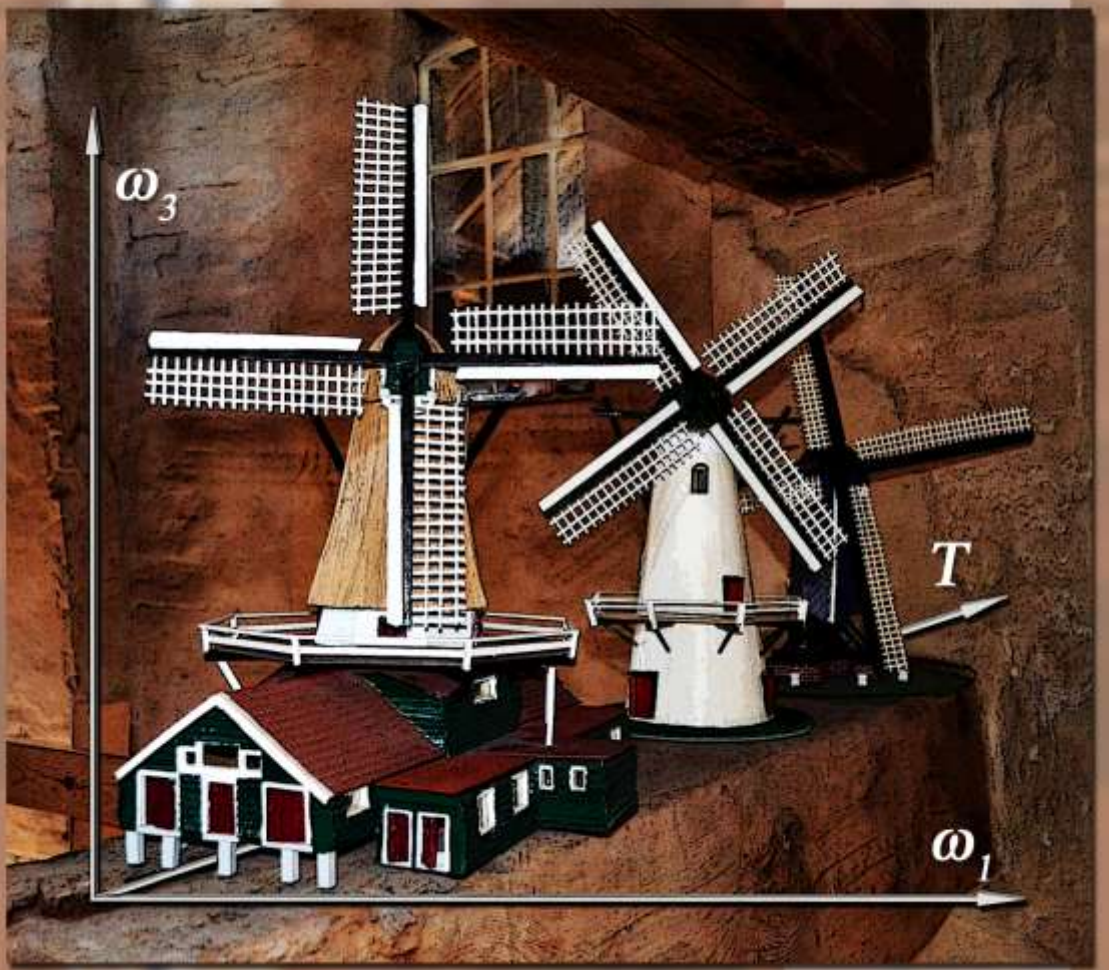
CMDS 2016

The 8th International Conference on Coherent Multidimensional Spectroscopy

CMDS 2016

June 29 - July 1 2016, Groningen, the Netherlands



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Welcome Message

We are pleased to welcome the 8th International Conference on Coherent Multidimensional Spectroscopy, CMDS 2016, to Groningen, the Netherlands! This meeting follows the CMDS conferences in Eugene, Berlin, Minneapolis, Kyoto, Rigi-Kulm, Madison, and Seoul.

The bi-annual CMDS conference is a major international forum for discussion of the latest and most important results in multidimensional optical spectroscopy. The meetings bring together scientists from different fields of science and serve as a venue for exchanging ideas between theorists and experimentalists. CMDS has become the premier event for researchers developing and applying state-of-the-art multi-dimensional optical, infrared, and THz spectroscopic methods to address a vast variety of problems in chemistry, biology, physics, and material science.

Groningen is a vibrant, one thousand year old city. With its comprehensive university, founded in 1614, it combines a rich academic tradition with an attractive city life, characterized by culture, history, and an exciting social scene.

We wish you a fruitful conference and pleasant stay in Groningen!

Thomas la Cour Jansen
Maxim S. Pshenichnikov
Conference Co-chairs

For further information, visit the conference website at
http://CMDS2016.ORG

Time		Tuesday, June 28	Wednesday, June 29		Time	
08	00		**Registration**		**08**	00
	30		**Opening**			30
	40		**Chemistry / Catalysis**	We01 **Kubarych**		40
09	00			We02 **Bredenbeck**	**09**	00
	20			We03 **Xiong**		20
	40		Chair: Carlos R. Baiz	We04 **Vöhringer**		40
10	00			We05 **Wright**	**10**	00
	20		**Coffee break**			20
	40					40
11	00		**Biomolecules I (DNA)**	We06 **Chergui**	**11**	00
	20			We07 **Hunt**		20
	40		Chair: Sander Woutersen	We08 **Prokhorenko**		40
12	00			We09 **Marcus**	**12**	00
	20		**Lunch**			20
	40					40
13	00		**Materials I**	We10 **Zanni**	**13**	00
	20			We11 **De Sio**		20
	40		Chair: Steven T. Cundiff	We12 **Kwak**		40
14	00			We13 **Ryu**	**14**	00
	20		**Coffee break**			20
	40					40
15	00		**Methods I**	We14 **Brixner**	**15**	00
	20	**Registration**				20
	40		Chair: R.J. Dwayne Miller	We15 **Davis**		40
16	00			We16 **Cina**	**16**	00
	20			We17 **El Khoury**		20
	40					40
17	00		**Dinner (on your own)**		**17**	00
18	00	**Reception**			**18**	00
19	00	**Dinner (on your own)**	**Poster session I (odd numbers)**		**19**	00
20	00				**20**	00
21	00				**21**	00
22	00				**22**	00

Color coding	Official	Refreshments	Social	Session topic	Invited talk	Contributed talk	Poster session

