

The 22nd International Conference on Ultrafast Phenomena (UP 2020)



Th1A.2 • 09:00

Heme Doming in Ferric Cytochrome c: Femtosecond X-ray Absorption and X-ray Emission Studies, Camila Bacellar⁴, Dominik Kinschel⁴, Giulia F. Mancini⁴, rebecca ingle⁴, Jérémy Rouxel⁴, Oliviero Cannelli⁴, Claudio Cirelli¹, Gregor Knopp¹, Jakub Szlachetko², Frederico Lima³, Samuel Menzi¹, Georgios Pamfilidis¹, Katharina Kubicek³, Dmitry Khakhulin³, Wojciech Gawelda³, Angel Rodriguez- Fernandez³, Mykola Biednov³, Christian Bressler³, Christopher Arrell¹, Philip Johnson¹, Christopher J. Milne¹, Majed Chergui⁴; ¹PSI, Switzerland; ²Inst. of Nuclear Physics, Poland; ³European XFEL, Germany; ⁴EPFL, Switzerland. The photoinduced dynamics of ferric Cytochrome c was investigated by ultrafast non-resonant X-ray emission (XES) and X-Ray Absorption (XAS) spectroscopies, and a cascade through high spin states accompanied by heme doming are observed for the first time. © 2020 The Author(s)

Th1A.3 • 09:15

Megahertz-Rate Pump-Probe Jitter and Drift Characterization at a Hard X-ray Free-Electron Laser, Romain Letrun¹, Tokushi Sato¹, Henry J. Kirkwood¹, Jia Liu¹, Jan Grünert¹, Adrian P. Mancuso^{1,2}; ¹European XFEL, Germany; ²Dept. of Chemistry and Physics, La Trobe Inst. for Molecular Science, La Trobe Univ., Australia. We report on the development and implementation of single-shot hard X-ray/optical cross-correlation at the European X-ray free-electron laser for characterization of timing jitter and drift at megahertz rate.

Th1A.4 • 09:30

Ultrafast Charge Transfer and Electron Delocalization in a Cyanide-Bridged Ru-Ru Dimer Investigated with Femtosecond Transient X-Ray and IR Spectroscopies, Benjamin I. Poulter¹, Elisa Biasin², Chelsea Liekhus-Schmaltz¹, Christopher Arrell³, Sven Augustin³, Claudio Cirelli³, Amy Cordones-Hahn², Philip Johnson³, Gregor Knopp³, Christopher J. Milne³, Roberto Alonso Mori⁴, Dmitry Ozerov³, Marco Reinhard², Jason W. Sandwisch¹, Dimosthenis Sokaras^{5,3}, Ivan Usov³, Robert B. Weakly¹, Niranjan Govind⁶, robert Schoenlein⁴, Munira Khalil¹; ¹Chemistry, Univ. of Washington, USA; ²Stanford Pulse Inst., SLAC National Accelerator Laboratory, USA; ³SwissFEL, Paul Scherrer Inst., Switzerland; ⁴Linac Coherent Light Source, SLAC National Accelerator Laboratory, USA; ⁵Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, USA; ⁶Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, USA. Transient IR and X-Ray spectroscopies were used to investigate excited state delocalization of a mixed valence Ru based donor-bridge-acceptor complex on a femtosecond timescale revealing the role of the electron density on the Ru-CN-Ru fragment.

Th1A.5 • 09:45

Femtosecond Molecular Flattening in [Cu(dmp)₂]⁺ Probed by X-ray Emission Spectroscopy and Solution Scattering, Tae-Kyu Choi¹, Dmitry Khakhulin¹, György Vankó², Zoltán Németh², Jakub Szlachetko³, Makina Yabashi⁴, Thomas Penfold⁵, Wojciech Gawelda^{1,6}, Tetsuo Katayama^{7,4}; ¹European XFEL, Germany; ²Wigner Research Centre for Physics, Hungarian Academy of Sciences, Hungary; ³Inst. of Nuclear Physics, Polish Academy of Sciences, Poland; ⁴RIKEN SPring-8 Center, Japan; ⁵Chemistry-School of Natural and Environmental Sciences, Newcastle Univ., UK; ⁶Faculty of Physics, Adam Mickiewicz Univ., Poland; ⁷Japan Synchrotron Radiation Research Inst., Japan. Femtosecond electronic and nuclear dynamics in [Cu(dmp)₂]⁺ complex upon 550 nm photoexcitation are studied with X-ray emission spectroscopy and X-ray solution scattering, revealing pseudo Jahn-Teller distortion (~410 fs) coupled with coherent vibrational motion.

