Towards Dynamical Pictures of Zeroth Order Vibronic States

Albert Stolow, Steacie Institute for Molecular Sciences, National Research Council, 100 Sussex Drive, Ottawa, ON Canada K1A 0R6.

Wavepackets, coherent superpositions of eigenstates formed by laser pulses, can be used to effectively create zeroth order states. Under certain conditions the evolution of wavepackets can give an intuitive picture of the dynamics of these states. We are particularly interested in using wavepacket methods to study fast non-adiabatic processes in the excited states of polyatomic molecules with a view towards disentangling zeroth order electronic dynamics from the coupled zeroth order nuclear dynamics. Time-resolved photoelectron spectroscopy, being sensitive to both orbital configurations and vibrational dynamics, is one approach to these problems. We discuss progress along these lines with examples chosen from linear polyenes, polyaromatic hydrocarbons, excited state proton transfer systems and model Molecular Electronic switches.