Abstract ID: 19

Controlling the Electrons in Excited State Chemistry: Studies using the Quantum Ehrenfest Method (QuEh).

Content

Attosecond spectroscopy has opened up the possibility of observing electron dynamics on timescale of a few attoseconds. We have been studying such electron dynamics together with the coupled nuclear motion, using our implementation of the Ehrenfest method with quantized nuclear motion (Quantum Ehrenfest QuEh method) (1) The initial electronic wavepacket is chosen as a superposition of eigenstates. If this superposition is chosen appropriately, it can be used to steer the coupled nuclear motion, and thus leads to attochemistry

We will review our methodology (1) for the combination of the Ehrenfest method with both classical and quantum dynamics (2) We will then focus on some model molecular systems (eg GLY+ see below) where the course of the nuclear motion is driven by the nature of the electron dynamics.

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Contribution Type: Invited talk