

Poster Session 1 - Tuesday, June 15, 9:00 - 11:00 am (Eastern Daylight Time)

The poster session will take place on Gather (links will be sent to all registered participants)

1	Klaas Wynne	University of Glasgow	School of Chemistry	United Kingdom of Great Britain and Northern Ireland	Characterization of locally ordered structures from the glass into the liquid	Phenomena from vitrification to crystal nucleation are governed by locally ordered structures, which are ephemeral, do not have distinct spectral features, and are therefore critically important but unobservable. Here we show that molecular symmetry in femtosecond optical Kerr-effect spectroscopy can be used to isolate the signal from such structures.
2	Ricardo Fernández-Terán	University of Zurich	Department of Chemistry	United Kingdom of Great Britain and Northern Ireland	A Closer Look into the Distance Dependence of Vibrational Energy Transfer on Surfaces Using 2D IR Spectroscopy	Using 2D-IR spectroscopy and simulations, we show that vibrational energy transfer becomes a collective phenomenon on the surface. We believe this work sets the stage for establishing VET in isotope-labelled molecules as a valuable tool to investigate, characterize and quantify the morphology of surface-bound catalysts, photosensitisers and mixtures of both.
4	Mark Stitch	University College Dublin	School of Chemistry	Ireland	Enantiomeric selective binding of a Ruthenium Polypyridyl complex to a quadruplex forming DNA sequence	We are interested in resolving the role of DNA structures in disease. TRIR is used to identify the quadruplex binding sites of photo-excited Ru(II)nitrilepolypyridyl enantiomers due to nucleobase perturbation. The linear frequency response of the transient nitrile vibration to H-bonding and solvent polarity further reports on the quadruplex binding environment.

5	Ravi Kumar Venkatraman	University of Sheffield	Department of Chemistry	United Kingdom of Great Britain and Northern Ireland	Ultrafast Dynamics at the Lipid–Water Interface: DMSO Modulates H-Bond Lifetimes.	Dimethyl sulfoxide (DMSO) is widely used as a cryoprotectant, and its interaction at the water-lipid interface remains contentious. Herein, we report that the addition of DMSO leads to a non-monotonic behavior of the water dynamics at the lipid membrane interface using 2D IR spectroscopy and MD simulations.
6	Danny Shaw	University of York	Chemistry	United Kingdom of Great Britain and Northern Ireland	Ultrafast 2D-IR assessment of the real-time conformational dynamics and binding of an anti-psoriasis drug target	Ultrafast 2D-IR spectroscopy is used to investigate the structural dynamics of three isoforms of a series of cytokine proteins that are associated with unwanted inflammatory responses within the human body. Differences in protein flexibility correlate with ligand binding affinities, providing valuable insight into the ongoing search for suitable therapeutics.
7	Barbara Procacci	University of York	Chemistry	United Kingdom of Great Britain and Northern Ireland	Sensing of bacterial spores with 2D-IR Spectroscopy	Application of 2D-IR spectroscopy for classification of bacterial spores is evaluated. Spectra of dry and liquid films of two species of Bacillus spore show signatures of the calcium dipicolinate biomarker for sporulation. Distinctive amide I off-diagonal peaks permitted species differentiation. Amide I vibrational lifetimes were compared with solution phase data.
8	Solomon Wrathall	University of York	Chemistry	United Kingdom of Great Britain and Northern Ireland	Ultrafast IR spectroscopy of EchHyd-1 hydrogenase	Ultrafast 2D-IR spectroscopy has been used to study the vibrational dynamics of the active site of a [NiFe]-hydrogenase enzyme. Vibrational lifetimes and energy transfer processes involving carbonyl and cyanide ligands are compared with solution phase models to identify the role of the protein matrix in determining the active site environment.
9	C. Peter Howe	University of York	Chemistry	United Kingdom of Great Britain and Northern Ireland	Comparison of RNA and DNA Tetraloop Melting Dynamics using Ultrafast T-jump IR Spectroscopy	Ultrafast time-resolved multiple-probe infrared spectroscopy with a nanosecond temperature jump was used to investigate the melting dynamics of DNA and RNA 12mer T/UACG tetraloops over the 1 ns – 4 ms time range. The extracted dynamics were used to determine base-specific contributions to the stability of the hairpins.

