



CONFERENCE PROGRAM

Saturday, August 14, 2004

- 4:00-6:00 Registration: Lobby of Chemistry, Charter Street Entrance
6:00- Registration: 8th floor, Fluno Center
6:00-8:00 Welcome Reception: Skyview Room, Fluno Center**
8:00-9:00 Meeting of the International Organizing Committee: Rm 810 Fluno Center**

Sunday, August 15, 2004

- 8:00-12:00 Registration: Lobby of Chemistry, Charter Street Entrance
8:50 Welcome and opening remarks – John Wright, University of Wisconsin-Madison
Session 1 Session Chair: John Wright, University of Wisconsin-Madison
9:00 -9:40 *Dual Frequency 2D IR of Amide Groups in Peptides and Liquids*
Robin Hochstrasser - University of Pennsylvania
9:40 -10:20 *Heterodyned Fifth-order 2D IR Spectroscopy of Model Condensed Phase Systems*
Martin T. Zanni - University of Wisconsin-Madison
10:20-10:40 Refreshment Break – Rm 1371
10:40-11:20 *Structures and Dynamics of Small Peptides by Two-Dimensional Infrared Spectroscopy*
Nien-Hui Ge, Denis Karaiskaj, Soohwan Sul, Ying Jiang, and Hiroaki Maekawa - University of California, Irvine
11:20-12:00 *Two-Dimensional Infrared Spectroscopy of Protein Conformation and Unfolding*
H. S. Chung, M. Khalil, A.W. Smith, Z. Ganim, **Andrei Tokmakoff** - Massachusetts Institute of Technology
12:00 PM Lunch – Tripp Commons, Memorial Union**
Session 2 Session Chair: Fleming Crim, University of Wisconsin-Madison
1:20 -2:00 *Mixed Quantum and Classical Methods for Ultrafast Vibrational Spectroscopy, with Applications to Water and Aqueous Solutions of Biologically Relevant Molecules*
James L. Skinner - University of Wisconsin-Madison
2:00 -2:40 *Ultrafast Infrared Vibrational Echo Correlation Spectroscopy: Hydrogen Bond Dynamics in Bulk Water and in Water Nanopools*
John S. Asbury, T. Steinel, I. R. Piletic, Howe-Siang Tan, **Michael. D. Fayer** - Stanford University
2:40 -3:00 Refreshment Break – Rm 1371
3:00 -3:40 *Femtosecond Mid-Infrared Spectroscopy of Water in Strong Molecular Confinement*
J. Gijljamse, A. Lock, **Huib. J. Bakker** - FOM Institute AMOF

- 3:40 -4:20 *Ultrafast Vibrational Dynamics and Anharmonic Couplings of Hydrogen-Bonded Dimers in the Condensed Phase*
Thomas Elsaesser, Karsten Heyne, Nils Huse, Jens Dreyer, Erik T. J. Nibbering - Max-Born-Institute
- 4:20 -5:00 *Cascaded Energy Redistribution Upon O-H Stretching Excitation in an Intramolecular Hydrogen Bond*
 Karsten Heyne, **Erik T. J. Nibbering**, Thomas Elsaesser - Max-Born-Institute and Milena Petkovic, **Oliver Kuehn** - Freie Universitaet Berlin
- 5:00 -7:00 **Poster Session** – Hallway, Chemistry
- 7:00-9:00 Thermo Electron Conference Banquet – Skyview Room, Fluno Center**

Monday, August 16, 2004

- Session 3** Session Chair: Ned Sibert, University of Wisconsin-Madison
- 8:00-8:40 *Two-dimensional Electronic Spectroscopy of Molecular Complexes*
 Igor Stiopkin, Tobias Brixner, **Graham R. Fleming** - University of California-Berkeley
- 8:40 -9:20 *Probing the Response of the Local Environment Directly Using Resonant Pump Third Order Raman Probe Spectroscopy*
 David F. Underwood, Sarah J. Schmidtke, **David A. Blank** - University of Minnesota
- 9:20 -9:40 *Views of Water's Energy Landscape from Nonlinear IR Spectroscopy*
Joel D. Eaves, Joseph J. Loparo, Christopher J. Fecko, Sean Roberts, Andrei Tokmakoff, Phillip Geissler - Massachusetts Institute of Technology
- 9:40 -10:00 Refreshment Break – Rm 1371
- 10:00 -10:40 *Transient 2D-IR Spectroscopy: Beyond the Two-Point Frequency Fluctuation Correlation Function*
Peter Hamm, Jens Bredenbeck, Jan Helbing - Universitat Zurich
- 10:40 -11:20 *Femtosecond 1D and 2D FT Experiments on Vibrational and Electronic Motions at a Conical Intersection*
David M. Jonas - University of Colorado-Boulder
- 11:20 -12:00 *Applications of High-Speed Pulse Shaping to Multidimensional Spectroscopy and Imaging*
Warren Warren - Princeton University
- 12:00 Lunch – Tripp Commons – Lakeside Deck, Memorial Union**
- Session 4** Session Chair: James Skinner, University of Wisconsin-Madison
- 1:20 -2:00 *Many-Body Approaches to Multidimensional Spectroscopies*
Shaul Mukamel, W. Zhuang, T. Hayashi, D. Abramavicius, T. la Cour Jansen - University of California-Irvine
- 2:00 -2:40 *Recent Progress in Calculation of Vibrational Spectra*
Jianshu Cao - Massachusetts Institute of Technology
- 2:40 -3:00 Refreshment Break – Rm 1371
- 3:00 -3:40 *Simulation Studies of Protein 2D Vibrational Spectroscopy and Novel Nonlinear Spectroscopies for Optical Activity Measurement*
Minhaeng Cho - Korea University

