

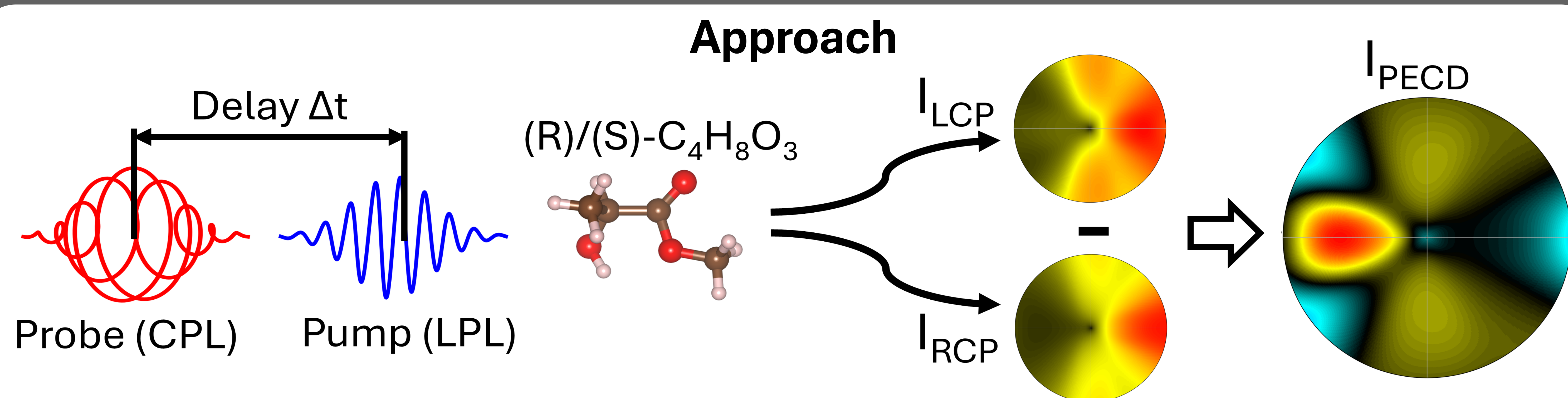
First-principles study of chiral spin dynamics and photoelectron circular dichroism