10	Luuk van Wilderen	Johann Wolfgang Goethe-Universität	Institut für Biophysik	Germany	Femtosecond to millisecond dynamics of photoactive yellow protein revealed by the vibrational label –SCN	The reversible photocycle of the photoreceptor photoactive yellow protein (PYP) comprises partial unfolding of its secondary structure. Insertion of the vibrational label thiocyanate (SCN) at key positions allows the extraction of detailed local information, revealing which parts of the protein undergo structural changes and at what time after photon absorption.
11	Kim van Adrichem	University of Groningen	Zernike Institute for Advanced Materials	Netherlands	AIM: a new tool for modelling of 2D-IR spectra of proteins	2D-IR spectroscopy can provide valuable insight in protein structure, but spectra can be hard to interpret. AIM is a new tool for modelling amide I FTIR and 2D-IR spectra using molecular dynamics simulations as a starting point. It will be freely available and support a wide range of MD software.
12	Julien Réhault	University Bern	Department of Chemistry, Biochemistry and Pharmaceutical Sciences (DCBP)	Switzerland	High resolution phase-sensitive sum frequency generation spectroscopy by time-domain ptychography	We demonstrate that time-domain ptychography, when applied to a set of broadband vibrational sum frequency spectra (BB-vSFG), reconstructs amplitude and phase of the vibrational free induction decay from an interfacial sample with a resolution that is independent of the up-converting pulse bandwidth and spectrometer resolution.
13	Sarah von Berg	Goethe University Frankfurt	Institute of Biophysics	Germany	Temperature dependent low-frequency modes in the active site of Carbonic Anhydrase II probed by 2D-IR spectroscopy	2D-IR spectral diffusion measurements of an IR label in the active site of carbonic anhydrase II resolve a low-frequency mode at 1 THz. Its frequency is viscosity dependent and correlates with the dynamics of the buffer, indicative of slaving. The frequency is lowered with increasing temperature as the protein's potential softens.
14	Seyyed Jabbar Mousavi	University of Zurich	Department of Chemistry	Switzerland	2D Raman-THz Spectroscopy of Binary CHBr3-MeOH Solvent Mixture	Two-dimensional Raman-terahertz spectroscopy is used to measure the interactions between two solvents pair in the binary CHBr3-MeOH mixture. The appearance of a new cross peak in the 2D spectrum of XMeOH = 0.3 indicates a coupling to a new set of low-frequency modes formed due to the hydrogen bond interactions.

15	Marta	Duchi	University of Zurich	Chemistry	Switzerland	2D-Raman-THz spectroscopy implemented with single-shot THz detection	Abstract: We present a novel Raman-terahertz setup with single-shot THz detection to reduce the acquisition time from many days to a few hours. The combination of finely made echelons, high repetition rate laser, fast scanning and 100 kHz camera allows a significant improvement in signal-to-noise. Liquid bromoform test measurements are reported.
16	Jan Gerrit	Löffler	Goethe University Frankfurt	Institute of Biophysics	Germany	Different Probes for a Common Purpose: Detection of Ultrafast Vibrational Energy Transfer in Proteins	Site selective measurements are crucial for understanding vibrational energy transfer (VET) in proteins and peptides. A powerful approach is ultrafast Vis-pump/IR-probe spectroscopy of flexibly positioned non-canonical amino acids (ncAAs). Here we investigate the advantages and drawbacks of five ncAA infrared labels as VET-probes in peptides and proteins.
17	Lara	Denninger	Goethe University Frankfurt/Main, Germany	Institute of Biophysics	Germany	Photochemistry of a Cyclopropanone-Caged Click Reagent	Click reagents caged by a cyclopropanone group release carbon monoxide upon UV excitation. This photochemical activation allows spatiotemporal control of the click labelling strategy. Here, we investigate the photoreaction of PhotoDIBO-OH by UV-pump IR-probe spectroscopy to resolve the lifetimes of the different reaction paths.
18	Jeannette	Ruf	University of Zurich	Department of Chemistry	Switzerland	From Picoseconds to Milliseconds: Unravelling the Dynamics of Protein Response by Transient IR Spectroscopy	Transient IR spectroscopy is a powerful method to explore the non-equilibrium dynamics of photoswitchable protein systems. Recently, we investigated the time-resolved protein response of a cyanobacterial GAF domain, a PDZ3 domain, and the RNase S complex. We analyzed the complex protein response with global fitting and lifetime analysis.
19	Kerstin	Oppelt	University of Zurich	Department of Chemistry	Switzerland	Flexible to rigid: IR spectroscopic investigation of a rhenium-tricarbonyl-complex at a buried interface	The solid-liquid interface of a rhenium-tricarbonyl complex (ReP-Cl) embedded in ALD-deposited ZrO ₂ revealed correlations between the oxide layer height and the spectroscopic response in (time resolved) IR spectroscopy. We observed a transition of the molecular environment from flexible to rigid, limitations to ligand exchange and excited state quenching.

