January 29 - 31, 2003, Asilomar Conference Center, Pacific Grove, CA

Meeting Schedule

All talks will be in the *Chapel*. All Poster Sessions will be nearby at *the Fred Farr Forum*. All meals will be served in the *Crocker Dining Hall*.

Wednesday, January 29th

3:00 – 6:00 p.m.	Registration in Main Lodge
4:00 – 5:00 p.m.	Set-up for Poster Session I in the Fred Farr Forum
5:00 – 6:00 p.m.	Poster Session I in the Fred Farr Forum
6:00 – 7:00 p.m.	Dinner in the Crocker Dining Hall
7:00 – 8:00 p.m.	Registration Continues in Main Lodge
8:00 – 9:00 p.m.	Registration continues in the Chapel
8:00 – 8:10 p.m.	Welcoming Remarks in the Chapel: **Geraldine Richmond** WSA Program Chairperson University of Oregon
8:10 – 9:00 p.m.	Opening Lecture in the Chapel: **F. Sherwood Rowland,** University of California, Irvine "The Changing Atmosphere 2003"
9:00 – 11:30 p.m.	Poster Session I continues in the Fred Farr Forum

Thursday, January 30th

7:30 a.m.	Breakfast (Crocker Dining Hall)
8:00 – 8:30 a.m.	Registration continues in the Chapel
8:30 – 10:30 a.m.	Lecture Session I in the Chapel Session Chair: **Joseph Nibler**, Oregon State University
8:30 – 9:30 a.m.	**Mostafa A. El-Sayed** Georgia Institute of Technology "Small is Different; Some Interesting Properties of Material Confined to the Nanometer Length Scale of Different Shapes"
9:30 – 10:30 a.m.	**William H. Miller** University of California, Berkeley "Using Semiclassical Theory to Include Quantum Effects in Classical Molecular Dynamics Simulations"
10:30 – 10:45 a.m.	Coffee Break
10:45 – 11:45 a.m.	**Margaret Murnane** University of Colorado, JILA "Ultrafast Spectroscopy of Small Molecules with Visible and EUV Pulses"
12:00 Noon	Lunch (Crocker Dining Hall)
1:30 – 2:00 p.m.	Set-up for Poster Session II in the Fred Farr Forum
2:00 – 4:00 p.m.	Poster Session II in the Fred Farr Forum
4:00 – 6:30 p.m.	Break
5:30 – 6:00 p.m.	Set-up for Poster Session III in the Fred Farr Forum
6:30 – 8:00 p.m.	BANQUET (Crocker Dining Hall)
8:00 – 9:00 p.m.	Banquet Address (in the Chapel): **Yuan T. Lee** Academia Sinica, Taiwan “From Chemical Dynamics to Spectroscopy”
9:00 – 11:30 p.m.	Poster Session III in the Fred Farr Forum

Friday, January 31st

7:30 a.m.	Breakfast (Crocker Dining Hall)
8:00 – 8:30 a.m.	Registration continues in the Chapel
8:30 – 10:30 a.m.	Lecture Session II in the Chapel Session Chair: **David Chandler**, Sandia National Laboratories
8:30 – 9:30 a.m.	**Richard N. Zare** Stanford University "Overview of Cavity-Enhanced Absorption Spectroscopies"
9:30 – 10:30 a.m.	**Geoffrey Blake** California Institute of Technology "Spectroscopy with Telescopes: Astrophysical & Atmospheric Puzzles, Laboratory Challenges"
10:30 – 10:45a.m.	Coffee Break
10:45 – 11:55 a.m.	**Panel Discussion:** "Optics and Spectroscopy: The Next 50 Years?" **Richard Zare**, Moderator, Stanford University **Geoffrey Blake**, California Institute of Technology **Steven Buratto**, University of California, Santa Barbara **David Chandler**, Sandia National Laboratories **Margaret Murnane**, University of Colorado, JILA, Boulder **Benjamin Schwartz**, University of California, Los Angeles
12:00 Noon	Lunch in the Crocker Dinning Hall

Abstracts of Contributed and Invited Talks

The Changing Atmosphere 2003

F. Sherwood Rowland
University of California, Irvine
Donald Bren Research Professor of Chemistry and Earth System Science
516 Rowland Hall, Irvine, CA 92697-2025

Earth's atmosphere is not an equilibrium system, but instead is much closer to a photochemical steady state under the influence of the sun. This average steady state can drift over time, at least in part to the direct influences of mankind. Three general effects are considered here; (1) smog created in urban environments (with similar chemistry from biomass burning), (2) depletion of stratospheric ozone by halogenated compounds, allowing more solar ultraviolet radiation to reach Earth's surface, and (3) increasing levels of greenhouse gases, hindering escape of terrestrial infrared radiation, with global warming as a consequence.

