

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

Directing Particles & Quasiparticles Coherently

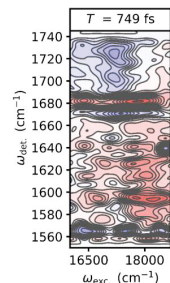
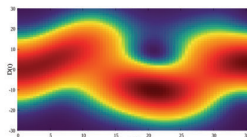
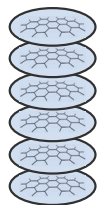
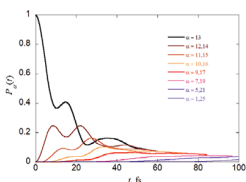
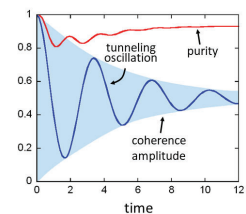
Role of molecular vibrations in sustaining/destroying coherence

- Calculation of state populations and coherences in models and specific molecules

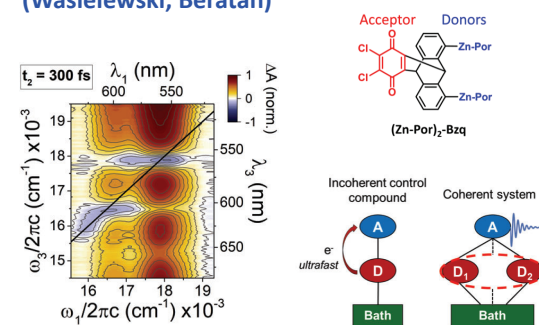
Optimal relation between electronic and vibrational parameters

- Simulation of/feedback from 2DES and 2DEV spectra
(Fleming, Therien, Beratan, Wasielewski)

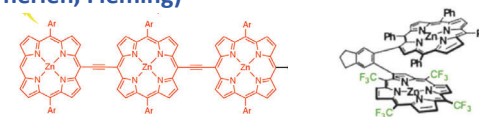
Structure/function-aimed design of coupled chromophore arrays



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



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



Engaging coherence - Producing Leaders