Time		Thursday, June 30		Friday, July 1		Time	
08	00					08	00
	20						20
	40	Water	Th01 **Backus**	Light Harvesting	Fr01 **Ogilvie**		40
09	00		Th02 **Inoue**		Fr02 **Paleček**	09	00
	20		Th03 **Tokmakoff**		Fr03 **Pullerits**		20
	40	Chair: Huib J. Bakker	Th04 **Tominaga**		Fr04 **Heisler**		40
10	00		Th05 **Elsaesser**	Chair: Tomáš Mancal	Fr05 **Tan**	10	00
	20				Fr06 **Collini**		20
	40	**Coffee break**			Fr07 **Shi**		40
11	00	Ions	Th06 **Hamm**	**Poster session II (even numbers)**		11	00
	20		Th07 **Zhuang**				20
	40	Chair: Amber T. Krummel	Th08 **Berg**				40
12	00		Th09 **Garrett-Roe**			12	00
	20	**Lunch + IOC meeting**		**Lunch**			20
	40						40
13	00					13	00
	20	Materials II	Th10 **Bakulin**	Methods II	Fr08 **Cho**		20
	40						40
14	00		Th11 **Grégoire**		Fr09 **Kemlin**	14	00
	20	Chair: Tobias Brixner	Th12 **Roberts**	Chair: Arend G. Dijkstra	Fr10 **Krummel**		20
	40		Th13 **Cundiff**		Fr11 **Gelin**		40
15	00	**Coffee break**		**Closing remarks**		15	00
	20			**Conference end**			20
	40	Biomolecules II (Proteins)	Th14 **Helbing**				40
16	00		Th15 **Rezus**			16	00
	20	Chair: Jianping Wang	Th16 **Moran**				20
	40		Th17 **Klug**				40
17	00	**Boat trip - Excursion**				17	00
18	00					18	00
19	00	**Conference dinner**				19	00
20	00					20	00
21	00					21	00
22	00					22	00

Color coding	Official	Refreshments	Social	Session topic	Invited talk	Contributed talk	Poster session

Tuesday, June 28

15:30 **Registration**

Location: "De Oosterpoort", Trompsingel 27

18:00 **Reception**

Location: Academigebouw, Broerstraat 5

This reception is offered to you by the University of Groningen, the Municipality of Groningen and the Province of Groningen.

Wednesday, June 29

08:00 **Registration**

08:30 **Opening**

Chemistry / Catalysis Chair: Carlos R. Baiz

08:40

We01 **Photocatalysis Reaction Dynamics Probed in Operando with 2DIR**

Kevin J. Kubarych

University of Michigan, USA

2D-IR can be used to track structural dynamics as well as mechanistic connectivity in functional photocatalytic reactors. Non-equilibrium 2D-IR, both transient and at steady-state reveals ultrafast intermolecular charge transfer, solvent exchange and catalyst dimerization.

09:10

We02 **How Catalysts Control Substrate Structure**

Jens Bredenbeck

Johann Wolfgang Goethe-Universität, Germany

The stereochemistry of substrate-catalyst-complexes in reaction mixtures is resolved by polarization-dependent 2D-IR spectroscopy and DFT computations, shedding light on the controversial reaction mechanism of an important textbook example of enantioselective synthesis. The influence of thermal fluctuations on 2D-IR structure determination is assessed by temperature-dependent measurements and *ab initio* MD simulations.

Wednesday, June 29

Chemistry / Catalysis

Chair: Carlos R. Baiz

09:30 **We03**

Measuring Orientation and Surface Interactions of Heterogeneous Catalysts using 2D SFG

Wei Xiong

University of California-San Diego, USA

Using 2D SFG spectroscopy, we characterize a CO_2 reduction catalyst on gold surface. We find that by analyzing lineshape of cross-peaks, the interactions between vibrational modes and gold surface can be revealed. Further, we demonstrate a general method to measure the molecular orientation and its distribution on surface.

09:50 **We04**

Ultrafast Dynamics of a Ferracyclobutadiene

Peter Vöhringer

University of Bonn, Germany

The photo-induced primary processes of a carbonyl-bearing ferracyclobutadiene are revealed by ultrafast time-resolved mid-infrared spectroscopy. Following optical excitation, a CO-dissociation occurs within several tens of picoseconds via barriercrossing on the electronically excited state. Solvent binding by the vacancy of a coordinatively unsaturated intermediate is faster than the initial CO-loss.

10:10 **We05**

Fully Coherent Electronic-Vibrational Spectroscopy of Transition Metal Complexes

John C. Wright

University of Wisconsin-Madison, USA

Three independently tunable OPAs create multiple quantum coherences (MQCs) using fully coherent pathways involving vibrational and electronic states. The MQCs create 3D electronic/vibrational spectra that can serve as multidimensional spectral signatures of transition metal complexes in complex biological systems. We report experiments using different methodologies to probe different biological systems.

10:30

Coffee break

Sponsored by Coherent

Wednesday, June 29

Biomolecules I (DNA) Chair: Sander Woutersen

11:00

We06

Ultrafast 2D UV and Visible Spectroscopy of (Bio)Chemical Systems

Majed Chergui

Ecole Polytechnique Fédérale de Lausanne, Switzerland

We review our recent studies, using 2D transient absorption deep-UV spectroscopy, on electron transfer in hemoproteins and on the charge carrier dynamics in Titanium dioxide. We then present our recent studies using visible coherent 2D on the energy transfer in diporphyrins and on pentacene crystals.

11:30

We07

Long-Range Vibrational Dynamics are Directed by Watson-Crick Base-Pairing in Duplex DNA

Neil T. Hunt

University of Strathclyde, UK

Ultrafast two-colour 2D-IR spectroscopy has been used to study vibrational coupling interactions and energy relaxation pathways linking DNA bases with the sugar phosphate backbone. We show that vibrational relaxation proceeds via modes located on the deoxyribose unit, while helix formation leads to unique coupling of base and phosphate vibrations.

11:50

We08

Two-Dimensional And Transient Absorption Spectroscopies of Single-Stranded DNA in The Deep UV

Valentyn I. Prokhorenko

Max Planck-Institute for the Structure and Dynamics of Matter, Germany

Ultrafast electronic dynamics in DNA and its nucleobases are studied with 2D-UV photon echo and transient absorption spectroscopies, covering a spectral range of 250-300 nm. Increasing the DNA length leads to significant changes in their 2D spectra.

Wednesday, June 29

Biomolecules I (DNA) Chair: Sander Woutersen

12:10

We09 **Studies of Vibronically Coupled Molecular Dimers in DNA by Timeresolved Two-Dimensional Fluorescence Spectroscopy**

Andrew H. Marcus

University of Oregon, USA

Two-dimensional fluorescence spectroscopy (2DFS) is used to study the local conformations and excited state dynamics of pairs of cyanine dyes, which are sitespecifically incorporated into the sugar-phosphate backbones of DNA replication fork constructs. A vibronic coupling model describes time-resolved 2DFS, circular dichroism (CD), and linear dichroism (LD) of these systems.

12:30 **Lunch**

Materials I Chair: Steven T. Cundiff

13:30

We10 **Ultrafast Exciton Transport Studied with 2D White-Light Spectroscopy at 100 Khz**

Martin T. Zanni

University of Wisconsin-Madison, USA

Exciton transport in thin films made from semiconducting carbon nanotubes was studied with a new 2D WL spectrometer operating at a repetition rate of 100 kHz. Exciton lifetimes are found to scale with the rate of energy transfer, which has implications for working devices.

14:00

We11 **Coherent Polaron Pair Formation in a Semiconducting Polymer**

Antonietta De Sio

Carl von Ossietzky Universität, Germany

Combining high-time resolution two-dimensional electronic spectroscopy with detailed theoretical simulations, we investigate the initial dynamics of excitons and polaron pairs in a semiconducting polymer thin film. We show that coherent vibronic coupling promotes charge delocalization and results in long-lasting coherent oscillatory dynamics of strongly coupled excitons and polaron pairs.

