

TUEIf • Poster II f - Chemistry

Poster Area

18:00–20:00

TUEIf • Poster II f - Chemistry

TUEIf.1 • 18:00

Coherently Enhanced Ionization and Fragmentation, •Xin Zhu, Vadim Lozovoy, and Marcos Dantus; Michigan State University, Department of Chemistry, East Lansing, Michigan 48823.

We report the observation of coherently enhanced fragment ion ejection pathway. The ions formed through this process exhibit very sensitive dependence upon the time-frequency structures of the laser pulses.

TUEIf.2 • 18:00

Single-Shot Time Domain Measurement of Phase Response of Ultrafast Vibrational Quantum Beating, •Jesse W. Wilson, Philip Schlup, and Randy A. Bartels; Electrical and Computer Engineering Department, Colorado State University, Fort Collins, CO 80523, USA.

Phase-sensitive time-domain Fourier transform spectroscopy is used to measure vibrational Raman spectra in solid, liquid and gas phase samples. The pump-probe configuration measures phase shifts directly via spectral holography in scanned or single-shot modes.

TUEIf.3 • 18:00

Vibrational Coherence Transfer in Metal Carbonyls: Solvent Dependence of Coherence Lifetimes Studies with MDIR, •Matthew J. Nee, Carlos R. Baiz, Jessica M. Anna, Robert McCanne, and Kevin J. Kubarych; Department of Chemistry, University of Michigan, Ann Arbor, Michigan, 48109, USA.

Multidimensional infrared spectra of metal carbonyls in different solvents are presented as a function of the waiting time. The evolution of each peak is discussed with reference to excited-state coherences and coherence transfer.

TUEIf.4 • 18:00

The finite duration of chemical exchange events can be observed using two-dimensional infrared spectroscopy,

•Thomas la Cour Jansen and Jasper Knoester; Center for Theoretical Physics and Zernike Institute for Advanced Materials, University of Groningen, Groningen, The Netherlands.

We use numerical Langevin simulations to calculate two-dimensional infrared spectra of chemical exchange. We demonstrate that the spectra are not only sensitive to the exchange rate, but also to the finite duration of the exchange.

TUEIf.5 • 18:00

Chain Length Dependence of Two-Dimensional Infrared Spectral Pattern Characteristic to 3_{10} -Helix Peptides, Hiroaki Maekawa¹, Fernando Formaggi², Claudio Toniolo², and •Nien-Hui Ge¹; ¹Department of Chemistry, University of California, Irvine, California 92697-2025, USA, ²Institute of Biomolecular Chemistry, CNR, Padova Unit, Department of Chemistry, University of Padova, 35131 Padova, Italy.

Two-dimensional infrared spectra of Z-(Aib)_n-OtBu (*n* = 3, 5, 8, and 10) were measured to investigate how they depend on the peptide chain length. The onset of the 3_{10} -helical spectral signature appears to occur at the pentapeptide.

TUEIf.6 • 18:00

Ultrafast Exciton Dynamics of J- and H-Aggregates of Porphyrin Catechol in Aqueous Solution, •Hirendra Ghosh and Sandeep Verma; Radiation & Photochemistry Division, Bhabha Atomic Research Centre, Trombay, Mumbai - 400 085, INDIA,.

Porphyrin catechol found to form J- and H-aggregates in different pH at certain concentration. Ultrafast exciton dynamics of J- and H-aggregates found to be 200 fs and 100 fs respectively as monitored by femtosecond spectroscopy.

TUEIf.7 • 18:00

Chirp Effects on Vibrational Wave Packets in Large Molecules: A Multimode Perspective, •Amir Wand¹, Ofir Shoshanim¹, Shimshon Kallush², Ronnie Kosloff², and Sanford Ruhman¹; ¹Department of Physical Chemistry and the Farkas Center for Light-Induced Processes, The Hebrew University, Jerusalem 91904, Israel., ²Department of Physical Chemistry and The Fritz Haber Research Center, The Hebrew University, Jerusalem 91904, Israel.

Linear chirp which optimally induces vibronic wave packets in large molecules is addressed by theory and experiment. Results allow better definition for "following" of nuclear dynamics by the instantaneous pump frequency in the multidimensional case.

TUEIf.8 • 18:00

Determining Vibrational Huang-Rhys Factors by Photon Echo Spectroscopy, •Niklas Christensson, Arkady Yartsev, and Tönu Pullerits; Department of Chemical Physics, Lund University, P.O. Box 124, Se-22100, Lund, Sweden.