Room 1

10:30 -- 12:30

Th2A • Excitons

President: Dongho Kim; Yonsei Univ., Korea (the Republic of)

Th2A.1 • 10:30 (Invited)

Coherent Two-dimensional Electronic Spectroscopy with Dual Mode-locked Lasers, Minhaeng Cho¹; ¹Dept. of Chemistry, Korea Univ., Korea (the Republic of). Abstract not available.

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Th2A.2 • 11:00

Molecular annihilation dynamics measured in the perturbative regime of excitation, Pavel Malevich¹, Constantin Heshmatpour^{1,2}, Harald Ceymann³, Maximilian Schreck³, Juergen Hauer^{1,4}; ¹*Technische Universität München, Germany*; ²*Charles Univ., Czechia*; ³*Universität Würzburg, Germany*; ⁴*Vienna Univ. of Technology, Austria*. We present a fully non-collinear 50 kHz shot-to-shot detected two-dimensional electronic spectroscopy setup for directly studying bi-exciton relaxation dynamics via 5th order signals. The measurements report on annihilation timescales at a single, perturbative excitation energy.

Th2A.3 • 11:15

Probing Exciton Transport in Squaraine Polymers Using Fifth-Order Two-Dimensional Spectroscopy, Julian Lüttig¹, Pavel Malý¹, Arthur Turkin², Katja Mayershofer¹, Simon Büttner¹, Christoph Lambert², Tobias Brixner¹; ¹*Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Germany*; ²*Institut für Organische Chemie, Universität Würzburg, Germany*. We use the technique of exciton–exciton-interaction two-dimensional spectroscopy to investigate exciton transport in squaraine copolymers. We reveal the influence of the polymer chain conformation by comparing the exciton dynamics in H-and J-type polymers.

Th2A.4 • 11:30

Packing Morphology-Dependent Singlet Fission in Single Crystal Anthradithiophene Derivatives, Gina Mayonado¹, Kyle Vogt¹, Jonathan Van Schenck¹, Oksana Ostroverkhova¹, Matthew W. Graham¹; ¹*Oregon State Univ., USA*. Single crystal excited state dynamics in functionalized anthradithiophene (ADT) derivatives were compared across four distinct packing morphologies. Using polarization-dependent transient absorption microscopy, morphology-dependent singlet fission was observed in only three of the four ADT derivatives.

Th2A.5 • 11:45

Probing atomic motions accompanying singlet exciton fission in pentacene, Hélène Seiler¹, Marcin Krynski¹, Daniela Zahn¹, Yoav William Windsor¹, Thomas Vasileiadis¹, Sebastian Hammer², Jens Pflaum², Mariana Rossi^{3,1}, Ralph Ernstorfer¹, Heinrich Schwörer³; ¹*Fritz Haber Inst., Germany*; ²*Julius-Maximilians-Universität, Experimental Physics VI, Univ. of Würzburg, Germany*; ³*MPI for Structure and Dynamics of Matter, Germany*. We investigate the structural dynamics accompanying singlet fission in pentacene single crystals with femtosecond electron diffraction. The data reveal incoherent and coherent contributions to the structural dynamics. We discuss the implications for singlet fission properties.

Th2A.6 • 12:00

Ultrafast Spectroscopy Reveals Structural Heterogeneity of Artificial Light-Harvesters, Maxim S. Pshenichnikov¹, Björn Kriete¹; ¹*Zernike Inst. for Advanced Materials, Univ. of Groningen, Netherlands*. Ultrafast 2D spectroscopy is combined with single-object spectroscopy to disentangle the structural heterogeneity of an artificial light-harvester. The dynamically (~50 fs timescale) fluctuating environment governs the system's properties, but not structural variations among different harvesters.