Wednesday, June 29

Materials I

Chair: Steven T. Cundiff

14:20 **We12**

Equilibrium Dynamics in Electrolytes of Li-Ion BatteryStudied by Two-Dimensional IR Spectroscopy

Kyungwon Kwak

Korea University, Korea

The solvation structures and dynamics of Li ions in liquid electrolyte play an essential role to Li-based battery performance. To mimic commercial electrolyte, Li+ were dissolved in diethylcarbonate and its solvation behavior was observed with time-resolved IR spectroscopies. 2D-IR experiments show that there is fast equilibrium solvation dynamics around Li-ion.

14:40 **We13**

Optical Inhomogeneity from 2D Spectra vs. Static Size Dispersion in an Ensemble of PbSe Nanocrystals

Jisu Ryu

University of Colorado, USA

The optical inhomogeneity of a PbSe QD sample is determined using 2DFT spectroscopy with the nodal line slope method and compared to size dispersions measured with TEM. Comparison between the two suggests that either TEM overestimates the size dispersion or the optical inhomogeneity does not directly reflect the size dispersion.

15:00

Coffee break

Sponsored by Fastlite

Methods I

Chair: R.J. Dwayne Miller

15:30 **We14**

New 2D Methods for Studying Molecular Interactions

Tobias Brixner

Universität Würzburg, Germany

We developed several methods concerning the study of molecular interactions: 1) A theorem states conditions for the unique inversion of electronic 2D spectra toward the complete population-transfer matrix; 2) we present 2D spectroscopy of exciton–exciton interactions; 3) we introduce 2D spectroscopy on interaction-free molecular beams using mass-resolved ion detection.

Wednesday, June 29

Methods I Chair: R.J. Dwayne Miller

16:00

We15 **Isolating Specific Pathways in Double Quantum 2D Spectroscopy**

Jeffrey A. Davis

Swinburne University of Technology, Australia

By combining spectral amplitude shaping and select pulse delays it is possible to filter out unwanted signal contributions in double quantum 2D spectra, analogous to techniques in multidimensional NMR. In coupled semiconductor quantum wells this allows removal of broad free-carrier contributions and isolation of the mixed 2-exciton states.

16:20

We16 **Relating Action- and Transmission-Detected Multidimensional Wave-Packet Interferometry Signals**

Jeffrey A. Cina

University of Oregon, USA

We report on our recent comparative studies of calculated fluorescence-detected wavepacket interferometry and heterodyne-detected four-wave-mixing signals. Special attention is given to the possible use of pulse-shaping methods to render more nearly equivalent differently measured time-resolved nonlinear optical signals.

16:40

We17 **Femtosecond Redox-Induced 2D-IR Difference Spectroscopy of Proteins and Biomolecules**

Youssef El Khoury

Institut de Physique et Chimie des Matériaux de Strasbourg, France

In analogy to redox-induced FTIR difference spectroscopy, we developed redox-induced 2D-IR difference spectroscopy to investigate ultrafast dynamics of redox-sensitive vibrational modes. Lifetimes, couplings, vibrational energy transfer and spectral diffusion can be investigated under redox control. The methodology and first applications including the protein cytochrome c are presented.

17:00 **Dinner** (on your own)

19:00 **Poster session I (odd numbers)**

Thursday, June 30

Water Chair: Huib J. Bakker

08:30

Th01

Energy Transfer in Water Underneath Oppositely Charged Surfactants

Ellen H. G. Backus

Max Planck Institute for Polymer Research, Germany

Energy transfer in water underneath both negatively and positively charged surfactants is studied with two-dimensional vibrational sum frequency generation spectroscopy. For the negatively charged surfactant, two distinct water sub-ensembles are identified with subpicosecond energy transfer between them. In contrast, water underneath a positively charged surfactant behaves like bulk water.

09:00

Th02

2D Heterodyne-Detected VSFG Spectroscopy of a Model Membrane Interface

Ken-ichi Inoue

RIKEN, Japan

2D HD-VSFG is applied for studying a zwitterionic lipid/water interface as a model membrane interface. The transient spectra in the OH stretch region reveal the presence of “H-down“ oriented water associated with a choline group in addition to “H-up“ oriented water in the vicinity of a phosphate group.

09:20

Th03

The Dynamics of Excess Protons in Liquid Water Viewed through 2D IR Spectroscopy

Andrei Tokmakoff

The University of Chicago, USA

We investigate the dynamics of protons in strong acid solutions using 2D IR spectroscopy of the acid continuum band. We observe a crosspeak between stretching and bending vibrations associated with the excess proton at (3200 cm^{-1}, 1760 cm^{-1}) that is assigned to a persistent Zundel complex.

Thursday, June 30

Water Chair: Huib J. Bakker

09:50

Th04

Frequency Fluctuations of Non-Ionic Vibrational Probe in Waterstudied by 2DIR Spectroscopy and Molecular Simulation

Keisuke Tominaga

Kobe University, Japan

Frequency fluctuations of the CN stretching mode of 2-nitro-5-thiocyanatobenzoic acid are examined by 2D-IR spectroscopy and classical molecular dynamics simulation. The 2D-IR experiment revealed that the frequency-frequency correlation function contained the decay component of 1.1 ps, which is attributed to the rearrangement of hydrogenbond network around the solute.

10:10

Th05

Short-Range Electric Interactions of the DNA Surface with its Hydration Shell

Thomas Elsaesser

Max-Born-Institut für Nichtlineare Optik und Kurzzeitspektroskopie, Germany

Electric interactions at the interface of native DNA and its aqueous environment are probed with two-dimensional infrared (2D-IR) spectroscopy of backbone vibrations. The fast fluctuations of electric forces from thermal water motions acting on these oscillators are limited in their range to the first two hydration layers.

10:30 **Coffee break**

Sponsored by Infrared Systems

Ions Chair: Amber T. Krummel

11:00

Th06

2D-Raman-THz Spectroscopy of Salt Solutions

Peter Hamm

University of Zurich, Switzerland

The 2D-Raman-THz repsonse of salt solutions reveals an echo, whose decay time correlates with the water structuring capability of the cation. Polarizable force fields of water and ions are developed to simulate the spectroscopic response.

Thursday, June 30

Ions Chair: Amber T. Krummel

11:30

Study the Spatial Range of Ion Effect Using 1D and 2D Vibrational Spectroscopy

Th07 Wei Zhuang

Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, China

The range of ion effect on water in ionic solutions was studied theoretically using 1D and 2D vibrational spectroscopy. Evidence of ion effect beyond its hydration shell was addressed in infrared photodissociation spectra and low frequency vibration spectra.

11:50

Heterogeneous Solvation Dynamics in an Ionic Liquid: Multidimensional Rate Spectra Yield Quantitative Measurements

Th08 Mark A. Berg

University of South Carolina, USA

Multidimensional correlation functions have been applied to simulations of solvation dynamics in an ionic liquid. Heterogeneity is found in both the rate of diffusive solvation and in the amplitude of inertial solvation. New methods for analyzing multidimensional kinetics have been developed to quantify these phenomena.

12:10

Ultrafast Vibrational Spectroscopy of Ionic Liquids

Th09 Sean Garrett-Roe

University of Pittsburgh, USA

Ultrafast dynamics in ionic liquids are studied with 2D-IR spectroscopy. Quantum chemistry and molecular dynamics simulations unravel the experimentally observed vibrational frequency fluctuation correlation functions of CO_2. Thiocyanate ionic liquids in reverse micelles respond to confinement depending on micelle size and surfactant.

