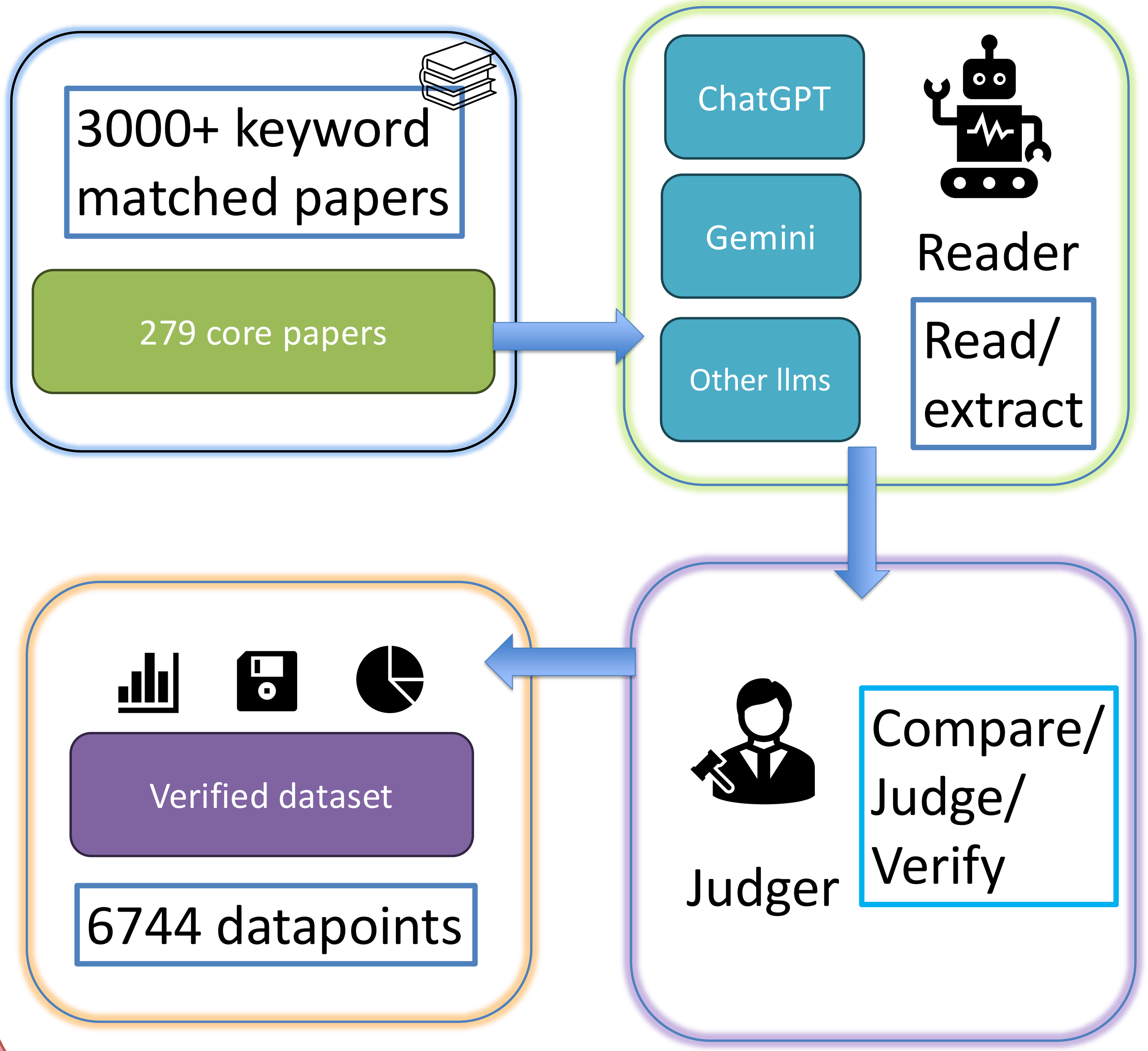
Yes, with the recent development of large language models (llms), it is completely duable.

In this study, we asked 3 llms to read 3000+ papers and select 279 of them that is containing meaningful data, and studies the statistical correlation between the physical quantities and the strength of the CISS effect, as well as the cross paper correlations.

