

화학고 세미나

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Deciphering Excited State Dynamics by MRSF-TDDFT

The coupling between molecular vibrations and electronic states is fundamental to excited-state dynamics, shaping the outcomes of ultrafast nonadiabatic processes and subsequent photochemical reactions. The recently developed Mixed-Reference Spin-Flip Time-Dependent Density Functional Theory (MRSF-TDDFT) offers unprecedented insights into these intricate interplays. Coupled with nonadiabatic molecular dynamics (NAMD), MRSF-TDDFT has demonstrated its versatility by uncovering the long lifetimes of dark states in thymine, the hidden ultrafast decay dynamics of uracil and aromatization dynamics in azulene. And it has proposed a novel mechanism for green fluorescent protein (GFP), among other achievements.

The success of MRSF-TDDFT lies in its ability to overcome the limitations of traditional linear response theories while delivering accuracy on par with advanced quantum mechanical methods. We begin by introducing MRSF-TDDFT as a groundbreaking quantum chemical framework capable of tackling challenging scenarios in both ground and excited states, such as diradicals, bond breaking, conical intersections, doubly excited states, and core-level excitations. This is followed by representative examples where MRSF-TDDFT has advanced our understanding of excited-state dynamics.

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