20	Hendrik	Brunst	Goethe University Frankfurt	Physics	Germany	Infrared Labels for Expanding 2D-IR Spectroscopy Beyond the Vibrational Lifetime	Measuring frequency fluctuations of IR labels by 2D-IR spectroscopy is limited by the vibrational lifetime (ps). VIPER-2D-IR spectroscopy overcomes this limitation by transferring vibrationally excited population to an electronically excited state. With a VIPER label the timescale for 2D-IR spectroscopy can be expanded to ns (singlet labels) or μ microseconds (triplet labels).
21	Georg	Wille	Goethe University Frankfurt/Main	Physics Dept.	Germany	SH - it happens	Cysteine S-H bonds have a spectroscopically convenient stretching frequency of ~ 2550 cm ⁻¹ . We employ Fourier-Transform 1D- and 2D-IR spectroscopy to identify cysteines with distinct H-bonds in pyruvate oxidase. Large anharmonicity and long life-time allow monitoring ultrafast spectral diffusion separately for both fundamental and overtone transition.
22	Erhan	Deniz	Goethe University Frankfurt	Institute of Biophysics	Germany	Through Bonds or Contacts? Mapping Protein Vibrational Energy Transfer Using Non-canonical Amino Acids	To disentangle backbone and contact pathways of vibrational energy transfer (VET), we equipped a tryptophan zipper beta-hairpin with a VET injector and a VET sensor at various positions. Femtosecond pump probe experiments together with MD simulations reveal backbone vs. contact transport efficiencies with H-bonds as dominant VET pathways.
23	Hafiz	Masood	Goethe University, Frankfurt	Institute of Biophysics	Germany	Vibrationally Promoted Electronic Resonance (VIPER) Spectroscopy Using Two-Photon Excitation	VIPER allows to carry out electronic excitation with the selectivity of IR spectroscopy for applications in photochemistry and time resolved spectroscopy. Here, we demonstrate two-photon VIPER spectroscopy, which opens the near infrared window for applications on biological samples. We discuss the results in comparison with the recently developed theoretical description.

