

# SYMPOSIUM ON MOLECULAR REACTION DYNAMICS IN CONDENSED MATTER

*March 3-6, 2004, Laguna Beach, CA*

Program Chairs: E. Chronister (UC Riverside) D. Dlott (Illinois) and V. A. Apkarian (UC Irvine)

Program sponsors: Air Force Office of Scientific Research, University of California, Riverside,  
UC Irvine, Offices of Research and Graduate Studies, and the UC Discovery Grant Program

## Wednesday, March 3

*Arrival and check in*

5:00 - 7:00 pm

Reception

7:30 - 9:10 pm

*Dynamics in Condensed Phases* -- Chair **Eric Chronister**

7:30	Keith Nelson	MIT	Terahertz polaritonics: Spatiotemporal coherent control over propagating lattice waves
8:20	Marcos Dantus	Michigan St.	Controlling nonlinear optical excitation of large molecules in condensed phase and multiphoton imaging
8:45	Harald Kauffman	Vienna	Quantum-stochastic relaxation of optical excitations in a conjugated polymer: experimental coherence and homogeneous dephasing

## Thursday, March 4

7:30 – 9:00 am

Breakfast

9:00 -12:15

*Condensed Phase Dynamics* -- Chair **Dana Dlott**

9:00	Ken Eisenhal	Columbia	Molecular Dynamics at Aqueous Interfaces
9:50	Alex Benderskii	Wayne State	Coherent time-resolved vibrational spectroscopy of surfaces and interfaces
10:15	John Deak	Scranton	Energy Transfer over self-assembled nanostructures
10:40	Break		
11:00	James Skinner	Wisconsin	Ultrafast spectroscopy and dynamics in water and aqueous solutions
11:50	David Blank	Minnesota	Direct probing of the local environment during dynamic events in solution

12:15 -2:00 pm

Lunch

2:00 –6:05 pm

*Multidimensional Spectroscopy* -- Chair **Alex Benderskii**

2:00	Andrei Tokmakoff	MIT	Hydrogen bond dynamics in water probed with IR echoes and 2D IR spectroscopy
2:50	Shaul Mukamel	Irvine	Multidimensional optical spectroscopies of molecules and aggregates: snapshots of electronic and vibrational coherence
3:40	Break		
4:00	Nien-Hui Ge	Irvine	Heterodyned 2D IR spectroscopy of short peptides
4:25	Richard Van Duyne	Northwestern	Nanoparticle Optics for Surface-Enhanced Sensing and Spectroscopy
5:15	Yoonsoo Pang	Illinois	Vibrational energy relaxation in water and HOD/D <sub>2</sub> O by ultrafast IR-Raman spectroscopy
5:40	Dana Dlott	Illinois	Molecular dynamics with ultrahigh time and space resolution with multidimensional vibrational spectroscopy

6:05 - 8:00 pm

Dinner

8:00 – 9:40 pm

*Condensed Phase Dynamics (cont.)* -- Chair **Benjamin Schwartz**  
& *Quantum Computing*

8:00	Eric Chronister	UC Riverside	Optically generated surface acoustic waves as a probe of liquid-solid interfaces - applied under variable high pressure conditions
8:25	Christopher Elles	Wisconsin	Solvent influence on the vibrational relaxation of CH <sub>3</sub> I
8:50	Ara Apkarian	Irvine	Quantum Coherent Dissipation - a glimpse of the "cat"

## Friday, March 5

7:30 – 9:00 am Breakfast

9:00 -12:15 pm *Molecular Dynamics Relevant to Quantum Computing* -- Chair **Marcos Dantus**

9:00	Regina de Vivie-Riedle	München	Quantum gates and quantum algorithms operating on molecular vibrational modes
9:50	Philip Bucksbaum	Michigan	Learning about Quantum Dynamics from Learning Control Algorithms
10:40	Break		
11:00	Birgitta Whaley	Berkeley	Nanoscale Superfluidity in Molecular Hydrogen
11:50	Leonard Mueller	Riverside	NMR Quantum Information Processing with a Single-Crystal Solid

12:15 -2:00 pm Lunch

2:00 – 5:40 pm *Collective motions probed by THz or X-rays* – Chair **Andrei Tokmakoff**

2:00	Steven Leone	Berkeley	Ultrafast Chemical Dynamics Probed by Soft X-Rays
2:50	Margaret Murnane	Colorado	Ultrafast EUV Probes of Surfaces: Charge Transfer and Photoacoustic Spectroscopies
3:40	Break		
4:00	Christoph Rose-Petruck	Brown	XANES spectroscopy of solvated transition metal complexes measured with ultrafast laser-driven x-ray sources
4:50	Ting Guo	UC Davis	Ultrafast selected energy x-ray absorption spectroscopy (USEXAS): Principle and applications
5:15	Eberhard Riedle	München	Real-time investigation of nuclear motion during primary chemical reactions

😊😊😊😊 5:40 watch sunset 😊😊😊😊

6:05 - 8:00 pm Dinner

8:00 – 9:40 pm

*Dynamics in Liquids* – Chair **David Blank**

8:00	J.T. Hynes	ENS, Paris/ Colorado	Dynamics in the Aqueous Solvation Shell of Anions
8:50	Steven Adelman	Purdue	Time Correlation Function Approach to Liquid Phase Vibrational Energy Relaxation: Dihalogen Solutes in Rare Gas Solvents
9:15	Hyung Kim	Carnegie Mellon	MD simulation study of solute and solvent dynamics in room-temperature ionic liquid

**Saturday, March 6**

7:30 – 8:30 am

Breakfast

9:00 - 12:35

*Chemical Dynamics in Condensed Phases* – Chair **Ara Apkarian**

9:00	Todd Martinez	Illinois	First Principles Studies of Photoinduced Isomerization and Proton Transfer
9:50	Adam Cohen	Irvine	Resonant enhancement and dissipation in nonequilibrium van der Waals forces
10:15	Wei Zhao	Arkansas	Doubly vibrationally enhanced four wave mixing spectroscopy in a metal ion-acetonitrile complex system
10:40	Break		
11:00	Benjamin Schwartz	UCLA	The Roles of Electron Exchange and Correlation in Condensed-Phase Dynamics: Nonadiabatic Mixed Quantum-Classical Computer Simulations of the Hydrated Dielectron
11:50	Steven Corcelli	Wisconsin	Combined electronic structure/molecular dynamics approach for ultrafast infrared spectroscopy of dilute HOD in liquid H <sub>2</sub> O and D <sub>2</sub> O

12:15

*Conference ends*