12:30

Lunch + IOC meeting

Thursday, June 30

Materials II

Chair: Tobias Brixner

13:30

Th10

Vibronic Effects in Singlet Fission Observed by Coherent Electronic 2D Spectroscopy

Artem A. Bakulin

University of Cambridge, UK

We use electronic 2D spectroscopy to study the intermediate states responsible for ultrafast singlet exciton fission in pentacene-/tetracene-based molecular crystals and in pentacene dimers. Our results show the vibrational coupling enhances interaction between the singlet and multiexcitonic double-triplet states, which greatly facilitates fission process.

14:00

Th11

Two-Dimensional Coherent Photocurrent Excitation Spectroscopy Of A Hybrid Lead-Halide Perovskite Solar Cell

Pascal Grégoire

Université de Montréal, Canada

We report two-dimensional coherent photocurrent excitation spectroscopy in efficient hybrid lead-halide perovskite solar cells. We identify weakly bound exciton and continuum excitation features in the total correlation spectrum. Via the absolute zero-time rephasing spectrum, we also measure the temperature-dependent homogeneous linewidth and thus address the proposed polaronic nature of photocarriers.

14:20

Th12

Extracting Solar Energy from Singlet Fission Materials

Sean T. Roberts

University of Texas at Austin, USA

Singlet Fission is a process wherein a highly excited spin-singlet exciton divides its energy to form a pair of spin-correlated triplet excitations. We report ultrafast transient absorption and electronic sum frequency generation experiments that establish structure-function relationships that allow triplet exciton formation and extraction from perylene diimide thin films.

Thursday, June 30

Materials II Chair: Tobias Brixner

14:40

Th13

Multi-Quantum Coherences Measure the Exciton-Polariton Ladder of States in a Microcavity

Steven T. Cundiff

University of Colorado, USA

Exciton-polaritons result when the coherent exchange of energy between excitons and light is strong, giving new eigenmodes. We study these eigenmodes using a collinear approach to 2D near-IR spectroscopy. Multi-quantum coherences reveal higher-order avoided crossings inaccessible in standard experiments. These avoided crossings reveal the structure of the cavity polariton.

15:00

Coffee break

Sponsored by Ultrafast Innovations

Biomolecules II (Proteins) Chair: Jianping Wang

15:30

Th14

2D-IR Versus VCD Spectroscopy of Artificial β-Sheet Forming Fibrils

Jan Helbing

University of Zurich, Switzerland

We discuss 2D-IR and VCD spectra of self-assembled nanostructures, which form monomeric right-handed parallel beta sheet helices, but exhibit the 'giant' amide I VCD signals typical of left-handed amyloid-like peptide aggregates. Isotope-labelling and strand-length variations cause dramatic changes in the VCD signal, which are only partially reflected in 2D-IR.

16:00

Th15

Temperature-Induced Collapse of Elastin-Like Peptides Studied by 2DIR Spectroscopy

Yves L.A. Rezus

FOM institute AMOLF, The Netherlands

We use 2DIR spectroscopy to study the conformational dynamics of elastin-like peptides in both their soluble and aggregated form. We find that the peptides remain surprisingly well hydrated in the aggregated state. In addition, we find evidence for the presence of an intramolecular hydrogen-bond in both states.

Thursday, June 30

Biomolecules II (Proteins) Chair: Jianping Wang

16:20

Th16

Dynamics of Substrate-Based IR Probes in Enzymes and Transporters

Sean D. Moran

Southern Illinois University Carbondale, USA

I will present our work characterizing substrate and binding pocket dynamics in enzymes and transmembrane transport proteins using 2D IR spectroscopy. We focus on developing vibrational probes that are close analogs of substrates for these proteins to understand how protein structure, dynamics, and environment guide reactivity and transport.

16:40

Th17

The Structure of a Drug-Protein Complex Detected and Analysed by EVV 2DIR Spectroscopy

David R. Klug

Imperial College London, UK

The geometry of a drug-bound to its protein target is measured with EVV 2DIR. Of the >200 resolvable peaks at least 7 are due to specific binding. By comparing the spectrum calculated from the crystal structure with that measured by EVV 2DIR we can determine whether the structure as observed by EVV 2DIR is the same as that of the complex in the crystal structure or not.

17:00 **Boat trip – Excursion**

Departure from "De Oosterpoort", Trompsingel 27

19:00 **Conference dinner**

Location: 't Feithhuis, Martinikerkhof 10

Friday, July 1

Light Harvesting

Chair: Tomáš Mancal

08:30

Fr01

Multidimensional Spectroscopic Studies of Photosynthetic Reaction Centers

Jennifer P. Ogilvie

University of Michigan, USA

We describe two-dimensional electronic spectroscopy studies of the primary processes of energy transfer and charge separation in photosynthetic reaction centers. We compare the observation of coherent dynamics in reaction centers with control studies in monomer pigments. To probe charge separation in reaction centers, we combine two-dimensional electronic and Stark spectroscopies.

09:00

Fr02

Coherence Shift Mechanism Explains Long-Lived Beatings in Bacterial Reaction Centers

David Paleček

Lund University, Sweden

We experimentally identified a new photophysical mechanism of coherence shift from the excited to ground electronic state, occurring during energy transfer process. It provides a clear explanation for the picosecond lifetimes of the coherences in the reaction centers.

09:20

Fr03

Fluorescence Detected 2D Spectroscopy of LH2

Tõnu Pullerits

Lund University, Sweden

Fluorescence detected coherent 2D spectroscopy on peripheral light harvesting complex of photosynthetic purple bacteria LH2 reveals clean cross peaks between two major absorption bands B800 and B850. The results together with quantum dynamics simulations allow new insight to the excitation dynamics in this system.

Friday, July 1

Light Harvesting Chair: Tomáš Mancal

09:40

Fr04

2D Electronic Spectroscopy Study of Coherent and Structural Dynamical Effects in Porphyrin Chromophores

Ismael A. Heisler

University of East Anglia, UK

In order to successfully create efficient novel porphyrin based artificial light harvesting materials the excited state dynamics associated with conformational heterogeneity have to be determined and understood. Multi-timescale processes are present in conjugated molecular structures as well as coherent phenomena. Here we address early time dynamics with 2D electronic spectroscopy.

10:00

Fr05

Excitation Energy Transfer Dynamics of LHCII complexes

Howe-Siang Tan

Nanyang Technological University, Singapore

We use ultrafast ultrafast pump-probe, 3rd order 2D electronic (2DES) and 5th order 3D electronic (3DES) spectroscopies to study the excitation energy transfer dynamics of plant light-harvesting complex II, LHCII. Studies on solubilized natural and mutant trimers, as well as aggregates will be presented.

10:20

Fr06

Electronic Coherences in Rhodamine Dimers: Vibronic Coupling and Distance Dependence

Elisabetta Collini

University of Padova, Italy

2D electronic spectroscopy experiments supported by theoretical modeling on rhodamines hetero-dimers characterized by different interpigment distances and electronic interactions have been performed to clarify the role of vibronic coupling in the coherent dynamics of the systems.

