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Using quantum dynamics simulations to understand motion around a conical intersection GRAHAM WORTH, University of Birmingham, U.K. — Quantum dynamics simulations provide a key support in understanding laser spectroscopy measurements. To do this, a model must first be able to reproduce, or be associated with, an observation. The model can then be analysed to provide a picture at the molecular level. Unfortunately the wavepacket propagation methods used in many quantum dynamics calculations are unable to treat more than a few degrees of freedom: a major bottleneck in photochemical systems where the dynamics is dominated by internal conversion through a conical intersection. The multi-configuration time-dependent Hartree (MCTDH) method is one approach that has been very successful in accurately treating non-adiabatic polyatomic systems. Combined with the vibronic coupling model Hamiltonian we have been able to study in detail the dynamics of a number of molecules as they pass through a conical intersection. Recent work, to be covered in this talk, focuses on the complex photochemistry of benzene, showing how a time-resolved photo-electron spectrum can be calculated and interpreted in terms of the underlying molecular dynamics.

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