**Excitation** **energy transfer using real-time path integral methods**

Real-time path integral methods offer a rigorous, fully quantum mechanical approach to the dynamics of many processes in condensed-phase or biological environments and large molecular aggregates. These include the quasi-adiabatic propagator path integral (QuAPI) and its small matrix formulation (SMatPI), which eliminates the need for tensor storage, the modular decomposition (MPI) and the quantum-classical path integral (QCPI). These methods are used to simulate excitation energy transfer (EET) in large molecular aggregates of perylene bisimide and in the photosynthetic light harvesting complex LH2 of purple bacteria.

****

**Prof. Nancy Makri**

University of Illinois at Urbana-Champaign

1985 B.S., University of Athens

1989 Ph.D., University of California at Berkeley

1989-92 Junior Fellow, Harvard University

1992- University of Illinois (currently Edward William and Jane Marr Gutgsell Professor)

Web: <https://chemistry.illinois.edu/nmakri>

ACS Award in Theoretical Chemistry, 2023; ACS Physical Chemistry Division Award in Theoretical Chemistry, 2021; Löwdin Lecture, Uppsala University, Sweden, 2019; Member, American Academy of Arts and Sciences; Member, International Academy of Quantum Molecular Science.