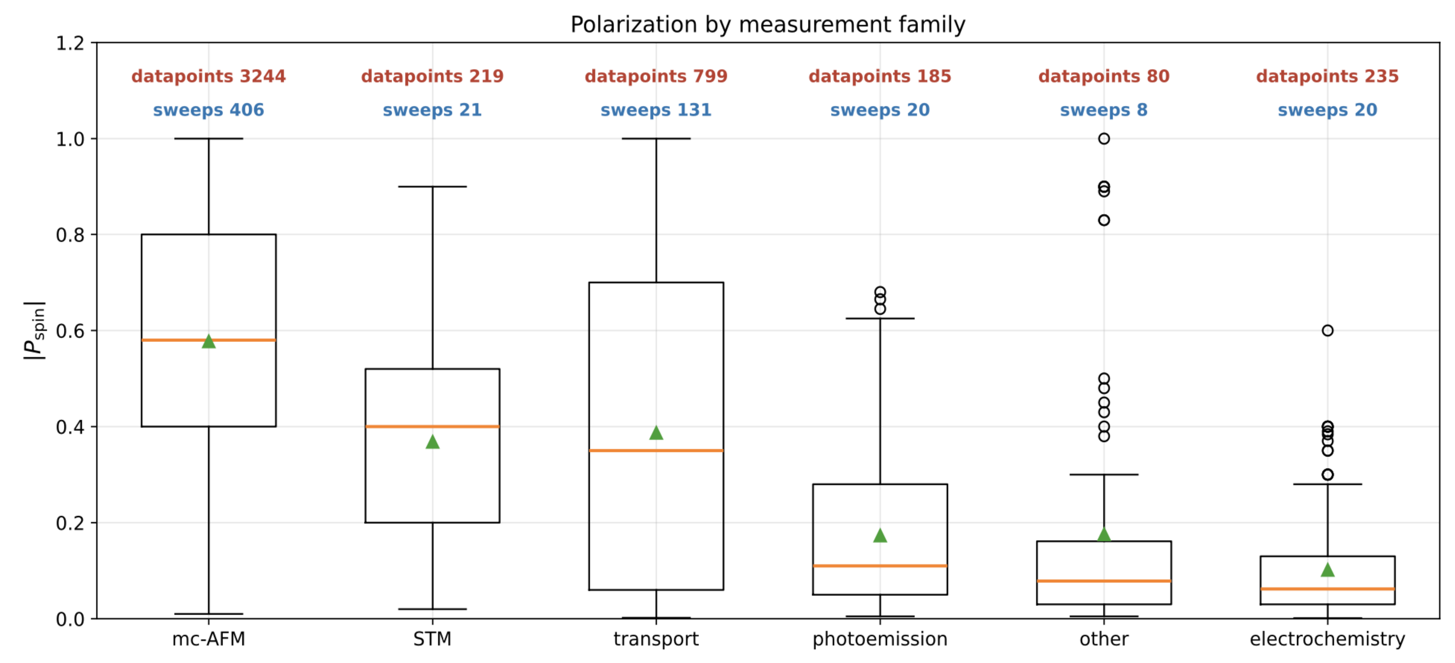
Definition of spin polarization/ CISS strength

$$P_{spin} = \frac{I_{\uparrow} - I_{\downarrow}}{I_{\uparrow} + I_{\downarrow}}, |P_{spin}| \in [0,1]$$