- 3:40 -4:20 *Probing the Structure and Dynamics of a Molecular Device by Two-Dimensional Vibrational Spectroscopy*
Olaf A. Larsen, Wybren Jan Buma, David A. Leigh, **Sander Woutersen** - FOM Institute for Atomic and Molecular Physics
- 4:20 -4:40 *Vibrational Coherence Transfer and Trapping as Sources for Long-lived Quantum Beats in Polarized Emission from Energy Transfer Complexes*
Jeffrey A. Cina, Graham R. Fleming - University of Oregon
- 4:40 -5:00 *Vibrational Substructure in the OH Stretching Transition of HOD*
Zhaohui Wang, Yoonsoo Pang, and Dana D. Dlott - University of Illinois at Urbana-Champaign
- 5:00 Session Ends
- 5:20 Depart for Mariners Inn and dinner cruise. Bus leaves on Mills St.
- 6:30-9:30 Spectra-Physics Eclipse Conference Dinner Cruise on Lake Mendota

Tuesday, August 17, 2004

- Session 5** Session Chair: Martin Zanni – University of Wisconsin-Madison
- 8:00-8:40 *Two-Dimensional Visible / Infrared Spectroscopy Applied to Doubly-Resonant Difference Frequency Mixing in Asymmetric Quantum Wells*
Manuel Joffre, Nadia Belabas - Ecole Polytechnique
- 8:40 -9:20 *Two Dimensional Resonantly Enhanced Coherent Raman Spectroscopy*
Peter C. Chen, Candace C. Joyner - Spelman College
- 9:20 -9:40 *Ultrafast Resonance Raman Observations of Heme Vibrational Dynamics in Five-Coordinate Iron Porphyrins*
J. Reddy Challa, Tissa Gunaratne, **M. Cather Simpson**, - Case Western Reserve University
- 9:40 -10:00 *Phase-Coherent Degenerate Four-Wave Mixing Spectroscopy Via Two-Dimensional Femtosecond Pulse Shaping*
Thomas Hornung, **Joshua Vaughan**, Thomas Feurer, Keith A. Nelson - Massachusetts Institute of Technology
- 10:00 -10:20 Refreshment Break – Rm 1371
- 10:20 -10:40 *DOVE Spectroscopy as a Potential Method for Fingerprinting of Amino Acids, Peptides, and Proteins*
Jason Palmer, Paul Donaldson, David Klug - Imperial College London
- 10:40 -11:00 *DOVE Four Wave Mixing Spectroscopy in an Acetonitrile-Magnesium Perchlorate Model System*
Wei Zhao - University of Arkansas
- 11:00 -11:40 *Frequency and Time Resolved Coherent Multidimensional Vibrational Spectroscopy*
Kent A. Meyer, **John C. Wright** – University of Wisconsin, Madison
- 11:40 Final Announcements
- 12:00 Lunch/Presentation – Rm 9341
Sponsored by Spectra Physics

Sunday, August 15, 2004 - [Poster Papers](#)

- P-1 *Molecular State Reconstruction by Nonlinear Wave Packet Interferometry*
Travis S. Humble, **Jeffrey A. Cina** - University of Oregon
- P-2 *Diffraction Optics Based 2-D Vibrational and Electronic Spectroscopy*
M. L. Cowan, B. D. Bruner, N. Huse, T. Elsaesser, E. T. J. Nibbering, R. J. D. Miller – University of Toronto
- P-3 *Characterizing Higher Quantum States with Fifth-order Two Dimensional Infrared Spectra*
Feng Ding, Eric C. Fulmer, Martin T. Zanni – University of Wisconsin, Madison
- P-4 *Ultrafast Dynamics of Nano-confined Water*
Adriaan M. Dokter, Sander Woutersen, Huib Bakker - FOM-Institute for Atomic and Molecular Physics
- P-5 *Molecular Dynamics Simulation of Polarizability Response in Solution*
M. Dolores Elola, Branka M. Ladanyi - Colorado State University
- P-6 *Calculating the Vibrational Echo of a Myoglobin Mutant, H64V*
Anne Goj, Roger F. Loring - Cornell University
- P-7 *Elucidating the Vibrational Coupling Mechanisms in DNA using 2D-IR Spectroscopy*
Amber T. Krummel, Prabuddha Mukherjee, Martin T. Zanni – University of Wisconsin, Madison
- P-8 *Studies of Molecular Center-of-Mass Translation by Fourier Imaging Correlation Spectroscopy*
Andrew H. Marcus, Kenneth V. Adair, Michael Fink – University of Oregon
- P-9 *Vibrational Echoes Calculated with Semiclassical Dynamics and Classical Feynman Diagrams*
W. G. Noid, G.S. Ezra, R.F. Loring - Cornell University
- P-10 *Probing the Solvent Dynamics During Ultrafast Excited State Proton Transfer In 1-(Acylamino)Anthraquinones*
Sarah J. Schmidtke, David F. Underwood, David A. Blank - University of Minnesota
- P-11 *Efforts to Realize the Two-Dimensional Concept: Sub-20fs Photon Echos Across the Visible*
Jaroslav Sperling, Franz Milota, Peter Baum, Eberhard Riedle, Harald F. Kauffmann - University Vienna
- P-12 *Probing Hydrogen Bonding Dynamics between Solvent and Solutes :Resonant Pump Third Order Raman probe Spectroscopy (R_A PTORS) of Coumarin 102 in Binary Mixtures of Acetonitrile:Water*
Nathan P. Wells, David F. Underwood, David A. Blank - University of Minnesota