24	Florian	Eigenmann	IRSWEEP	spectroscopy	Switzerland	Non-repetitive protein dynamics on microsecond to second time-scales monitored by mid-infrared dual comb spectroscopy (DCS)	Dual-comb spectroscopy (DCS) can be used to monitor protein dynamics on a microsecond time-scale. Kinetics of irreversible protein reactions require an analytical technique that provides time-dependent infrared spectra in a single shot. We compare caged compound induced reactions monitored by FTIR and DCS and observe good data quality with 4 μ s time resolution, three orders of magnitude faster than any FTIR measurements..
25	Florian	Eigenmann	IRSWEEP	Spectroscopy	Switzerland	Need for Speed: Protein Dynamics in Stopped Flow Applications with Dual Comb Spectroscopy	Protein chemists have always wanted to follow kinetics in the mid infrared region in order to gain more insights than with conventional techniques. Traditionally, the stopped-flow is coupled to a FTIR spectrometer. The main limitation is often the time resolution of the scanning interferometer. Dual-comb spectrometers however do not have any movable parts and can therefore obtain kinetics with microsecond time resolutions.
26	David	Buhrke	Universität Zürich	Chemistry	Switzerland	H-bonding in a Photoreceptor Protein observed with Isotope Labeling and 2D-IR Spectroscopy	We studied a photoreceptor protein with isotope labeling and two dimensional infrared (2D-IR) spectroscopy. Isotope labeling allows us to isolate two site-specific marker modes from the overall mid-IR signal of the protein. 2D-IR is used as a sensitive method to study the vibrational line shapes in different photo-states.
27	Soumen	Ghosh	Politecnico di Milano	Physics	Italy	Phonon Mediated Exciton-Polaron Spin Dynamics in Layered Metal Halide Perovskites	We have employed femtosecond Faraday rotation and transient absorption spectroscopy to study the ultrafast spin depolarization dynamics in layered metal halide perovskites. We observe that excitation with excess photon energy leads to a distinct spin relaxation mechanism due to the polaron formation, mediated by coherent phonon vibrations.
28	Ho-Wah	Siu	University of Konstanz	Chemistry	Germany	Constrained polyQ rich peptides to elucidate the exceptional role of glutamine side chains in polyQ aggregation	Expanded polyQ sequences are responsible for many neurodegenerative diseases. We have designed a set of constrained polyQ rich peptides and demonstrated the enormous effect of single glutamines on the hairpin structure by NMR, CD and IR spectroscopic approaches. We could access sub-ms dynamics of the peptides by laser-excited temperature-jump spectroscopy.

29	Paul	Stritt	University of Konstanz	Department of Chemistry	Germany	Mid-IR quantum cascade laser spectroscopy to resolve lipid-mediated dynamics in the photocycle of bacteriorhodopsin	Time-resolved infrared spectroscopy provides insights into the interaction of the light-driven transmembrane proton pump bacteriorhodopsin and the lipid membrane. Tunable quantum cascade lasers were used to resolve minor changes of vibrational modes during the photocycle by single wavenumber measurements in a broad spectral region covering protein, chromophore, and lipid vibrations.
30	Charles	Sayers	Politecnico di Milano	Physics	Italy	Understanding phase transitions in transition metal dichalcogenides via the coherent phonon response	The metallic transition metal dichalcogenides are layered materials which are host to numerous charge density wave (CDW) phases, characterized by a reconstruction of the electronic and lattice structure. Using a combination of ultrafast spectroscopy techniques, we observe strong coherent phonon oscillations in the out-of-equilibrium response of these systems which gives an insight into the origin of the CDW phase.
31	Francesco	Segatta	Università di Bologna	Dipartimento di Chimica Industriale "Toso Montanari"	Italy	Visualizing Molecular Vibrations via Ultrafast UV-pump (soft) X-ray probe Spectroscopy; Theory and Experiment	A quantum chemistry based computational protocol to unravel (low-frequency) vibrations in molecular systems via time-resolved X-ray spectroscopy is presented: a UV (pump) pulse induces the wave-packet dynamics, which is then monitored by an X-ray (probe) pulse. The protocol is validated on hydroxychloroquine at the chlorine L-edge.
32	Yannik	Pfeifer	University of Potsdam	Institute of Chemistry	Germany	Investigation of the pH dependent reaction mechanism of pHP by ultrafast vibrational spectroscopies	Photocaging compounds are molecules releasing a part of their structure upon a light trigger. They are used as tools in biophysical applications like time-resolved serial crystallography. I am investigating the pH dependency of photouncaging reactions in para-hydroxyphenacyl (pHP) compounds by femtosecond stimulated Raman and transient (2D) infrared spectroscopy.
33	Andrea	Chiuri	Italian National Agency for New Technologies, Energy and Sustainable Economic Development (ENEA)	Nuclear Fusion and Safety Technologies Department (FSN)	Italy	Experimental performances of optical Kerr cells for Raman fast gating	Optical Kerr cells can be employed for fast gating in Raman spectroscopy to reject the fluorescence contribution. The performances of an Optical Kerr Cell are discussed and a review of the state of the art is presented after theoretical considerations and MonteCarlo simulations describing the possibilities offered by this approach.