Data extraction pipeline

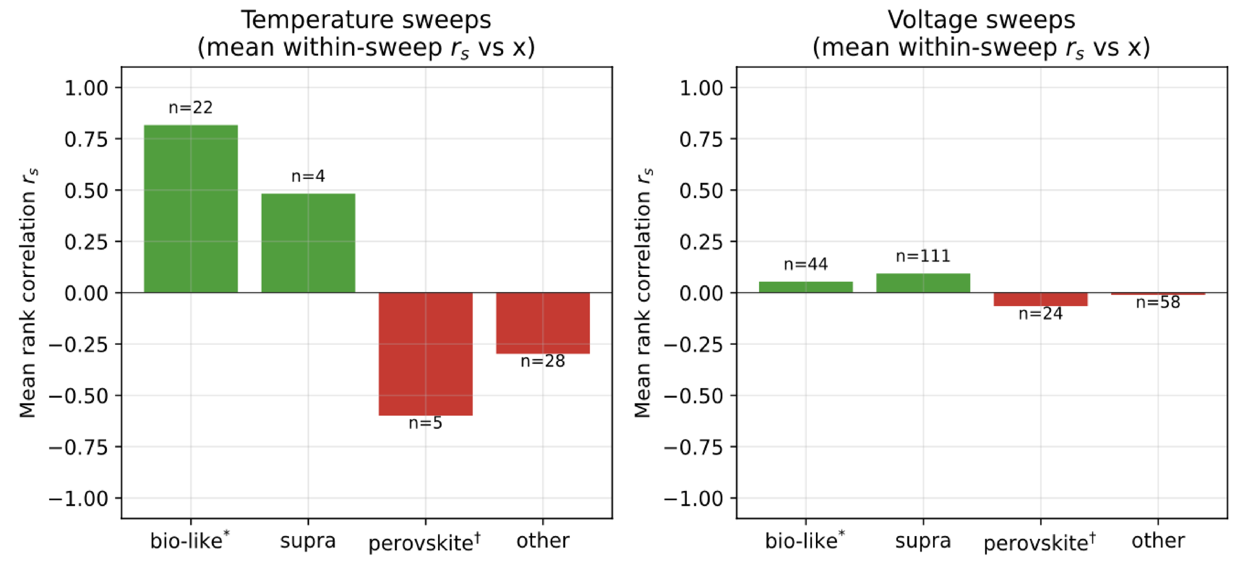


Polarization values by measurement family



We should not naively compare CISS strength across different materials, as they might be measured by different method such that the strength are having different meanings.

Temperature dependence of CISS



*bio-like = strict biomolecule (DNA, peptide, protein) + helicene / organic-cage / chiral-knot. †perovskite = chiral hybrid (formula-tagged, (R/S-MBA)$_2$PbI$_4$, (R-NEA)PbI$_3$, etc.).

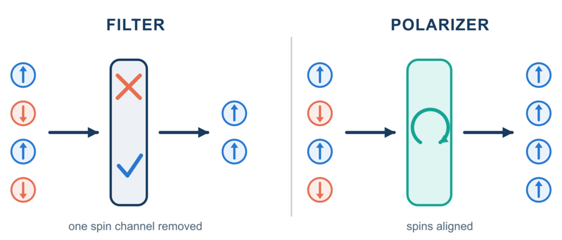
Biomolecules shown positive correlation, while perovskites shown negative correlation with temperature.

Longer chiral path, stronger spin filter

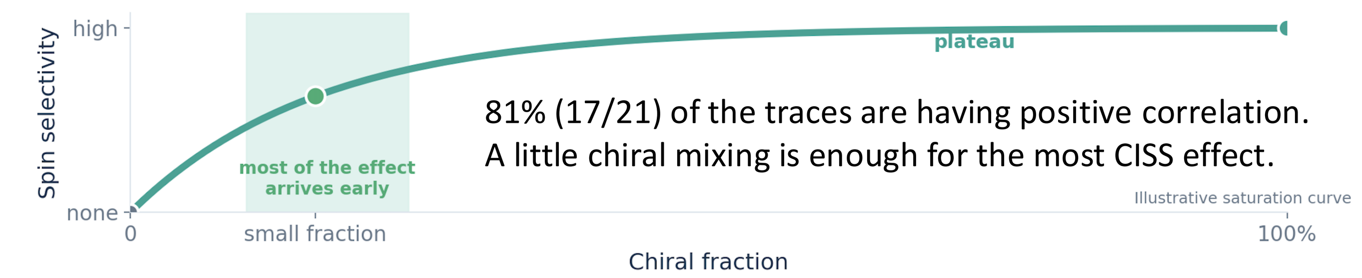
76% of the traces are having positive correlation.

Polarizer or filter?

Filter: 56% (155/278)
Polarizer: 17% (48/278)
Both: 14% (38/278)
Not committed: 13% (37/278)

