

The speaker will present a strategy for the simulation of nonadiabatic excited state dynamics, based on the direct calculation of electronic energies and wavefunctions by a semiempirical method. The semiempirical SCF-CI procedure has been adapted to represent bond breakings, orbital degeneracies and other multi-configurational open-shell situations of interest in photochemistry. The semiempirical parameters can be calibrated with respect to experimental or ab initio data. A QM/MM extension of the method is suitable to treat a chromophore interacting with a condensed phase medium, a macromolecule or a supramolecular environment. An application to azobenzene photoisomerization will be reviewed.