34	Federico	Angelini	ENEA	FSN-TECFIS-DIM	Italy	Time-gated methods for fluorescence rejection in Raman Spectroscopy	An analysis of the methods for time-gated Raman spectroscopy is presented, from the analysis of expected performances to a review of the devices realized and employed in the last decades.
35	Giuseppe	Fumero	Sapienza, University of Rome	Department of Physics	Italy	2D Impulsively Stimulated Resonant Raman Spectroscopy of Molecular Excited States	We bring together some of the key advantages of vibrational and electronic multidimensional spectroscopies in a multidimensional Raman scheme to study the vibronic properties during excited-state dynamics in a selective manner, an open problem in ultrafast science which cannot be tackled by lower order techniques.
36	Zhengjun	Wang	Division of Chemical Physics	Department of Chemistry	Sweden	Quantum beating of CdSe QDs measured by 2D spectroscopy at low temperature	This work is to study the quantum beating in the vibrational energy level of CdSe QDs at 77K by 2D electronic spectroscopy. We find that quantum beating comes from the ground state coherence and excited state coherence in the QDs at a wavelength of 230 nm.
37	Selflando	Shehaj	University of Potsdam	Chemistry	Germany	Vibrational Spectroscopy to study Proton Mobility in Ionic Liquids	Ionic Liquids (ILs) are very promising materials in future due to their properties. Protic ILs are prone to proton exchange and hydrogen bonded network. However, the detailed mechanism of proton conduction in PILs remains to be determined. Our study intends to identify the proton transfer pathway/mechanism of proton transport in PILs.
38	Florian	Bartonitz	Freie Universität Berlin	Experimentelle Physik	Germany	Strong Spectral Modulation of the Proton Continuum Band after Ultrafast Photoinduced Dissociation of Delphinidin-3-Rutinoside	Photodissociation of cationic Delphinidin-3-Rutinoside (D3R) was studied by fs pump-probe spectroscopy in Vis and IR spectral ranges. Ultrafast formation of a highly structured proton continuum band is observed in heavy water and methanol.
39	Marius	Horch	Freie Universität Berlin	Department of Physics	Germany	Understanding Metalloenzyme Catalysis by Advanced Experimental and Computational IR Spectroscopy	Using hydrogenase as a model system, I will illustrate how the structure and dynamics of complex metalloenzymes can be studied by ultrafast and two-dimensional IR spectroscopy. Supported by computations, unexpected aspects of energy transfer, cofactor-protein interactions, and ligand bonding were unraveled. These findings provide new perspectives for understanding (bio)inorganic catalysis.

40	Luiz	Schubert	Freie Universitaet Berlin	Physics	Germany	Protein Conformational and Protonation Dynamics Monitored by Single-Shot IR Spectroscopy	In this study we used quantum cascade laser (QCL) based dual-comb spectroscopy to study protein conformational and protonation dynamics of bacteriorhodopsin. We provide a comparison between a commercially available dual-comb spectrometer and our homebuilt tunable QCL based spectrometer to showcase the possibility of probing non-repetitive protein dynamics.
41	Clark	Zahn	FU Berlin	Experimental Physics	Germany	Spectral decomposition of Qx and Qy absorption bands- Resolving Q band mixing in chlorophyll a by fs Vis-pump IR-probe spectroscopy	Polarization resolved femtosecond VIS pump - IR probe spectroscopy provides detailed insight into Q band mixing of Chlorophyll a. Measuring the anisotropy of the Keto C=O at 1700 cm ⁻¹ for different excitation wavelength allows for direct decomposition of the Q band and assignment of Qx and Qy absorption.
42	Till	Stensitzki	Universität Potsdam	Physikalische Chemie	Germany	Ultrafast Backbone Protonation in Channelrhodopsin-1	Proton-transfer reactions are an essential part of the mechanism in many proteins. In general, only certain amino-acid sidechains take part in these reactions. Here we present spectroscopic evidence, that a backbone amide-group acts as a transient proton acceptor in the initial photoreaction of Channelrhodopsin-1.
43	Jakob	Schauss	Max-Born-Institute, Berlin	C1 - Femtosecond Spectroscopy of Molecular Systems	Germany	Phosphate Vibrations Reveal Contact Ion Interactions: 2D-IR Spectroscopy of the Dimethyl Phosphate Model System	Phosphate vibrations of the nucleic acid backbone allow non-invasive probing of electric interactions with the hydration shell. The dimethyl phosphate anion (DMP ⁻) is a model system relevant in this context. Vibrational properties of DMP ⁻ and metal ion pairs are examined using 2D-IR spectroscopy and interpreted using microscopic density functional theory.
44	Hanna	Orlikowska	Poznan University of Technology	Faculty of Materials Engineering and Technical Physics	Poland	Modulation transfer approach: on the way to routine fluorescence-free imaging of biomimetic membranes	The presentation outlines the first steps we took to provide fluorescence-free imaging of biomimetic membrane components. We used an intensity-modulated pump beam to excite the sample and a probe beam to monitor the induced changes. We show that the signal results from the interplay between different contrast mechanisms.

