

# Poster list

## Poster Session 1: Tuesday, June 13

## Theme 1 - Intra- and intermolecular vibrational excitations in (ionic) liquids, polymers and hydrogels

- P1-1 Effects of Reorientation Induced Spectral Diffusion in Ionic Liquids **Sean Garrett-Roe** (University of Pittsburgh, Pittsburgh, USA)
- P1-2 Effect of Ca<sup>2+</sup> Carboxylate Interaction on the Amide Bond of Zwitterionic Alanylalanine **Carola Krevert** (Max Planck Institute for Polymer Research, Mainz, Germany)
- P1-3 Density Functional Modelling of Conducting Polymer Backbone Torsions to Predict Charge Conductivity Measured by Time-Resolved Terahertz Spectroscopy **Edwin Heilweil** (National Institute of Standards & Technology, Gaithersburg, USA)
- P1-4 2D-IR of SCN-labeled Carbohydrates **Philip Gasse** (Universität Potsdam, Potsdam, Germany)
- P1-5 2D Raman THz Spectroscopy of Ionic Liquids Saurabh Shukla (University of Zurich, Zurich, Switzerland)
- P1-6 Vibrational Dynamics of Poly-(*N*,*N*-diethylacrylamide) and Its Monomer Unit in Water Investigated by 2D-IR Spectroscopy and MD Simulations **Yuki Fujii** (Kobe University, Kobe, Japan)
- P1-7 Monitoring Chemical Exchange Dynamics of Highly Concentrated Salt Solutions Using 2D-IR Spectroscopy

Vivian Crum (University of Michigan, Ann Arbor, MI, USA)

## Theme 2 - Phonon and vibrational dynamics in solids, nonlinear 'phononics'

- P1-8 THz Pump Activation of Anharmonic Coupling in CdWO4 **Megan Nielson** (Brigham Young University, Provo, Utah, USA)
- P1-9 Vibrationally Promoted Electronic Resonance Spectroscopy for Probing Vibronic Coupling in Hybrid Perovskites

Navendu Mondal (Imperial College London, London, UK)

P1-10 2D Raman-THz Spectroscopy of Beta Barium Borate

Seyyed Jabbar Mousavi (University of Zurich, Zurich, Switzerland)

### Theme 3 - Vibrations in nanoparticles (quantum dots) and metal complexes

- P1-11 Excited State Dynamics of Sterically Different Carboxylate Ligands on Inp Nanoclusters Casey Bisted (University of Washington, Seattle, USA)
- P1-12 Vibrational Response of Activated C-D Bonds in a Chloroform-Platinum(II) Complex **Jia Zhang** (Max Born Institute for Nonlinear Optics and Short Pulse Spectroscopy, Berlin, Germany)

P1-13 Ir-Ir Bond Formation in Excited Iridium Complex Observed by FSRS Spectroscopy **Miroslav Kloz** (The Extreme Light Infrastructure ERIC, Dolní Břežany, Czech Republic)

### Theme 4 - Vibrations at surfaces and membranes

P1-14 Time-Resolved Vibrational Sum-Frequency Generation for Opto-Acoustic Interferometry to Investigate the Interface of Aqueous Electrolyte Solutions

Alessandro Greco (Max Planck Institute For Polymer Research, Mainz, Germany)

- P1-15 Development and Characterization of Electrodes for 2D IR Spectroelectrochemistry **Melissa Bodine** (University of Chicago, Chicago, USA)
- P1-16 Orientational Coupling of Molecules at Interfaces Revealed by Two-Dimensional Electronic-Vibrational Sum Frequency Generation (2D-EVSFG)

  Yi Rao (Utah State University, Logan, USA)
- P1-17 Protein Structure at Nanoparticle Interfaces Probed by Sum Frequency Scattering **Thaddeus Golbek** (Aarhus University, Aarhus, Denmark)

### Theme 5 - Biophysical processes (proteins, DNA/RNA) and molecular motors

- P1-18 Electron-Vibration-Vibration 2DIR Spectroscopy to Study G-Quadruplex DNA Formation A. Larasati Soenarjo (Imperial College London, London, UK)
- P1-19 Probing Local Changes to  $\alpha$ -Helical Structures with 2D IR Spectroscopy and Isotope Labeling **Alisa Shmidt** (Vanderbilt University, Nashville, USA)
- P1-20 pH Dependent IR Spectroscopy to Study Intrinsically Disordered Peptides **Anna Zehle** (University of Potsdam, Potsdam, Germany)
- P1-21 Transient 2D IR Spectroscopy Reveals Vibrational Couplings in the Cyanobacteriochrome SIr-G3 **David Buhrke** (Humboldt University, Berlin, Germany)
- P1-22 Non-Equivalence of  $\alpha$  and  $\beta$  Subunits of Human Hemoglobin in Conformational Relaxation and Ligand Rebinding