Th2A.7 • 12:15

Charge generation mediated by bound polaron pairs and delocalized charge transfer states in non-fullerene organic photovoltaics, Yin Song¹, Xiao Liu¹, Yongxi Li¹, Hoang Nguyen¹, Rong Duan¹, Kevin J. Kubarych¹, Stephen Forrest¹, Jennifer Ogilvie¹; ¹*Univ. of Michigan, USA*. Using two-dimensional electronic and electronic-vibrational spectroscopies, we find that charge generation via both electron and hole transfer pathways are mediated by bound polaron pairs and delocalized charge-transfer states in non-fullerene organic photovoltaics.

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Room 1

14:00 -- 16:15

Th3A • Chemical Reactions

Presider: Tobias Brixner; Universität Würzburg, Germany

Th3A.1 • 14:00 (Invited)

Ultrafast Dynamics of Molecular Motors Driven by Near-Infrared Light, Nong V. Hoang¹, Lukas Pfeifer², Ben L. Feringa², Maxim S. Pshenichnikov¹; ¹*Zernike Inst. for Advanced Materials, Univ. of Groningen, Netherlands*; ²*Stratingh Inst. for Chemistry, Univ. of Groningen, Netherlands*. Dye-sensitization of a molecular motor allowed its functioning under two-photon near-infrared excitation. Ultrafast transient absorption spectroscopy was used to verify energy transfer from the sensitizer to the motor and motor's subsequent rotation

Th3A.2 • 14:30

Probing Ultrafast Photochemical Reaction at Water Surface by Heterodyne-Detected Vibrational Sum Frequency Generation, Ryoji Kusaka¹, Satoshi Nihonyanagi¹, Tahei Tahara¹; ¹*RIKEN, Japan*. Heterodyne-detected vibrational sum frequency generation (HD-VSFG) is a powerful probe to reveal structure and dynamics at interfaces. We present femtosecond time-resolved vibrational tracking of a photochemical reaction at water surface realized for the first time.

Th3A.3 • 14:45

Vibrational relaxation of water at the air/H₂O interface revealed by time-resolved heterodyne-detected vibrational sum-frequency generation in the OH stretch hot-band region, Woongmo Sung¹, Ken-ichi Inoue¹, Satoshi Nihonyanagi^{1,2}, Tahei Tahara^{1,2}; ¹*Molecular Spectroscopy Laboratory, RIKEN, Japan*; ²*RIKEN Center for Advanced Photonics (RAP), RIKEN, Japan*. Vibrational relaxation (T₁) time of hydrogen-bonded OH of interfacial water was determined by TR-HD-VSFG spectroscopy to be 250 - 400 fs contrary to the previous report, while free-OH stretch shows noticeably slow (~1 ps) T₁.

Th3A.4 • 15:00

Manipulating Ultrafast Conical Intersection Dynamics by Optical Cavities, Bing Gu¹, Shaul Mukamel¹; ¹*Chemistry, Physics and Astronomy, Univ. of California, Irvine, USA*. Optical cavities provide a novel means to manipulate photochemical processes. Real-time dynamical/spectroscopic simulations of pyrazine molecules strongly coupled to a cavity mode show that the polariton effects can influence significantly the conical intersection dynamics.

Th3A.5 • 15:15

Probing Delayed C–I Bond Fission in the UV Photochemistry of 2-Iodothiophene with Core-to-Valence Transient Absorption Spectroscopy, Benjamin W. Toulson¹, Mario Borgwardt¹, Davide Faccialà², Daniel M Neumark^{3,1}, Stephen R Leone^{3,1}, Oliver Gessner¹; ¹*Lawrence Berkeley National Laboratory, USA*; ²*Istituto di Fotonica e Nanotecnologie—CNR, Italy*; ³*Univ. of California, Berkeley, USA*. The UV photodissociation dynamics of 2-iodothiophene are monitored by an XUV probe pulse that promotes iodine 4d core-to-valence transitions. Absorption changes from molecular iodine species conclusively show that dissociation requires up to ~1 picosecond. © 2020 The Authors

Th3A.7 • 15:30

Ultrafast Conical Intersection Dynamics Monitored Through Electronic Coherences by Stimulated X-Ray Raman Signals, Shaul Mukamel¹, Thomas Schnappinger², Regina de Vivie-Riedle², Daniel Keefer¹; ¹*Chemistry and Physics and Astronomy, Univ. of California, Irvine, USA*; ²*Chemie, Ludwig-Maximilians-Universität München, Germany*. Coherences at conical intersections are probed by X-Ray stimulated Raman signals. Contrary to the common picture of short femtosecond and precisely timed non-adiabatic passages, the distinctly visible coherence signature survives for a much longer time.