45	Emilia	Krok	Poznan University of Technology	Faculty of Materials Engineering and Technical Physics	Poland	Water interacting with biomimetic cell membranes – can anhydrobiosis be recreated in the lab?	Nature equipped some of the organisms with a very sophisticated system which allows them to undergo the anhydrobiosis. Our research presents a novel method for preparation of lipid membranes that can survive complete dehydration conditions. By using slow, gradual dehydration process we successfully dehydrated the membrane without any structural damages.
46	Madhurima	Chattopadhyay	Poznan University of Technology	Faculty of Materials Engineering and Technical Physics	Poland	Water Facilitating Lateral Diffusion in Biomembranes	By fluorescence microscopy and FRAP experiments, we show that the lateral diffusion of lipids is controlled by only few water molecules in the water clathrate structure around the lipid headgroups ¹ . At lower hydration conditions, the clathrate structure is broken resulting in ~twofold increase in activation energy of diffusion of lipids.
47	Arghyadeep	Basu	Technion Israel Institute of Technology	Chemistry	Israel	Understanding Molecular Structure of L-Glutathione on Silver Nanoparticle Surface by 2D IR Spectroscopy	Understanding the molecular structure of peptide-functionalized nanoparticles is very important for their efficient use in modern scientific and technological applications. Using 2D IR spectroscopy and isotope labeling on the cysteine unit of Glutathione, we studied the secondary structure of glutathione (γ -Glu-Cys-Gly, GSH) on silver nanoparticle surfaces.
48	Srijan	Chatterjee	NCL,pune	Department of chemistry	India	Quantitative Estimation of Local Electrostatics and Dynamics in Choline Based Deep Eutectic Solvents	A combined approach of vibrational Stark Spectroscopy, 2D IR spectroscopy, and molecular dynamics simulations have been utilized to estimate the residue specific electrostatic interactions and dynamics in alcohol-based deep eutectic solvents.
49	Chi-Jui	Feng	University of Chicago	Chemistry		Conformational Variation of Insulin Dimer Studied by Amide I Spectroscopy and Computational Spectroscopy	To study coupled unfolding and unbinding process in insulin dimer dissociation, we investigated the dimer conformational variation using site-specific isotope labeling, amide I 2D IR spectroscopy and computational spectroscopy. Two dominant conformers are experimentally found: native dimer and twisted dimer, with the detailed dynamics revealed from a Markov State Model.

50	Juno	Kim	Yonsei University	Department of Chemistry	Republic of Korea	Non-Adiabatic Pathway Governs Nuclear Rearrangements: Exciton Self-trapping and Delocalization in Organic Nanoring	Monitoring ultrafast processes from high-lying excited states are at the frontier of field of photophysics. Ultrafast structural evolutions in organic nanoring during non-adiabatic transitions were scrutinized via time-resolved impulsive stimulated Raman spectroscopy. By accessing high-lying excited states of different wavefunction symmetry, key reaction coordinates for ultrafast exciton self-trapping are provided.
51	Yuki	Fujii	Graduate School of Science, Kobe University	Chemistry	Japan	Vibrational Frequency Fluctuation of Carbonyl Compounds in Water Studied by Two-Dimensional Infrared Spectroscopy	We used two-dimensional infrared spectroscopy to obtain detailed information on frequency fluctuation of carbonyl compounds in D2O. It is suggested that collective orientation of dipole moment of water molecules with respect to transition dipole moment of the vibrational probe play a key role in the frequency fluctuation.
52	Yuki	Fujii	Graduate School of Science, Kobe University	Chemistry	Japan	Vibrational Frequency Fluctuation of Carbonyl Compounds in Water Studied by Two-Dimensional Infrared Spectroscopy	We used two-dimensional infrared spectroscopy to obtain detailed information on frequency fluctuation of carbonyl compounds in D2O. It is suggested that collective orientation of dipole moment of water molecules with respect to transition dipole moment of the vibrational probe play a key role in the frequency fluctuation.
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54	Tomomi	Shionoya	Osaka University	Department of Chemistry, Graduate School of Science	Japan	Interaction between retinal chromophore and opsin to enable proton transport in a light-driven proton pump GR	We studied dynamics of protein structure of a light-driven proton pump, Gloeobacter rhodopsin using time-resolved resonance Raman spectroscopy. Our results showed that the atomic contacts between the retinal chromophore and Trp222 residue in the retinal binding pocket are required to drive the proton transfer in the protein.