Igor Sazanovich (Harwell Science and Innovation Campus, Harwell, UK)

P1-23 The Molecular Mechanism of Light-induced Bond Formation and Breakage in the Cyanobacteriochrome TePixJ

Jeannette Ruf (University of Zurich, Zurich, Switzerland)

- P1-24 External Manipulation of the Absorption Spectrum of a Photoreceptor Luuk van Wilderen (Goethe University Frankfurt, Frankfurt am Main, Germany)
- P1-25 A Detailed View on the Retinal Dynamics of the Light-Driven Sodium Pump KR2 **Marvin Asido** (Goethe University Frankfurt, Frankfurt am Main, Germany)
- P1-26 Common Structural Mechanism of Inward Proton Transport in Schizorhodopsins **Taito Urui** (Osaka University, Toyonaka, Osaka, Japan)
- P1-27 Investigating the Time Scales of Protein Interaction of MCL-1 and its Binding Partners via Time-Resolved IR Spectroscopy **Philipp Heckmeier** (University of Zurich, Zurich, Switzerland)
- P1-28 Biofluid Protein Analysis with 2D-IR Spectroscopy; Pre-Processing Steps and Applications towards a Protein Library

Neil Hunt (University of Strathclyde, Glasgow, UK)

### Theme 6 - (Plasmonic) photochemistry, photocatalysis, and electrochemistry

- P1-29 Molecular Insights into Tailored [Ru(Bpy)<sub>3</sub>]<sup>2+</sup> Photosensitizers in Aqueous Surfactant Environments **Christoph Kaiser** (AMOLF, Amsterdam, the Netherlands)
- P1-30 Two-Dimensional Electronic Spectroscopy Reveals Excited State Displacements **Giovanni Bressan** (UEA, Norwich, United Kingdom)
- P1-31 Switch? Isomerization of Singly Reduced RePON and ReAsON Tricarbonyl Complexes **Kerstin Oppelt** (University of Zürich, Zürich, Switzerland)
- P1-32 Oxidation State Dependent Vibrational Dynamics of TCNQ Investigated by 2DIR Spectroelectrochemistry

Ranadeb Ball (University of Pennsylvania, Philadelphia, USA)

P1-33 Can TRVS Guide Us to Make Next Generation Efficient LED Devices? **Pratyush Ghosh** (University of Cambridge, Cambridge, UK)

### Theme 7 - Novel (nonlinear) spectroscopic phenomena and techniques

P1-34 A 2D-IR Setup for High Spectral Resolution **Armel Jouan** (ISMO, CNRS, Université Paris-Saclay, Orsay, France)

P1-35 Vibrational Coherences in Broadband 2D Electronic Spectroscopy: Spectral Filtering vs. Excited State Displacement.

Dale Green (University of East Anglia, Norwich, UK)

P1-36 Tracking Molecular Vibrational Dynamics in Individual Plasmonic Nanocavities through Coherent and Incoherent Raman Scattering

Lukas Jakob (University of Cambridge, Cambridge, UK)

- P1-37 Toward Solution-Phase Single-Molecule Chemistry with Fluorescence-Encoded Infrared Spectroscopy **Seung Yeon Lee (**The University of Chicago, Chicago, USA)
- P1-38 Silicon Metasurface-enhanced Ultrafast Vibrational Spectroscopy **Soheila Kharratian** (University of York, York, UK)
- P1-39 Scattering Removal of 2D IR Spectra Using Mechanical Methods and Their Application to Studying Various Types of Samples

Yung Sam Kim (Ulsan National Institute of Science and Technology, Ulsan, Republic of Korea)

P1-40 Field-Resolved Infrared Detection at Kilohertz Rates **Daniel Gerz** (Leibniz Institute of Photonic Technology, Jena, Germany)

P1-41 Exploring Vibronic Couplings by Ir-Pump White-Light-Probe 2d Spectroscopy **Hafiz Muhammad Ahmed Masood** (Goethe University, Frankfurt am Main, Germany)