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Th3A.6 • 15:45

Extreme-ultraviolet time-resolved photoelectron spectroscopy of the photoisomerisation dynamics of cis-stilbene in the gas and liquid phases, Chuncheng Wang¹, Max Waters¹, pengju zhang¹, Tran Trung Luu¹, Vit Svoboda¹, Conall Perry¹, Zhong Yin¹, Hans Jakob Woerner¹; ¹ETH Zurich, Switzerland. Measuring time-resolved photoelectron spectra of liquids, and achieving photon energies to probe electronic ground states is challenging. We present gas- and liquid-phase XUV-TRPES of cis-stilbene, providing new insight into this prototype of molecular photoisomerisation dynamics.

Th3A.8 • 16:00

Relaxation and Coherence Transfer in Dual-Mode Vibrational Polaritons Tracked with 2DIR, Rong Duan¹, Kevin J. Kubarych¹, Josephy Mastron¹, Yin Song¹; ¹Univ. of Michigan, USA. Strong coupling between microcavities and molecular vibrations may enable direct, external control over chemical dynamics. We use ultrafast 2DIR to probe a unique system with two vibrational modes strongly coupled to two distinct cavity modes.

Room 2

14:00 -- 16:00

Th3B • High-Harmonic Generation and Applications

Presider: Katsumi Midorikawa; RIKEN, Japan

Th3B.1 • 14:00

Attosecond spectral singularities in solid-state high-harmonic generation, Ayelet J. Uzan¹, Gal Orenstein¹, Barry D. Bruner¹, Álvaro Jiménez-Galán², Chris McDonald³, Rui E.F. Silva⁴, Nikolai Klimkin^{5,6}, Valerie Blanchet⁷, Talya Arusi-Parpar^{1,8}, Michael Krüger^{1,9}, Alexey Rubtsov^{5,6}, Olga Smirnova^{2,10}, Misha Ivanov^{2,11}, Binghai Yan¹², Thomas Brabec³, Nirit Dudovich¹; ¹Dept. of Physics of Complex Systems, Weizmann Inst. of Science, Israel; ²Max-Born-Institut, Germany; ³Dept. of Physics, Univ. of Ottawa, Canada; ⁴Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, Spain; ⁵Russian Quantum Center, Russia; ⁶Dept. of Physics, Lomonosov Moscow State Univ., Russia; ⁷CNRS, CEA, CELIA, Universite de Bordeaux, France; ⁸Applied Physics Dept., NRC Soreq, Israel; ⁹Dept. of Physics and Solid State Inst., Technion, Israel; ¹⁰Technische Universität Berlin, Germany; ¹¹Imperial College London, UK; ¹²Dept. of Condensed Matter Physics, Weizmann Inst. of Science, Israel. Using high-harmonic generation spectroscopy, we reveal the underlying attosecond dynamics in multi-band solid-state systems. We identify the mapping of spectral caustics into the high-harmonic spectrum, and probe the structure of multiple unpopulated high conduction bands.

Th3B.2 • 14:15

Electron-vibrational coupling dynamics in SF₆, Patrick D. Rupprecht¹, Lennart Aufleger¹, Alexander Magunia¹, Simon Heinze², Thomas Ding¹, Marc Rebholz¹, Stefano Amberg¹, Nikola Mollov¹, Felix Henrich¹, Maurits W. Haverkort², Christian Ott¹, Thomas Pfeifer¹; ¹Max Planck Inst. for Nuclear Physics, Germany; ²Inst. for theoretical physics, Heidelberg Univ., Germany. We report on soft x-ray transient absorption spectroscopy in SF₆. The influences of strong SWIR fields and of impulsive stimulated Raman scattering initiated ν_1 vibrational breathing mode dynamics on the $6a_{1g}(S\ 2p_{1/2, 3/2})^{-1}$ resonance are investigated.

