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

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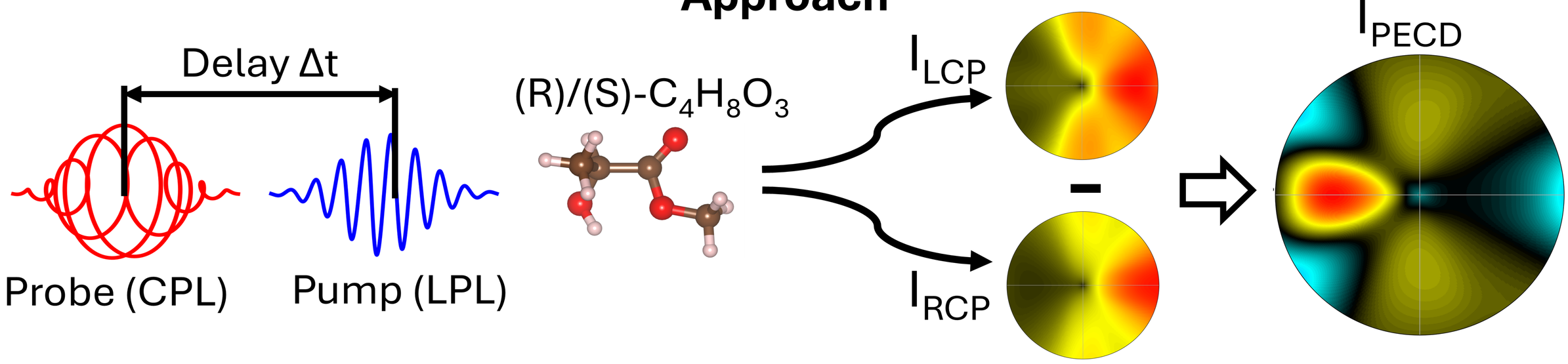
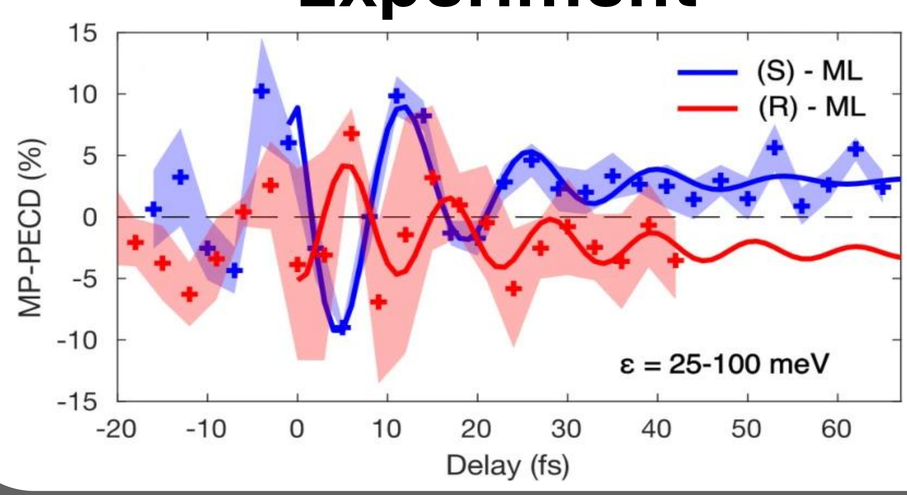
Investigation of electron dynamics in chiral structures are crucial in understanding chirality-dependent processes in chemistry and biology, in particular via the chiral induced spin selectivity (CISS) effect. Recent advances in attosecond science enabled real-time observation of electron dynamics using 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.

