Path Integral Studies of Coherent Transport

- Simulation aids the interpretation of experimental spectra and guides the design of structures that exploit coherent transport.
- Quantum coherence is a delicate phenomenon, arises from constructive interference among an astronomical number of phase terms.
- We employ highly accurate, phase-sensitive, real-time path integral methods that fully account for electronic interactions and hundreds of finite-temperature intramolecular vibrations in chromophore aggregates.

Building Coherence with Strong Electronic Coupling

- Role of molecular vibrations in sustaining/destroying coherence
- Optimal relation between electronic and vibrational parameters
- Structure/function-aimed design of coupled chromophore arrays

Directing Particles & Quasiparticles Coherently

- Calculation of state populations and coherences in models and specific molecules
- Simulation of feedback from 2DES and 2DEV spectra
  (Fleming, Therien, Beratan, Wasielewski)

- Coherence and exciton diffusion in porphyrin arrays
  (Beratan, Therien, Fleming)

- Interference among identical pathways in dimer with degenerate electron donor states
  (Wasielewski, Beratan)

Engaging coherence - Producing Leaders