



**EIXHMYΘ-ITE**

# ΣΕΜΙΝΑΡΙΟ

- ΟΜΙΛΗΤΗΣ: Nancy Makri, Professor of Chemistry and Physics  
Department of Chemistry  
University of Illinois
- ΘΕΜΑ: The path integral formulation of quantum mechanics: theory  
and numerical aspects
- ΤΟΠΟΣ: Αίθουσα Σεμιναρίων EIXHMYΘ - ITE
- ΗΜΕΡΟΜΗΝΙΑ: 17 Ιουλίου 2000
- ΩΡΑ: 12:00

## ***OVERVIEW OF RESEARCH IN THE MAKRI GROUP***

The central goal of our research is to advance the theoretical understanding of quantum mechanical processes in large molecules and the condensed phase. Unless severe approximations are introduced, direct solution of the Schrödinger equation is feasible only for small molecules, as it requires numerical effort that increases exponentially with the number of particles. We develop new theoretical descriptions and simulation methods based on Feynman's path integral formulation of quantum dynamics and its semiclassical limit and apply them to investigate proton and electron transfer reactions or relaxation processes in condensed-phase and biological systems as well as the possibility of manipulating transport in nanodevices using coherent laser light.