Light-induced molecular spin dynamics via time-dependent spin-orbit configuration interaction theory

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Spin transitions in molecules have a number of important applications including solar energy conversion, sensing, and information technology. These processes often involve transition metal complexes, and theoretical treatments have proven challenging due to the inherent static and dynamic correlation which generally require the use of multiconfigurational wavefunctions. The time-dependent spin-orbit configuration interaction (TDSOCI) method [1] is a real-time multiconfigurational relativistic electron dynamics method for simulating spin transitions of molecules in an external time-dependent electric field. The inclusion of spin-orbit coupling allows for a mapping between spin-mixed and spin-pure states in an explicitly time-dependent manner. The method is applied to study the effects of ultrafast laser pulses on spin transitions in Fe-containing molecules.

References

[1] I.S. Ulusoy and A.K. Wilson, Phys. Chem. Chem. Phys. 21, 7265 (2019).