Friday, July 1

Light Harvesting Chair: Tomáš Mancal

10:40

Fr07 **Revealing Quantum Coherence in Photosynthetic Complexes Using Ultrafast Spectroscopy: Simulation Studies**

Qiang Shi

Institute of Chemistry, Chinese Academy of Sciences, China

Simulations are performed to study quantum coherence in photosynthetic complexes using ultrafast spectroscopy. It is found that: (1) Different types of quantum coherence can be distinguished in pump-probe polarization anisotropy measurements. (2) Specific pulse shaping schemes are important in observing coherent energy transfer in the single molecule two-color double-pump experiment.

11:00 **Poster session II (even numbers)**

12:30 **Lunch**

Methods II Chair: Arend G. Dijkstra

13:30

Fr08 **Vibrational Solvatochromism, Intermolecular Interaction, and Femtosecond Vibrational/Electronic Spectroscopy**

Minhaeng Cho

Korea University, Korea

Current multidimensional vibrational spectroscopy in time domain provides critical information on vibrational frequency fluctuation dynamics, which is one of the vibrational solvatochromism phenomena. We here discuss a recent systematic development in vibrational solvatochromism theory and its applications to a few different systems.

Friday, July 1

Methods II Chair: Arend G. Dijkstra

14:00

Transient 2DIR Spectroscopy in a Vibrational Ladder

Fr09 Vincent Kemlin

Université Paris-Saclay, France

We perform transient two-dimensional Fourier-Transform infrared spectroscopy after vibrational ladder climbing in carboxy-hemoglobin. We will discuss how the observed diagonal and cross-peak dynamics can be related to population relaxation in this non-stationary system brought far from equilibrium.

14:20

Contact Ion-Pairing of LiOCN Under Multiple Solvent Conditions Enabled by Interfacing Microfluidics with 2D IR Spectroscopy

Fr10 Amber T. Krummel

Colorado State University, USA

We present the interfacing of IR compatible microfluidics with 2D IR spectroscopy to examine the solvatochromic pseudo-halide anion, cyanate (OCN^-) in cosolvent environments. 2D IR spectra are collected laterally across the device to capture the vibrational dynamics of OCN^- in methanol/dimethyl formamide cosolvent environments.

14:40

Alternative View of Two-Dimensional Spectroscopy

Fr11 Maxim F. Gelin

Technische Universität München, Germany

We show that femtosecond two-dimensional (2D) signals can alternatively be measured and computed as four-wave-mixing signals generated with two femtosecond pulses and two one-sided continuous-wave pulses. This alternative view allows a computationally more efficient evaluation of 2D signals and clarifies the relationship of 2D spectroscopy with other time-domain and mixed time-frequency-domain techniques.

15:00 **Closing remarks**

15:30 **Conference end**

Poster Session I (Odd Numbers)

19:00 **Wednesday, June 29**

P01

Water Hydrogen-Bonding Dynamics at Different Phases of Lipid Multibilayer: Femtosecond Mid-IR Pump-Probe Spectroscopy

Achintya Kundu, Minhaeng Cho

Institute for Basic Science, Korea University, SEOUL, Korea

The water hydrogen-bonding dynamics at different phases of lipid-multibilayer are studied by femtosecond Mid-IR pump-probe spectroscopy. We observe existence of two different vibrational lifetime components (phosphate-associated water and choline-associated water). Vibrational lifetime of phosphate-associated water remains constant, whereas other component slows down in a sigmoidal fashion upon lipid phase transition.

P03

Dynamics of the Excited Electronic States of Pyrene in the Deep UV

Alessandra Picchiotti[1], Valentyn I. Prokhorenko[1], Artur Nenov[2], Angelo Giussani[2], Marco Garavelli[2], R.J. Dwayne Miller[1]

[1]Max Planck Institute for the Structure and Dynamics of Matter, HAMBURG, Germany

[2]University of Bologna, BOLOGNA, Italy

We investigated pyrene using electronic two-dimensional, heterodyne transient grating, and transient absorption spectroscopies in a 250-300 nm spectral range. We resolved several cross-peaks and oscillations providing an insight to the S_3 vibronic excited state. Our findings are corroborated by theoretical simulations resulting in multiple oscillating diagonal and off-diagonal peaks.

P05

Benchmarking Spectral Simulation Protocols for Amide I

Ana V. Cunha, Anna S. Bondarenko, Thomas L.C. Jansen

University of Groningen, GRONINGEN, The Netherlands

A benchmark of amide I spectral simulation protocols is presented. Results allow choosing the optimal frequency mapping and coupling model for the tested force fields. We further find that due to the sensitivity of two-dimensional spectroscopy there is room for improving the protocols.

2D Raman-THz Spectroscopy of Aqueous Salt Solutions

P07 Andrey Shalit, Saima Ahmed, Peter Hamm

Universitat Zurich, ZURICH, Switzerland

The ultrafast time-resolved 2D Raman-THz spectroscopy was applied to study the dynamics of hydrogen bond networks in the aqueous solutions of the chloride salts. We demonstrate that the extent of the echo signal along the correlated $t_1=t_2$ coordinate correlates with the viscosity of the solution.

New Simulations of 2D spectra of Photosystem II Reaction Center

P09 Andrius Gelzinis[1], S. Seckin Senlik[2], Jennifer P. Ogilvie[2], Darius Abramavicius[1], Leonas Valkunas[1]

[1]*Vilnius University, VILNIUS, Lithuania*

[2]*University of Michigan, ANN ARBOR, United States of America*

Two dimensional spectra of photosystem II reaction center are simulated and compared with experimental results. Significant improvement comparing with previous simulations is achieved, by using a more suitable theoretical approach and updated model parameters.

Excitation Energy Transfer in Multichromophoric Systems

P11 Anna S. Bondarenko, Thomas L.C. Jansen, Jasper Knoester

University of Groningen, GRONINGEN, The Netherlands

Different methods are tested for determining the excitation energy transfer rate in a model of coupled ring systems, a situation where conventional Förster theory is breaking down. The study on simple systems can help better understanding of validity and applicability of different approaches, when studying bigger systems.

Modeling 2DUV Spectra of Nucleobases: Damped Dynamics Through Conical Intersections

P13 Arend G. Dijkstra, Jason D. Biggs, Michal A. Kochman, Alessandra Picchiotti, Valentyn I. Prokhorenko, R.J. Dwayne Miller

Max Planck Institute for the Structure and Dynamics of Matter, HAMBURG, Germany

We propose a model of damped dynamics on potential energy surfaces that exhibit conical intersections. The resulting ultrafast populations are compared with experimental 2DUV spectra.

Towards 2D Spectroscopy of Molecular Aggregate Formation

P15

Björn Kriete, Maxim S. Pshenichnikov

University of Groningen, GRONINGEN, The Netherlands

The self-assembly dynamics of tubular J-aggregates were investigated by combining time-resolved spectroscopy and microfluidics. By projecting the aggregate formation process into space, this novel lab-on-a-chip approach could reveal intermediate aggregation species.

A Robust, Fully Automated Algorithm to Collect High Quality OPA Tuning Curves

P17

Blaise J. Thompson, Schuyler Kain, Daniel D. Kohler, Paul Hebert, John C. Wright

University of Wisconsin-Madison, MADISON, United States of America

Motorized optical parametric amplifiers (OPAs) are increasingly common, but frequency domain experiments remain difficult, due in part to unreliable and irreproducible OPA tuning curves. We have developed an automated OPA tuning routine that produces robust, high quality tuning curves quickly.