# Poster Session 2: Wednesday, June 14

### Theme 1 - Intra- and intermolecular vibrational excitations in (ionic) liquids, polymers and hydrogels

P2-1 Probing Amide I – Water Vibrational Coupling in Hydrated Peptide Films with Two-Color Two-Dimensional Infrared Spectroscopy

Fani Madzharova (Aarhus University, Aarhus, Denmark)

P2-2 Hydrogen Bonds under Stress: Strain-Induced Structural Changes in Polyurethane Revealed by Rheological Two-Dimensional Infrared Spectroscopy

Giulia Giubertoni (University of Amsterdam, Amsterdam, the Netherlands)

P2-3 On the Origin of the Hydrogen-Bond Asymmetry of Water: Anti-correlated Hydrogen-Bonds of D2O evidenced by 2D-IR spectroscopy

Lucas Gunkel (Max Planck Institute for Polymer Research, Mainz, Germany)

P2-4 From Networked to Isolated: Water Hydrogen Bonds and Vibrational Relaxation in Electrolytes from the Dilute to the Superconcentrated Regime

Nicholas Lewis (University of Chicago, Chicago, USA)

P2-5 Exploring Reorientation Induced Spectral Diffusion of Nitrous Oxide in Alkylmethylimidazolium Ionic Liquids using 2D-IR and Calculated Spectra

Tyler Parrack (University of Pittsburgh, Pittsburgh, USA)

P2-6 Two-Dimensional Terahertz-Infrared-Visible Spectroscopy of Molecular C-H Groups **Pankaj Seliya** (Max Planck Institute for Polymer Research, Mainz, Germany)

## Theme 2 - Phonon and vibrational dynamics in solids, nonlinear 'phononics'

P2-7 Controlling the Electro-Optic Response of a Semiconducting Perovskite Coupled to a Phonon-Resonant Cavity

Lucia Di Virgilio (Max Planck for Polymer Research, Mainz, Germany)

P2-8 Photoluminescence Vibrationally Promoted Electronic Resonance Spectroscopy of High Quality Rubrene Single Crystals

Dmitrii Maslennikov (Imperial College London, London, UK)

P2-9 Direct Probing of Vibrational Interactions in UiO-66 Polycrystalline Membranes with Femtosecond Two-Dimensional Infrared Spectroscopy

Alexander A. Korotkevich (AMOLF, Amsterdam, the Netherlands)

## Theme 3 – Vibrations in nanoparticles (quantum dots) and metal complexes

P2-10 Ultrafast IR Spectroscopy of [CpFe(CN)<sub>2</sub>(CO)]K as a Probe of Structure, Dynamics & Solvation of the [NiFe] Hydrogenase Active Site

Barbara Procacci (University of York, York, UK)

- P2-11 Two-Dimensional Vibrational-Electronic Spectroscopy of a Charge-Delocalized Ruthenium Dimer Caroline Loe (University of Washington, Seattle, USA)
- P2-12 Probing The Stabilization of Formyl Intermediates by Lewis Acids in Catalytic CO<sub>2</sub> Reduction with Ultrafast 2DIR Spectroscopy

James Shipp (University of Pennsylvania, Philadelphia, USA)

P2-13 Ligand Exchange Kinetics in the First Reduction Step of CO<sub>2</sub> Catalyst: Trans(Cl)-Ru[Dimethyl-Bipyridine](CO)<sub>2</sub>Cl<sub>2</sub>

Sergio Aranda Ruiz and Luka Tatarashvili (University of Zurich, Zurich, Switzerland)

### Theme 4 - Vibrations at surfaces and membranes

P2-14 Cholesterol Decreases the Orientational Bias of Water Molecules at the Surface of a Model Cell Membrane

Hanna Orlikowska-Rzeznik (Poznan University of Technology, Poznan, Poland)

P2-15 Surface-Enhanced 2D IR Spectroscopy to Investigate Structural Dynamics of Voltage-Gated Ion Channels

Kiera Wilhelm (University of Wisconsin-Madison, Madison, USA)

P2-16 Time-resolved in situ Electrochemical SFG and SERS Studies of the Electrode Induction Effects on the Dynamics and Reactivities of Adsorbed Molecules

Tianquan Lian (Emory University, Atltanta, Georgia, USA)