Th3B.3 • 14:30

Detecting electronic coherences by the multidimensional HHG spectroscopy, Shicheng Jiang¹, Markus Kowalewski², Konstantin Dorfman¹; ¹East China Normal Univ., China; ²Dept. of physics, Univ. of Stockholm, Sweden. We propose an all-optical method based on pump-probe HHG to detect electronic coherence. Based on a new developed semi-perturbative approach, coherence between bound states is observed in Fourier transformed harmonic spectra using noncollinear geometry setup

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Th3B.4 • 14:45

Symmetry of Molecular Rydberg States Revealed by XUV Transient Absorption Spectroscopy, Peng Peng¹, Claude Marceau¹, Marius Hervé¹, Paul Corkum¹, Andrei Naumov¹, David Villeneuve¹; ¹*National Research Council of Canada, Canada*. We studied Rydberg states of N₂ and O₂ by XUV transient absorption spectroscopy. We were able to determine the polarization direction of the electronic transitions, and hence identify the symmetry of the final states.

Th3B.5 • 15:00

High-order Harmonic Generation in Femtosecond Laser Micromachined Devices for Ultrafast X-ray Spectroscopy, Anna Gabriella Ciriolo¹, Rebeca Martínez Vázquez¹, Valer Tosa², Aldo Frezzotti³, Eugenio L. Cinquanta¹, Gabriele Crippa⁴, Davide Faccialà¹, Michele Devetta¹, Roberto Osellame⁴, Caterina Vozzi¹, Salvatore Stagira⁴; ¹*CNR - Istituto di Fotonica e Nanotecnologie, Italy*; ²*National Inst. for R&D of Isotopic and Molecular Technologies, Romania*; ³*Dept. of Aerospace Science and Technology, Politecnico di Milano, Italy*; ⁴*Dept. of Physics, Politecnico di Milano, Italy*. We demonstrate efficient high-order harmonic generation in fused-silica chips fabricated by femtosecond laser micromachining. This work provides a route toward the miniaturization of HHG beamlines and the implementation of X-ray spectroscopy with attosecond temporal resolution.

Th3B.6 • 15:15

Role of intraband dynamics on circularly polarized high-harmonic generation from solids, Nicolai Klemke^{1,2}, Nicolas Tancogne-Dejean^{1,3}, Angel Rubio^{1,3}, Franz Kärtner^{1,2}, Oliver D. Mücke^{1,4}; ¹*DESY, Germany*; ²*Physics Dept., Univ. of Hamburg, Germany*; ³*Max Planck Inst. for the Structure and Dynamics of Matter, Germany*; ⁴*The Hamburg Centre for Ultrafast Imaging, Germany*. We perform single-particle intraband-only calculations to study the origin of circularly polarized higher-order harmonics from solids. The simulation results are compared to new experimental data on high-harmonic generation in zinc sulfide.

Th3B.7 • 15:30

Tracking Ultrafast Solid-State Dynamics in VO₂ Using High Harmonic Spectroscopy, Mina Bionta¹, Elissa Haddad¹, Adrien Leblanc¹, Vincent Gruson^{1,2}, Philippe Lassonde¹, Heide Ibrahim¹, Jérémie Chaillou¹, Nicolas Émond¹, Martin R. Otto³, Bradley J. Siwick³, Mohamed Chaker¹, François Légaré¹; ¹*INRS-EMT, Canada*; ²*The Ohio State Univ., USA*; ³*McGill Univ., Canada*. We extend time-resolved high harmonic spectroscopy to solid-state systems by investigating the dynamics of the insulator-to-metal phase transition in the strongly correlated material, VO₂, revealing all electronic states involved.

Th3B.8 • 15:45

Phase matched high-harmonic generation in macroscopic single-layer graphene, Roberto Boyero-García¹, Óscar Zurrón-Cifuentes¹, Luis Plaja¹, Carlos Hernandez Garcia¹; ¹*Universidad de Salamanca, Spain*. We study the macroscopic build-up of the high-harmonic signal in single-layer graphene. Our results show that the emission is dominated by a phase-matched ring.