Ab initio-based quantum studies of nonadiabatic molecular photodynamics.

A short outline is given of the ab initio quantum dynamical treatment of molecular processes following UV/Vis photoexcitation. Nonadiabatic coupling effects represent an important feature of these processes and are typically associated with conical intersections of potential energy surfaces. The methodology of their theoretical description is indicated. Illustrative examples comprise the five-membered heterocycles furan, pyrrole and thiophene, and related systems.