55	Taito	Urui	Osaka University	Department of Chemistry	Japan	Resonance Raman Determination of Chromophore Structures of Heliorhodopsin Photointermediates	Upon photoexcitation, photoreceptive proteins undergo structural changes, which are essential to their functioning. Here, we revealed retinal chromophore structures of heliorhodopsin by using time-resolved resonance Raman spectroscopy and discussed about the change of hydrogen bond strength at retinal Schiff base in the photocycle of heliorhodopsin.
56	Hajime	Torii	Shizuoka University	Applied Chemistry and Biochemical Engineering	Japan	Role of Intermolecular Charge Fluxes in the Hydrogen-Bond-Induced Frequency Shifts of the OH Stretch of Water	Mechanisms of the hydrogen-bond-induced frequency shifts of the OH stretch of water are analyzed to pursue the generality or the extent of applicability of the frequency vs electric field correlation. It is shown that the delocalized electronic motions related to both the dipole first and second derivatives play important roles.
57	Ahmed	Mohammed	RIKEN, Japan	Molecular Spectroscopy Laboratory	Japan	Capturing Hidden Isolated OH at the Charged Hydrophobic Interface by 2D Heterodyne-Detected VSFG Spectroscopy	2D HD-VSFG is applied for studying the femtosecond hydrogen-bond dynamics of water at oppositely charged hydrophobic ion/water interfaces. The obtained results unveiled the existence of energetically isolated distinct OH groups at the aqueous interface, depending on the sign of the charge of the hydrophobic ion on the water surface.
58	Woongmo	Sung	RIKEN	Tahara Molecular Spectroscopy Laboratory	Japan	Reliable vibrational relaxation time of OH stretch at the air/H₂O interface determined by time-resolved heterodyne-detected VSFG spectroscopy	Reliable vibrational relaxation (T ₁) time of OH stretch of interfacial H ₂ O was determined by TR-HD-VSFG spectroscopy. The obtained T ₁ times of hydrogen-bonded OH lie in the range of 200 - 400 fs, and they are comparable to the T ₁ times of bulk H ₂ O. Only free-OH stretch shows noticeably slow (~1 ps) T ₁ time.
59	Pavel	Kolesnichenko	Swinburne University of Technology	Department of Physics and Astronomy	Australia	Bridging time-resolved coherent Raman and coherent 2D spectroscopy: heterodyne detection of low-energy vibrational modes and recognizing excited-state contributions	Here we use coherent 2D spectroscopy and the formalism based on Feynman diagrams to explain complementarity of coherent Stokes and anti-Stokes Raman scattering spectra. We detect low-energy Raman modes (below kT at room temperature) without fluorescence or non-resonant background and identify excited-state contributions.

60 Christopher Hall

University of
MelbourneSchool of
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Australia

**The role of
conformational
heterogeneity on excited-
state dynamics in linked
diketopyrrolopyrrole
dimers**

In this work we investigated processes competing with singlet fission in dimers of Diketopyrrolopyrrole (DPP) derivatives with varying linker structures. Ultrafast spectroscopy (electronic and IR) and calculations reveal different populations of molecular conformations which mediate the formation of a charge-separated state.