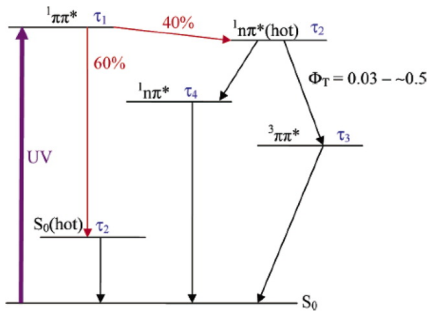
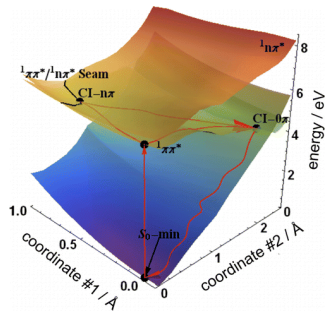
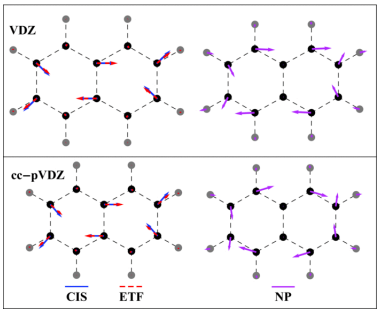
Q-CHEM™
A Quantum Leap Into the Future of Chemistry

Exploring Excited-State Potential Energy Surfaces: Nonadiabatic Couplings and Minimum-Energy Crossing Points

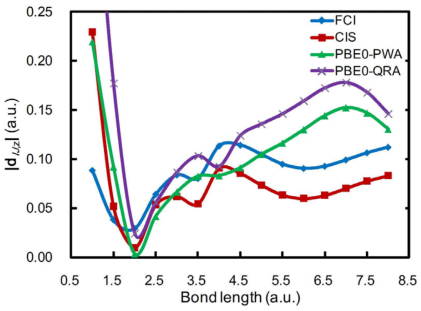




- Nonadiabatic coupling (NAC) is the most important physical quantity governing transitions between electronic states, such as internal conversion and radiationless relaxation.
- The minimum-energy crossing points (MECPs) in the seam space where multiple electronic states are degenerate are the most important points which connect photochemical reaction pathways.
- NACs can be computed with standard CIS and TDDFT methods, as well as with the spin-flip (SF) CIS and TDDFT variants, which afford correct topology around conical intersections.
- NACs can also be computed with EOM-EE/IP/EA-CCSD methods.
- Multiple algorithms for MECP location are available, including those that do not require NACs.



(a) Calculated NAC vectors for naphthalene



(b) Calculated z-component of the derivative coupling between the $3^1\Sigma_g^+$ and $5^1\Sigma_g^+$ states of He_2

Request a free trial at www.q-chem.com