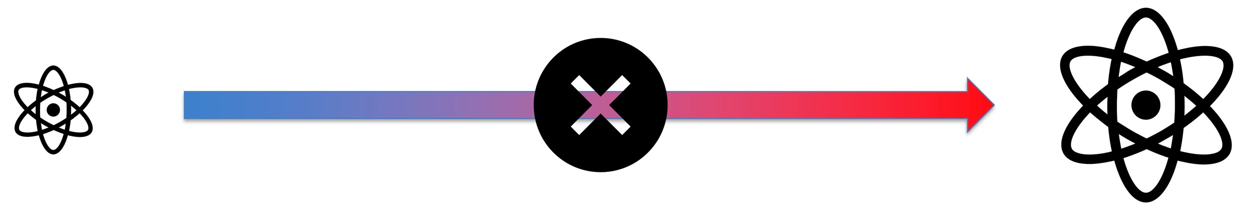


Polarization rises with the chiral fraction



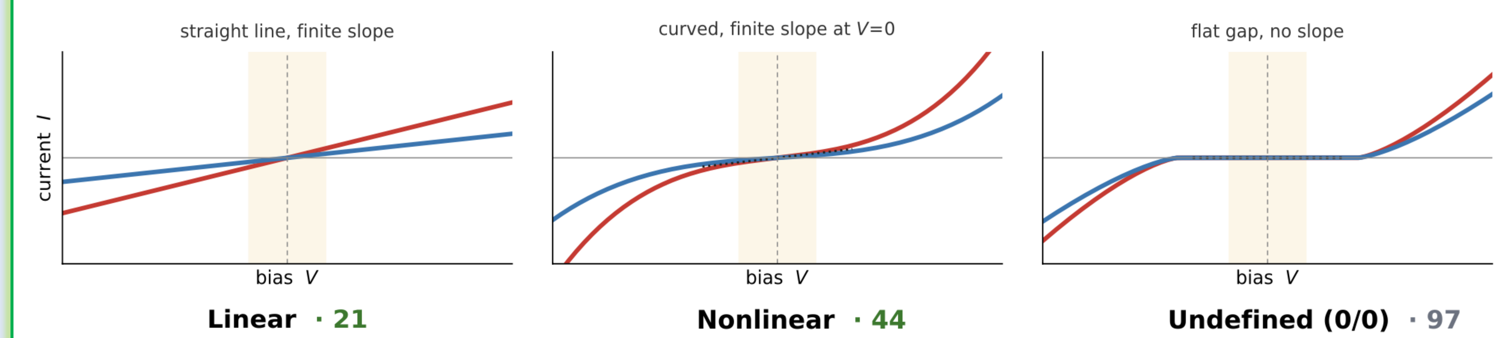
81% (17/21) of the traces are having positive correlation.
A little chiral mixing is enough for the most CISS effect.

Heavier atom does not give bigger CISS



The rank correlation of the heaviest atom atomic number vs the CISS strength is (Z, |P|) = −0.10, with $p = 3 \times 10^{-11}$. Note that this is also a consequence of the measurement difference.

Does the polarization survive at zero bias?



A finite zero-bias slope is present in 65 of 162 (linear 21 + nonlinear 44), which means around 40% of the cases survives at zero bias, while the rest of them (97/162) shown undefined (0/0).

Other take home messages

Robust positive findings.

- Bio-like T-sweeps (biomolecules + helicenes / organic cages): $|P|$ rises with T (20/22, median $r_s = +1.00$); chiral hybrid perovskites: opposite (1/6, $r_s = -1.00$).
- Length sweeps: $|P|$ rises with chiral-path length (16/21, median $r_s = +0.99$).
- Concentration sweeps: $|P|$ rises with chiral fraction (17/21, $r_s = +0.94$); ~30% sergeant-and-soldiers shape.
- Within-family α vs $|P|$: positive (length is monotonic proxy for α).
- Within-family μ vs $|P|$: positive in α-helices and perovskite n-series.
- Optical chirality g-factor and CISS $|P|$ are correlated: $r_s(g_{CD}, |P|) = +0.71$.
- Hybrid systems highest median $|P| = 0.62$ (vs organic 0.41, inorganic 0.42).

Robust nulls / negatives.

- Cross-paper T and V trends: artifacts, vanish within-paper.
- Heaviest-atom Z: weakly negative ($r_s = -0.08$).

Methodological observations.

- Measurement method is the biggest single predictor of $|P|$ (mc-AFM 0.58 vs electrochem 0.08).
- ICC(paper) = 0.72: most spread is between papers, not within.
- 24% of literature reports $|P| < 5\%$; 46% $< 10\%$.

Acknowledgement

This research is supported by the Air Force Office of Scientific Research under award number FA9550-23-1-0368.

Word of Caution: one should be very careful on treating the AI provided dataset and analysis. AI will make mistakes without being noticed by human. AI may confuse 2 physical quantities that share the same name but are conceptually completely different in different contexts. It will also miss a lot of really important environment settings that are mentioned in the context but not the raw data/ plots. We use 3 different most powerful llms to read the same paper and only pick the data that they shares to avoid this problem. AI will also make up multiple fake negative/ positive correlations between physical quantities especially when studying the cross paper correlations because: a) it does not realize the measurement difference; b) The majority of the data are from a single or two papers/ labs. We try to avoid the problem by studying the trends within the papers and less study the cross paper data correlation unless the quantity is very clean. We also only study the experimental results because many computational/ theoretical results are actually from adjustable model parameters and it is extremely difficult to determine the validity of the data representing the real world even for human readers.