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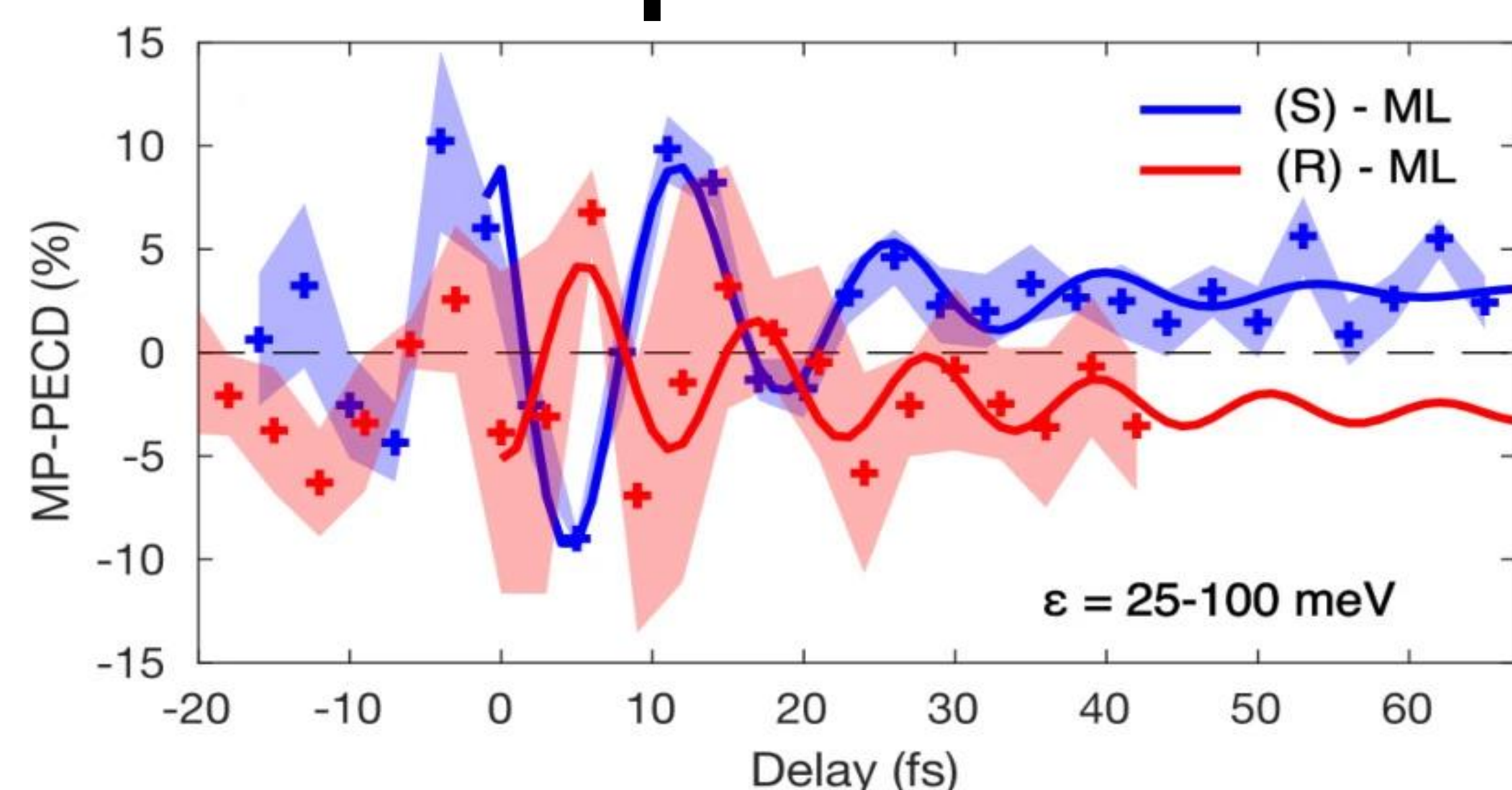
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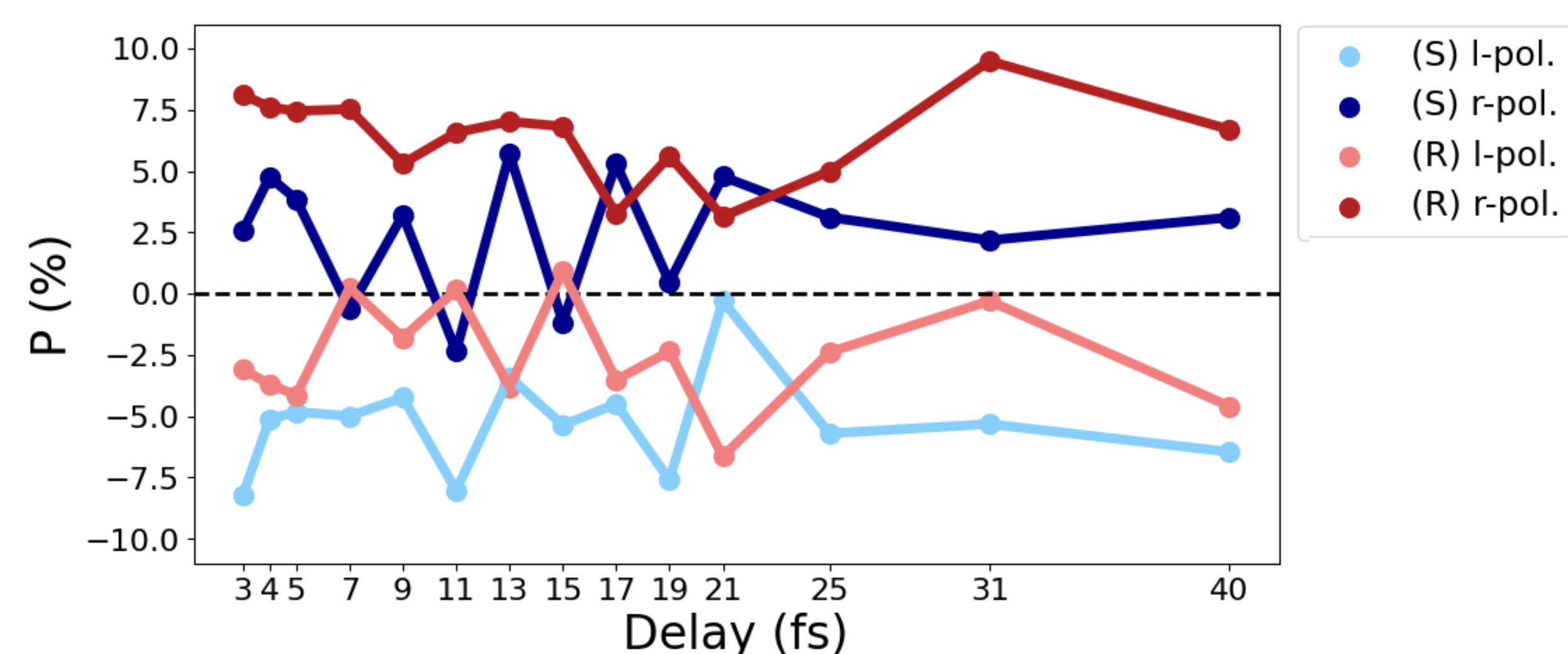
Investigation of electron dynamics in chiral structures are crucial in understanding chirality-dependent processes in chemistry and biology, in particular via the chiral induced spin selectivity (CISS) effect. Recent advances in attosecond science enabled real-time observation of electron dynamics using time-resolved photoelectron circular dichroism (TR-PECD). By employing real-time time-dependent density functional theory, we simulate TR-PECD spectra for (R)/(S)-methyl lactate. In addition, the photoelectron currents are examined for time- and chirality-dependent spin behaviour.