### Theme 5 - Biophysical processes (proteins, DNA/RNA) and molecular motors

- P2-17 Expanding the Horizon of Protein Vibrational Energy Transfer with Novel Energy Donors Carolin Feid (Goethe University, Frankfurt/Main, Germany)
- P2-18 Analysis of TRIR Data for Vitamin B12 Derivatives and the B12-dependent Photoreceptor, CarH. **Emma Wall** (The University of Manchester, Manchester, UK)
- P2-19 Study of the Transient hIAPP Oligomers by Mutagenesis and 2D-IR **Harrison Esterly** (University of Wisconsin Madison, Madison, USA)
- P2-20  $\mu$ s to Minute Protein Dynamics in Sensory Rhodopsin and Bacteriorhodopsin Studied by Single-shot Mid-infrared Dual-comb Spectroscopy

Jakob Hayden (IRsweep AG, Staefa, Switzerland)

- P2-21 Retinal Chromophore Twisting Regulates Channel Opening and Closing of Channelrhodopsin C1C2 **Keisei Shibata** (The University of Tokyo, Kashiwa, Japan)
- P2-22 How Anyone Can Predict Infrared Spectra of Complex (Biological) Systems **Kim van Adrichem** (University of Groningen, Groningen, the Netherlands)
- P2-23 Dual-Comb-IR-Spectroscopy as a New Method in Temperature-Jump Experiments to Study Polyq Peptide Dynamics

Lorenz Mattes (Universität Konstanz, Konstanz, Germany)

P2-24 Photoinduced Electron Transfer from a NAD(P)H Analog to Oxidized FMN in an Ene-Reductase Flavoenzyme

Magnus Speirs (Manchester Institute of Biotechnology, Manchester, UK)

P2-25 Lipid Dynamics During the Photocycle of Bacteriorhodopsin Studied by Time-Resolved QCL Spectroscopy

Paul Stritt (University of Konstanz, Konstanz, Germany)

- P2-26 Two-Dimensional Infrared Raman Spectroscopy Simulations of Proteins **Thomas La Cour Jansen** (University of Groningen, Groningen, the Netherlands)
- P2-27 ATP Accelerates Alpha-Synuclein Aggregation by Dissolving Off-Pathway Oligomers **Steven Roeters** (Aarhus University, Aarhus, Denmark)

### Theme 6 - (Plasmonic) photochemistry, photocatalysis, and electrochemistry

- P2-28 Vibronic Coherences in Light Harvesting Nanotubes: Unravelling the Role of Dark States **Andrea Lapini** (Università di Parma & LENS, Parma, Italy)
- P2-29 Singlet Fission in Pentacene Dimers: Coherent 2D Spectroscopy View **Haoqing Ning** (Imperial College London, London, UK)

- P2-30 Vibrational Energy Transfer between Photoexcited  $\alpha$ -Terthiophene and Metal Nanoparticles Probed with Picosecond Time-resolved Raman Spectroscopy **Koichi Iwata** (Gakushuin University, Tokyo, Japan)
- P2-31 Observing a Ti-based Photoredox Catalyst in-situ with Time-resolved IR-spectroscopy **Peter Vöhringer** (University of Bonn, Bonn, Germany)
- P2-32 Acceleration by Deprotonation: How the pH Affects Reaction Dynamics of a Photolabile Protection Group

Yannik Pfeifer (University of Potsdam, Potsdam, Germany)

### Theme 7 – Novel (nonlinear) spectroscopic phenomena and techniques

- P2-33 Coherence Transfer and Destructive Interference in Two-dimensional Coherence Maps **Amitev Sahu** (Indian Institute of Science, Bangalore, India)
- P2-34 VIPER Labels for Measuring IR Spectral Diffusion with Electronic Lifetimes **Lara Denninger** (Goethe University, Frankfurt am Main, Germany)
- P2-35 Time-Resolved Vibrational Spectroscopy Using Chirped-Pulse Upconversion of Mid-Infrared Pulses Generated by iDFG with a 250-kHz Yb Fiber Laser **Mindaugas Jonusas** (Ecole Polytechnique, Palaiseau, France)
- P2-36 Real-time Atomic Movie of Chemical Bond Formation Using Ultrafast Electron Diffraction: A Proof of Concept for Reduction in Dimensionality in Chemistry

  Nita Ghosh (University of Toronto, Toronto, Canada)
- P2-37 Displaced Sagnac Interferometer for Passive Phase-Stabilization in 2D IR Spectroscopy **Sofie Mika** (University of Vienna, Vienna, Austria)
- P2-38 Photoenhancement of Vibration Intensity of Probes **Wenkai Zhang** (Beijing Normal University, Beijing, China)
- P2-39 Development of a 100 kHz 2D SFG Spectrometer **Ashley Stingel** (Ruhr University Bochum, Bochum, Germany)