Small is Different;
Some Interesting Properties of Material Confined to the Nanometer Length Scale of Different Shapes

Mostafa A. El-Sayed
Georgia Institute of Technology

Using Semiclassical Theory to Include Quantum Effects in Classical Molecular Dynamics Simulations

William H. Miller
Department of Chemistry, University of California, Berkeley, CA 94720 USA

Semiclassical (SC) theory provides a good description of essentially all quantum effects (interference, tunneling, symmetry effects of identical particles, quantization of bounded motion, etc.) in molecular dynamics; this has been long appreciated and validated by many applications to small molecular systems [cf. Adv. Chem. Phys. **25**, 69-177 (1974)]. Since SC theory is built on the classical trajectories of the dynamical system, it should in principle be possible to use it also to add quantum effects to classical trajectory simulations of *complex* molecular systems (i.e., those with many degrees of freedom), e.g., chemical reactions in solution, clusters, proteins, or any complex environment. The practical implementation of SC theory for complex systems is based on various initial value representations (IVRs), which have recently undergone a re-birth of interest in this regard. This talk reviews the basic idea of the SC-IVR approach and describes a variety of recent applications that have been carried out using it. [For a recent overview, see J. Phys. Chem. A **105**, 2942-2955 (2001).]

Ultrafast Spectroscopy of Small Molecules with Visible and EUV Pulses

Margaret Murnane
University of Colorado, JILA

In this talk, I will discuss the use of shaped, broadband, femtosecond pulses to selectively excite vibrational modes and their overtones at room temperature and pressure. Relatively high spectral selectivity of $15cm^{-1}$ is achieved by carefully designing the shape of the excitation pulse. I will also discuss the use of ultrafast x-ray pulses to monitor charge transfer processes and molecular oscillations on surfaces on femtosecond timescales.

From Chemical Dynamics to Spectroscopy

Yuan T. Lee
Academia Sinica, Taiwan

In this lecture I will give my personal accounts of how I used photoexcitation to investigate the process of chemical reaction dynamics of excited species, and how the knowledge of molecular photodissociation was used for developing the tool to investigate IR spectroscopy of ionic clusters.

Overview of Cavity-Enhanced Absorption Spectroscopies

Richard N. Zare
Stanford University, Department of Chemistry

Absorption spectroscopy dates back to the beginning of the last century. It tends to be universal in that almost all matter (dark matter excepted!) absorbs electromagnetic radiation at some frequency, but it also tends to be rather insensitive. Typical absorption measurements cannot see a change in the absorption better than one part in 10,000 or one part in 100,000. This situation has dramatically changed for the better with the introduction of various absorption measurements using optical cavities. This talk will present a review of cavity ring-down spectroscopy and related techniques, emphasizing its use for the detection of absorbing species in gases, liquids, solids, and plasmas.

Spectroscopy with Telescopes: Astrophysical & Atmospheric Puzzles, Laboratory Challenges

Geoffrey A. Blake
Professor of Cosmochemistry & Planetary Science, Professor of Chemistry, and Deputy Director, Owens Valley Radio Observatory, gab@gps.caltech.edu
Division of Geological and Planetary Sciences, California Institute of Technology, MS 150-21, Pasadena, CA 91125, http://www.gps.caltech.edu/~gab/

The continuing development and deployment of large aperture telescopes and high performance spectrographs has produced spectra of natural environments with unprecedented sensitivity and resolution. Our understanding of processes as diverse as star formation and ozone destruction has been correspondingly enhanced. This talk will overview recent results from and near-future capabilities in remote sensing at optical through millimeter-wavelengths. Existing and new missions pose severe challenges to laboratory spectroscopy, the bedrock upon which progress is based, and so areas of greatest need in both astrophysics and atmospheric science will be highlighted.