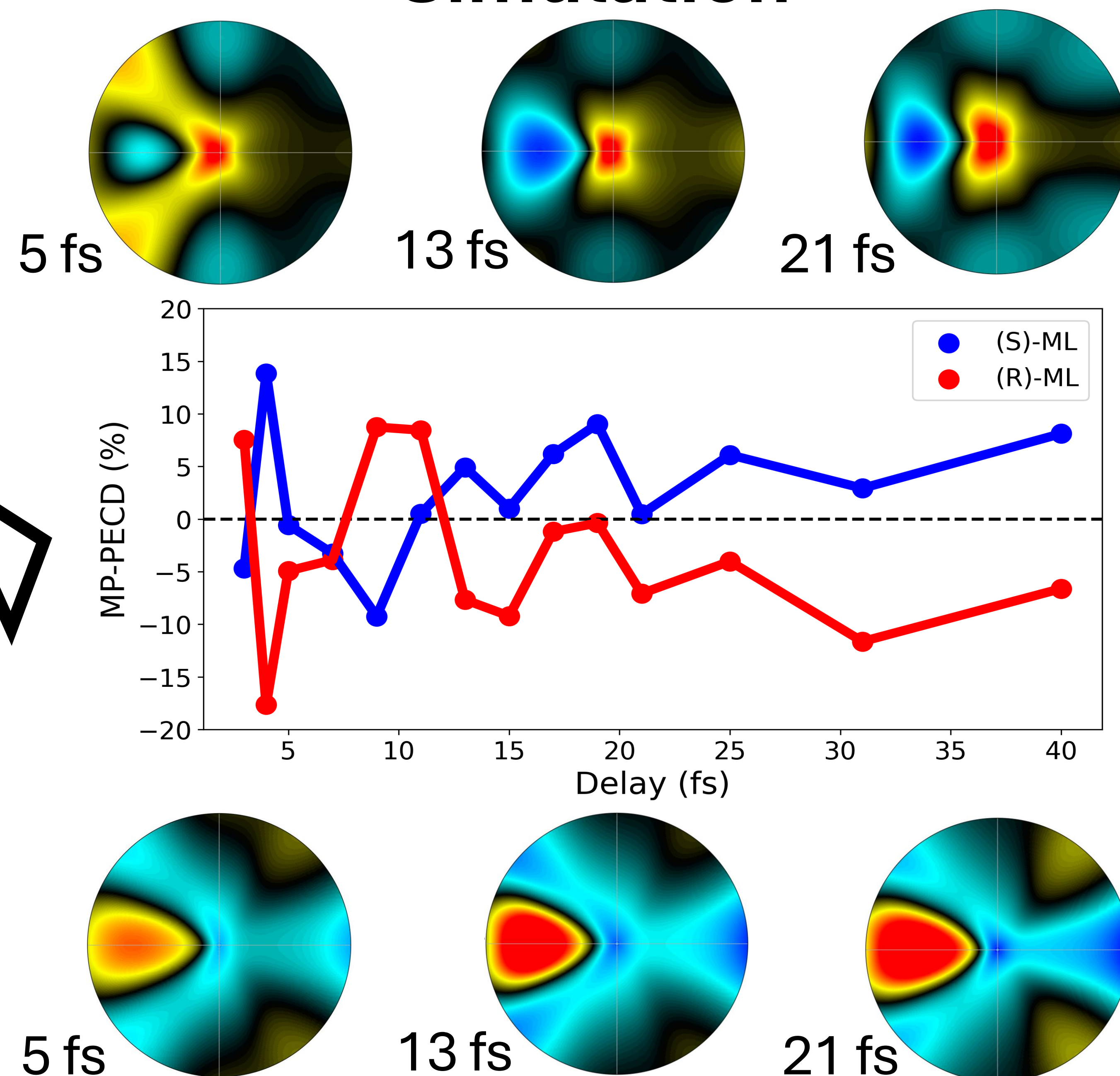
Experiment



Spin



Simulation



References

- [1] A. Comby et al., "Relaxation Dynamics in Photoexcited Chiral Molecules Studied by Time-Resolved Photoelectron Circular Dichroism: Toward Chiral Femtochemistry," *The Journal of Physical Chemistry Letters*, vol. 7, no. 22. American Chemical Society (ACS), pp. 4514–4519, Oct. 31, 2016. doi: 10.1021/acs.jpclett.6b02065.
- [2] V. Wanie et al., "Capturing electron-driven chiral dynamics in UV-excited molecules," *Nature*, vol. 630, no. 8015. Springer Science and Business Media LLC, pp. 109–115, May 22, 2024. doi: 10.1038/s41586-024-07415-y.
- [3] P. V. Möllers et al., "Spin-Polarized Photoemission from Chiral CuO Catalyst Thin Films," *ACS Nano*, vol. 16, no. 8. American Chemical Society (ACS), pp. 12145–12155, Aug. 09, 2022. doi: 10.1021/acsnano.2c02709.

Conclusion

First results for simulated TR-PECD spectra are in good agreement with experimental results [2]. Photoelectrons exhibit chirality-dependent spin polarization, which agrees with [3]. Future studies will attempt to deepen the understanding of the correlation between photoelectrons, chirality and spin for different systems.

We would like to express our sincere gratitude to Dr. Vincent Wanie and Prof. Francesca Calegari for their invaluable assistance and guidance in conducting this research.

Funded by the European Union, in the framework of the Marie Skłodowska-Curie Actions - CISS Doctoral Network, under Grant Agreement n° 101071886. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the European Research Executive Agency (REA). Neither the European Union nor the granting authority can be held responsible for them.