Water and Oil Do Mix: Structure and Dynamics of Water in Triglyceride Oils

P19

Carien C.M. Groot[1], K.P. Velikov[2], H.J. Bakker[1]

[1]*FOM Institute AMOLF, AMSTERDAM, The Netherlands*

[2]*Utrecht University, UTRECHT, The Netherlands*

The hydrogen-bond structure and dynamics of water in triglycerides triacetin, tributyrin and trioctanoin are studied using linear IR and 2D IR spectroscopy. We identify several stable (>20ps) water configurations: water clusters, waters with a single hydrogen bond to the triglyceride and waters with two hydrogen bonds to the triglyceride.

Investigating the Dynamics of Interfacial Ester Carbonyls in Lipid Bilayers

P21

Carlos R. Baiz, Sean C. Edington, Mason L. Valentine, Jennifer C. Flanagan

University of Texas-Austin, AUSTIN, United States of America

We present a general approach for parameterizing vibrational maps using input from experimental FTIR and 2D IR spectra. We develop an electrostatic map to model IR linear and nonlinear spectra of ester C=O vibrations in lipids, and we apply it to simulate spectra of lipid bilayers under different hydration conditions.

Understanding the Two-dimensional Electronic Spectra Peak Shapes of CdSe Quantum Dots

P23

Cheng Zhang, Thanh Nhut Do, Howe-Siang Tan

Nanyang Technological University, SINGAPORE, Singapore

CdSe nanocrystal quantum dots are studied by Two-dimensional Electronic Spectroscopic technique with a pump-probe geometry. Zero Line Slope analysis is performed to investigate the homogeneous and inhomogeneous broadening effects in the 2D spectra.

Ultrafast Dynamics of Carboxy-Hemoglobin: Two-Dimensional Infrared Spectroscopy Experiments and Simulations

P25

Cyril Falvo[1], Louis Daniault[2], Thibault Vieille[2], Vincent Kemlin[2], Jean-Christophe Lambry[2], Christoph Meier[3], Marten Vos[2], Adeline Bonvalet[2], Manuel Joffre[2]

[1]*Université Paris Sud, ORSAY, France*

[2]*Ecole Polytechnique, PALAISEAU, France*

[3]*Université Paul Sabatier, TOULOUSE, France*

We present high-resolution 2D-IR measurements and detailed simulations of HbCO with a good agreement between theory and experiment. The simulation shows the strong effect of the distal histidine through a hydrogen bond, which is responsible for the slow decay of the frequency-frequency correlation function.

Calculation of Two-Dimensional Spectra Using the Stochastic Hierarchy of Pure States (HOPS)

P27

Z. Li, P.-P. Zhang, A. Eisfeld

Max-Planck Institute, DRESDEN, Germany

Reliable theoretical calculations necessary for the correct interpretation of two-dimensional spectra are impeded by large system sizes and vibrational degrees of freedom Here we demonstrate that a numerical approach based on a stochastic hierarchy of pure states (HOPS) does allow to calculate two-dimensional spectra, notwithstanding the stochasticity of our method.

Theory of Femtosecond Double-Pulse Single-Molecule Spectroscopy

P29

Elisa Palacino González, Maxim F. Gelin, Wolfgang Domcke

Technical University of Munich (TUM), GARCHING, Germany

We have performed simulations of single-molecule fluorescence signals, excited by two phase-locked pump pulses, for several models with strong intramolecular electronic and electron-vibrational couplings. The signals can be decomposed into population and coherence contributions. We explored how the initial preparation of the molecular system manifests itself in the fluorescence signal.

2D IR Spectroscopy on OH Stretch in Diluted Alcohols

P31

Evgeniia Salamatova[1], Keisuke Shinokita[2], Ana V. Cunha[3], Thomas L.C. Jansen[3], Maxim S. Pshenichnikov[3]

[1]*Zernike Institute for Advanced Materials, GRONINGEN, The Netherlands*

[2]*Max-Born-Institut für Nichtlineare Optik und Kurzzeitspektroskopie, BERLIN, Germany*

[3]*University of Groningen, GRONINGEN, The Netherlands*

Hydrogen bond (HB) dynamics of strongly diluted alcohols were studied with 2D IR spectroscopy and combined molecular dynamics - spectral simulations on the OH stretching mode. For eight studied alcohols, the HB dynamics have similar behavior with fast (~200 fs) initial relaxation and long (3 ps) tail.

Impact of the Double-Single Strand Transition on Vibrational Coupling and Spectral Diffusion in an AT-15mer

P33

Gordon Hithell[1], Daniel J. Shaw[1], Gregory M. Greetham[2], Paul M. Donaldson[2], Michael Towrie[2], Glenn A. Burley[1], Anthony W. Parker[2], Neil T. Hunt[1]

[1]*University of Strathclyde, GLASGOW, United Kingdom*

[2]*STFC Central Laser Facility, DIDCOT, United Kingdom*

Ultrafast 2D-IR spectroscopy has been used to study the double-single strand transition of an AT-15mer DNA duplex. Changes in the 2D-IR spectra with temperature correlate with duplex melting and provide new insight into changes in vibrational coupling and spectral diffusion accompanying loss of Watson-Crick base pairing.

2D Infrared Spectroscopy of High Pressure Phases of Ice

P35

Halina Tran[1], Ana V. Cunha[2], Jacob J. Shephard[3], Andrey Shalit[1], Thomas L.C. Jansen[2], Christoph G. Salzmann[3], Peter Hamm[1]

[1]*University of Zürich, ZÜRICH, Switzerland*
[2]*University of Groningen, GRONINGEN, The Netherlands*
[3]*University College London, LONDON, United Kingdom*

The OH-stretch vibration of ice is complex and the assignment of distinct peaks of the OH-band remains controversial. We present 2D IR spectra of hydrogen ordered phases of ice. They exhibit distinct features that can aid the understanding of the coupling processes that underlie the OH-stretch mode.

Signatures of Charge Separation in the Reaction Center of PSII Revealed by 2D Electronic Spectroscopy

P37

Hong-Guang Duan[1], Emilie Wientjes[2], Roberta Croce[2], Michael Thorwart[3], Valentyn I. Prokhorenko[1], R.J. Dwayne Miller[1]

[1]*Max-Planck Institute, HAMBURG, Germany*
[2]*University of Groningen, GRONINGEN, The Netherlands*
[3]*University of Hamburg, HAMBURG, Germany*

Charge separation in the Photosystem II (PSII) reaction center (RC) was studied with 2D electronic spectroscopy at ambient conditions. Primary charge separation and associated timescale (1.5 ps) are identified by comparison of measured and calculated 2D decay-associated-spectra (2DDAS). For the modelling, we applied a tight-binding Hamiltonian.

Vibration-Mediated Coherent Mixing of Exciton and Polaron Pair In a Conjugated Polymer

P39

James Lim[1], Antonietta De Sio[2], Filippo Troiani[3], Ephraim Sommer[2], Margherita Maiuri[4], Julien Réhault[4], Susana F. Huelga[1], Martin B. Plenio[1], Giulio Cerullo[4], Elisa Molinari[3], Christoph Lienau[2]

[1]*Universität Ulm, ULM, Germany*
[2]*Carl von Ossietzky Universität, OLDENBURG, Germany*
[3]*Istituto Nanoscienze - CNR, MODENA, Italy*
[4]*IFN-CNR, MILANO, Italy*

Coherent electronic and vibronic features in the two-dimensional (2D) electronic spectra of a conjugated polymer where polaron pairs are formed on a sub-100 fs timescale are investigated theoretically. We identify signatures of coherent couplings and demonstrate that incoherent models cannot account for 2D spectra that have recently been obtained experimentally.