Approach

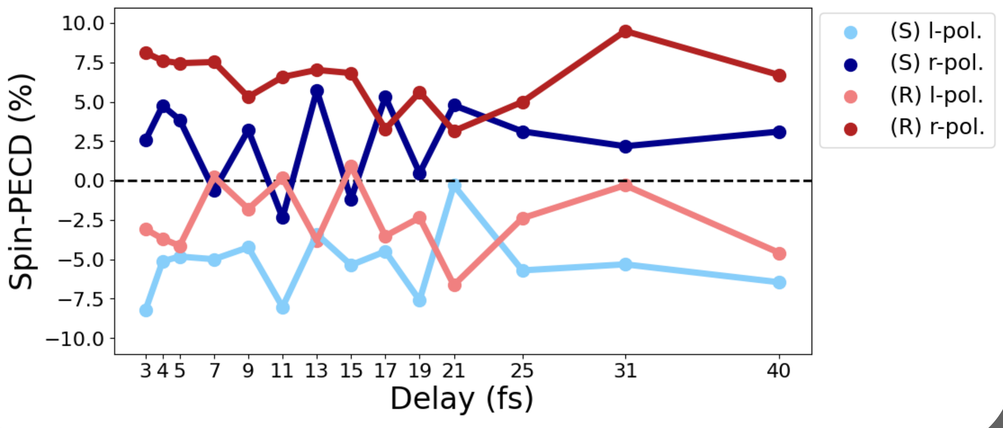


Experiment

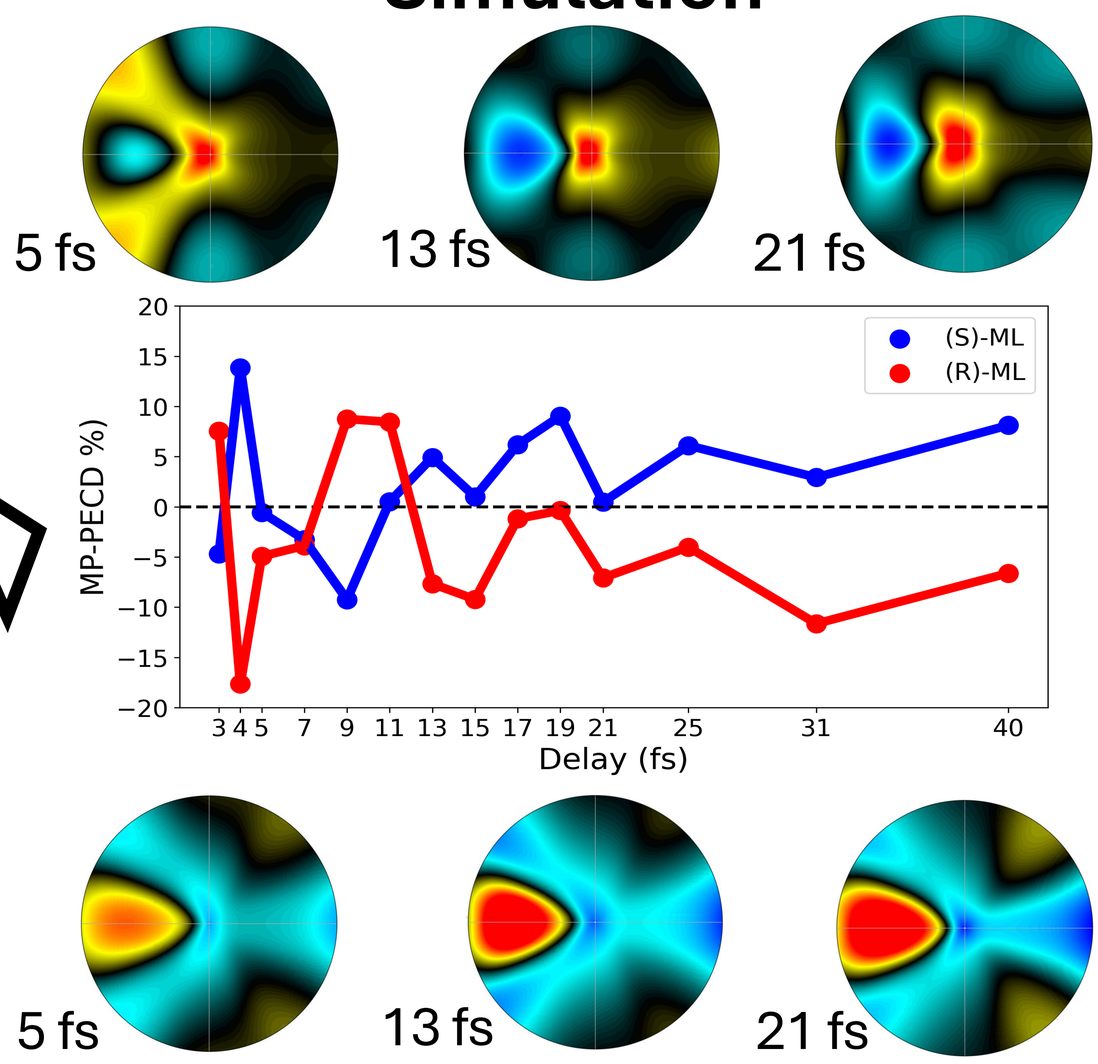


[2]

Spin



Simulation



References

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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.

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