Electronic and vibrational dephasing dynamics of Rhodamine 800 has been studied with 3PEPS. With careful analysis, the S-factors of the vibrational modes can be accurately determined. The vibrational dephasing rate displays abnormal frequency dependence.

TUEIf.9 • 18:00

The solvent dependent conformations of a Glycine-Alanine dipeptide: A two-dimensional infrared study, •Marco Candelaresi¹, Paolo Foggi^{1,2}, and Manuela Lima¹; ¹Via Nello Carrara 1 50019 Sesto Fiorentino (FI), ²Via Elce di Sotto 8 06100 Perugia.

The D₂O and DMSO solutions of the Glycine-Alanine-Methylamide are investigated by two-dimensional pump-probe infrared spectroscopy. Differences in the dynamics and in the intensity of the cross peaks are observed between the two solutions.

TUEIf.10 • 18:00

Observation of High-Frequency Coherent Vibrational Motion with Strongly Chirped Probe Pulses, •Dario Polli, Daniele Brida, Guglielmo Lanzani, and Giulio Cerullo; Dipartimento di Fisica, Politecnico, Milano, Italy.

We observe time-domain coherent vibrational wavepackets at 1585-cm⁻¹ frequency (21-fs period) using broadband probe pulses strongly chirped up to 150-fs duration. The results are explained using the chronocyclic (Wigner) representation of the chirped pulse.

TUEIf.11 • 18:00

Coherent Transfer of Molecular Vibrations in the Electronic Excited States, Chul Hoon Kim, Sohyun Park, Intae Eom, and

•*Taiha Joo; Pohang University of Science and Technology, Pohang, South Korea.*

Coherent wave packet motions in the electronic excited states prepared by impulsive nuclear rearrangement such as electronic transition, internal conversion, and chemical reaction are observed directly by ultrafast 35 fs time-resolved spontaneous fluorescence

TUEIIf.12 • 18:00

Ultrafast isomerization dynamics of biomimetic

photoswitches, •*Julien Briand¹, Divya Sharma¹, Jérémie Léonard¹, Jan Helbing², Andrea Cannizzo³, Majed Chergui³, Vittorio Zanirato⁴, Stefan Haacke¹, and Massimo Olivucci⁵*;
¹*Institut de Physique et Chimie des Matériaux de Strasbourg, UMR 7504 ULP CNRS, F-67034 Strasbourg, France,*
²*Physikalisch-Chemisches Institut, Universität Zürich Winterthurerstr. 190, CH-8057 Zürich (CH),*
³*Laboratoire de Spectroscopie Ultrarapide, ISIC - EPFL, BSP, CH-1015 Lausanne (CH),*
⁴*Dipartimento di Scienze Farmaceutiche, Università di Ferrara, 44100 Ferrara (I),*
⁵*Dipartimento di Chimica, Università degli Studi di Siena, 53100 Siena (I).*
Femtosecond UV-VIS and mid-IR experiments show that a new class of biomimetic photoswitches photo-isomerizes in less than

300 fs. In close analogy to rhodopsin, the isomerization is driven by motion along stretch and torsional coordinates.

TUEIIf.13 • 18:00

Exchange Transient 2D-IR Spectroscopy probes the remixing of vibrational eigenstates upon electronic excitation - a benchmark for DFT calculations, •

Andreas Messmer^{1,2}, Peter Hamm¹, Ana Maria Blanco Rodríguez³, Antonín Vlček Jr.^{3,4}, Stanislav Zális⁴, and Jens Bredenbeck²;
¹*Institute for Physical Chemistry, University of Zurich, Winterthurerstr. 190, CH-8057 Zurich, Switzerland,*
²*Institute for Biophysics, Johann Wolfgang Goethe-University Frankfurt, Max von Laue-Str.1, D-60438 Frankfurt (Main), Germany,*
³*School of Biological and Chemical Sciences, Queen Mary, University of London, Mile End Road, London E1 4NS, United Kingdom,*
⁴*J. Heyrovský Institute of Physical Chemistry, Academy of Sciences of the Czech Republic, Dolejškova 3, CZ-18223 Prague, Czech Republic.*

The composition of excited state vibrations can be disentangled by projecting the groundstate vibrations on them using exchange transient two-dimensional IR spectroscopy. The results challenge time-dependent DFT calculations.