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Relativisitc real-time electron dynamics-based approaches for chiroptical properties

In this talk, I will present real-time time-dependent density functional theory (RT-TDDFT) methods for simulating ground- and transient-state chiroptical properties [1,2]. For studies focused on high energy X-ray regions and systems containing heavy elements, incorporating relativistic effects is essential. Full four-component relativistic methods, while accurate, are often computationally challenging. To address this, we recently formulated and implemented the atomic mean-field exact two-component (amfX2C) approach [3] within the ReSpect software package [4], achieving four-component accuracy at a fraction of its computational cost, while variationally including scalar and spin-orbit relativistic corrections.

Beyond ground-state UV-vis and X-ray electronic circular dichroism (ECD) spectroscopy, we extended the RT-TDDFT framework to capture pump-probe transient ECD signals. Here, a pump pulse generates a chiral electronic wavepacket, followed by a probe pulse that captures the response of the chiral non-stationary state, providing insights into ultrafast chiral dynamics. I will also highlight novel applications in which symmetry-breaking is achieved with a circularly polarized pump pulse in attosecond timescales, manipulating only pure electron dynamics [2].

[1] L Konecny, et al, J. Chem. Phys., 2018, 149, 204104.
[2] T. Moitra, et al., submitted, 2024.
[3] S. Knecht, et al., J. Chem. Phys., 2022, 157, 114106.
[4] www.respectprogram.org

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