P41 Surface-Enhanced 2D Attenuated Total Reflectance IR Spectroscopy for Studying Surface-Sensitive Ultrafast Vibrational Dynamics

Jan Philip Kraack, Peter Hamm

University of Zürich, ZÜRICH, Switzerland

We present our latest developments towards establishing 2D attenuated total reflectance (ATR) IR spectroscopy as a versatile, surface-sensitive method for obtaining ultrafast vibrational signals from solid-liquid interfaces. Surface-enhancement mechanisms are characterized in detail and we report the development of 2D ATR IR for spectroelectrochemistry at electrode surfaces.

P43 Rotational Dynamics of Solutes with Multi-Rotational Axes in 1-Alchohol Solutions Studied by Infrared Pump-Probe Spectroscopy

Masaki Okuda, Kaoru Ohta, Keisuke Tominaga

Kobe University, KOBE, Japan

We observed the anisotropy decays of N_3 derivatized amino acids in the primary 1-alcohols with infrared pump-probe spectroscopy. From the temperature dependence of the rotational relaxation time, it is suggested that there are some correlations between rotational motions of the azide group and the nearby alkyl chain.

P45 Photocurrent Detected Two-Dimensional Spectroscopy of InP Nanowire Array Solar Cell

Khadga J. Karki, Gaute Otnes, Magnus Borgström, Tõnu Pullerits

[1]Lund University, LUND, Sweden

Photocurrent detected two-dimensional spectroscopy is used to study the effect of excitations in InP nanowire array solar cell. Results show instantaneous changes in the band structure of the semiconductor material due to the excitation of electrons into the conduction band. Possible mechanisms that lead to the changes are discussed.

P47 Solvation Dynamics of Concentrated Aqueous Polymer Mixtures: A Two-Dimensional Infrared Spectroscopy Study

Kimberly R. Daley, Kevin J. Kubarych

University of Michigan, ANN ARBOR, United States of America

Two-dimensional infrared spectroscopy is used to explore the chemical dynamics of crowded polymer mixtures. Using a transition metal carbonyl probe in solution, we find unexpected polymer length and concentration dependent dynamics in D_2O.

Investigating Nonadiabatic Photoisomerization Dynamics of Phytochrome Cph1 Using 2D ES

P49

Laurie A. Bizimana, Johanna Brazard, Daniel B. Turner

New York University, NEW YORK, United States of America

We use high-sensitivity two-dimensional electronic spectroscopy (2D ES) to directly probe the conformational heterogeneity of the ground state populations in phytochromes. The sub-100 fs population dynamics of the P_{fr} to P_r reaction indicate photoisomerization proceeds through a conical intersection.

Time-Resolved Vibrational Spectroscopy of Coumarin Cages Which Can Trigger Fast Bio/Chemical Reactions

P51

Luuk J.G.W. van Wilderen[1], Carsten Neumann[2], Daniela Kern-Michler[2], Nicole Seibert[2], Alexandre Rodrigues Correia[3], Matiss Reinfelds[3], Alexander Heckel[3], Jens Bredenbeck[2]

[1]*Johann Wolfgang Goethe-University, FRANKFURT AM MAIN, Germany*

[2]*Institute of Biophysics, Johann Wolfgang Goethe-University, FRANKFURT AM MAIN, Germany*

[3]*Institute of Organic Chemistry and Chemical Biology, Goethe-University, FRANKFURT AM MAIN, Germany*

The uncaging mechanism of the coumarin cage DEACM has been investigated and uncaging was resolved on a picosecond time scale, putting DEACM among the fastest known photocages. The influence of the solvent environment is investigated for two different attached leaving groups (LGs), i.e. azide and thiocyanate.

General Vibrational Spectroscopies with Wilson

P53

Magnus Ringholm, Dan Jonsson, Kenneth Ruud

Centre for Theoretical and Computational Chemistry, TROMSØ, Norway

We present an approach to simulate any elastic frequency-resolved vibrational spectroscopy where the incident lasers are in the infrared or ultraviolet/visible range, detuned from any electronic resonances, using a recursive scheme to identify the relevant contributions to the spectroscopic process. The approach is implemented in the computer program Wilson.

Signatures of Förster and Dexter Couplings between Quantum dots in 2D Spectroscopy

P55

Marten Richter, Judith F. Specht

Institut für Theoretische Physik, Technische Universität Berlin, BERLIN, Germany

Two major types of coupling mechanism lead to excitation energy transfer between nanostructures: Dexter- and Förster coupling. We show theoretically, that both couplings between two quantum dots can be distinguished by the double quantum coherence spectroscopy technique.

Structure and Dynamics of Solvated Protons in Water Studied with 2D IR Spectroscopy

P57

Martin Thämer[1], Luigi De Marco[2], Andrei Tokmakoff[2]

[1]*Fritz-Haber-Institut der Max-Planck-Gesellschaft, BERLIN, Germany*

[2]*University of Chicago, CHICAGO, United States of America*

Using ultrafast 2D IR spectroscopy we investigated the structures adopted by excess protons in water and their dynamics which drive the proton transfer process. Our results give insight into the role of the Zundel complex in the proton transfer mechanism.

Detection of Conical Intersection from the Vibrational Coherences

P59

Marwa Farag, Thomas L.C. Jansen, Jasper Knoester

Zernike Institute for Advanced Materials, GRONINGEN, The Netherlands

Vibrational coherences can be considered as a tool to detect the Conical Intersection (CI), because the wavepacket motion is affected by the surface crossing. Here, we identify the spectroscopic signatures associated with CI by analyzing the coherent wavepacket motions extracted from the linear absorption (1D) and two-dimensional electronic spectra (2DES).

Two-Dimensional Terahertz-Spectroscopy on Aspirin

P61

Giulia Folpini, Klaus Reimann, Michael Woerner, Thomas Elsaesser

Max Born Institute, BERLIN, Germany

Ultrafast phonon dynamics in polycrystalline Aspirin is studied with 2D THz spectroscopy. The hybrid mode of the CH3-rotations with collective oscillations of the p-electrons shows a nonlinear absorption around 1.4 THz that leads to a coherent emission at 1.9 THz pointing to a dynamic breakup of the strong electron-phonon correlations.

Wavelet filter for Femtosecond Stimulated Raman Spectroscopy: a new approach brings new horizons

P63

Miroslav Kloz[1,2], Jörn Weißenborn[1], Yusaku Hontani[1], John T.M. Kennis[1]

[1]*VU University Amsterdam, AMSTERDAM, The Netherlands*
[2]*Institute of Physics ASCR, PRAGUE, Czech Republic*

A new method for recording Raman spectra was developed that dramatically improves and automatizes baseline problems. Instead of using a narrowband Raman source, the experiment is performed using shaping of a broadband source. This allows locking the signal into carefully crafted watermarks that can be recognized from background.

Studying Energy Transfer Dynamics in Light Harvesting Complex II using 2D Electronic-Vibrational Spectroscopy

P65

Nicholas H.C. Lewis[1], Thomas A.A. Oliver[2], Matteo Ballottari[3], Natalie L. Gruenke[1], Roberto Bassi[3], Graham R. Fleming[1]

[1]*University of California, Berkeley, BERKELEY, United States of America*
[2]*School of Chemistry, University of Bristol, BRISTOL, United Kingdom*
[3]*Dipartimento di Biotecnologie, Facoltà di Scienze, Università di Verona, VERONA, Italy*

Excitation energy transfer dynamics in the photosynthetic protein LHCII from spinach, are studied using 2D electronic-vibrational spectroscopy. We show how energy transfer from Chl *b* to Chl *a* and can be directly observed in LHCII using this multidimensional technique, revealing previously unobserved steps in the excitation transfer pathway.

Coherent 2D Spectroscopy of Pentacene Thin Films

P67

Lars Mewes, André Al Haddad, Paul Gratia, Philippe Bugnon, Christopher A. Arrell, Frank Van Mourik, Majed Chergui

EPFL, LAUSANNE, Switzerland

We present our results on the photo induced dynamics inside a prototypical organic thin film semiconductor, namely pentacene. Measurements were performed on our recently commissioned visible 2D photon echo spectrometer, which covers a spectral range between 500 to 950 nm and provides sub-10 fs passively phase stabilized pulses.

Two-Dimensional Infrared Spectroscopy of a Site-Specifically Labeled Photoswitchable Allosteric Protein

P69

Olga R. Bozovic, Brigitte Stucki-Buchli, Philip J.M. Johnson, Klemens L. Koziol, Claudio Zanobini, Peter Hamm

University of Zürich, ZURICH, Switzerland

We have measured 2D-IR difference spectra for several different mutants of the PDZ2 domain protein using azidohomoalanine as a label. The 2D-IR difference spectra upon inducing the conformational change of a site-specifically labeled protein, as well as difference spectra for temperature depending unfolding of the protein are reported.

100 kHz 2D-IR Spectroscopy. Applications of a Fast, Sensitive Spectrometer to Chemical and Biochemical Problems

P71

Paul Donaldson, Greg Greetham, Rex Manurung, Tony Parker, Mike Towrie

Central Laser Facility, DIDCOT, United Kingdom

We present a 2D-IR spectrometer with a 100 kHz acquisition rate built around Yb:KGW amplifier technology. We demonstrate that the increased sensitivity and speed is a significant step forward for on the fly spectroscopy of chemical reactions and for the sensitive detection of protein labels at low concentrations.

Multistate DNA Oligonucleotide Dissociation Revealed Through FTIR, 2D IR, and t-HDVE Spectroscopy

P73

Paul J. Sanstead, Paul Stevenson, Andrei Tokmakoff

University of Chicago, CHICAGO, United States of America

The dehybridization of DNA oligonucleotides is studied with a combination of FTIR, 2D IR, and temperature jump t-HDVE spectroscopies. Nucleobase sequence is found to dictate the dissociation mechanism, with timescales of ~10 μs assigned to strand dissociation and ~70 ns assigned to premelting events such as duplex fraying.

Heterogeneous Protein-Ligand Binding Determined by 2D IR Spectroscopy with the Unnatural Amino Acid Azidohomoalanine

P75

Philip J.M. Johnson, Klemens L. Koziol, Peter Hamm

University of Zürich, ZURICH, Switzerland

Using azidohomoalanine as a vibrational probe of local protein structure, we observe multiple ligand binding conformations for C-terminal Aha mutated ligands when bound to a PDZ2 domain, manifest as multiple distinct frequency shifts from the unbound ligand bleach response as observed by 2D IR spectroscopy.

Mapping the Evolution of Spatial Exciton Coherence Through Time-Resolved Fluorescence

P77

Roel Tempelaar[1], Frank C. Spano[2], Jasper Knoester[3], Thomas L.C. Jansen[3]

[1]*Columbia University, NEW YORK, United States of America*

[2]*Temple University, PHILADELPHIA, United States of America*

[3]*University of Groningen, GRONINGEN, The Netherlands*

We demonstrate that time-resolved fluorescence allows one to continuously monitor exciton coherence between molecules featuring a pronounced vibronic progression. The degree of coherence is shown to be directly reflected in the spectral vibronic peaks. Fluorescence excludes ground state vibrations, which makes this excited state coherence measure unambiguous to interpret.

Tracking Electron and Hole Relaxation Dynamics in CdTe Nanorods by 2D Electronic Spectroscopy

P79

Tatjana Stoll[1], Federico Branchi[1], Ilka Kriegel[2], Francesco Scotognella[1], Giulio Cerullo[1]

[1]*Politecnico di Milano, MILAN, Italy*

[2]*Instituto Italiano di Tecnologia (IIT), MILAN, Italy*

We present new insights into the exciton dynamics from two-dimensional electronic spectroscopy on CdTe nanorods. Tracing of state-resolved energy relaxation dynamics allowed us to resolve the dynamics of both electron and hole transitions.

P81 Spectral Manifestation of C_2 Modulation of the LH2 Complex of Purple Bacteria

Tenzin Kunsel, Thomas L.C. Jansen, Jasper Knoester

Zernike Institute for Advanced Materials, GRONINGEN, The Netherlands

C_2 modulation in the B850 rings was suggested from single-molecule studies. It can manifest in various forms; five of which are discriminated based on single-molecule, linear and two-dimensional spectroscopy. We find that a model with C_2 modulated diagonal disorder fits best with all the experimental results.

Probing State- and Size-Dependent Line Broadening in CdSe Nanocrystals Using 2D ES

P83

Tobias A. Gellen, Daniel B. Turner

New York University Department of Chemistry, MANHATTAN, United States of America

Two-dimensional electronic spectroscopy (2D ES) can separate the homogeneous and inhomogeneous linewidths of CdSe nanocrystals. We find that, in contrast to inhomogeneous linewidths, homogeneous linewidths are relatively insensitive to both electronic state and nanocrystal size. This suggests that solvent effects dominate homogeneous line broadening.

Vibronically Mediated Exciton Transfer in Perylene Dimers

P85

Václav Perlík[1], Vladislav Sláma[1], Tomáš Mančal[1], František Šanda[1], Eberhard Riedle[2], Craig Lincoln[3], Jüergen Hauer[3]

[1]Charles University Prague, PRAHA 2, Czech Republic

[2]LS fur BioMolekulare Optik, LMU MUNCHEN, Germany

[3]Photonics Institute, TU Wien, VIENNA, Austria

Exciton transfer in molecular dyads depends critically on the spatial arrangement of donor and acceptor. Orthogonal perylene bisimide dimers exhibit transfer faster than expected from Förster theory. We show how the interplay of electronic dynamics with underdamped high frequency vibrational modes acts as a mechanism for fast transfer.

Intra- and Intermolecular Vibrational Coupling in a Polymerization Reaction

P87

Valeri Kozich, Theodore von Haimberger, Karsten Heyne

Freie Universität Berlin, BERLIN, Germany

Vibrational coupling of N=C=O stretching vibration at 2270 cm^{-1} with lower frequency modes in two reactants of a polymerization reaction are studied with 2D IR spectroscopy. The observed coupling with 1530 cm^{-1} modes indicates that this vibration could contribute to the chemical reaction coordinate.

Interfacial Hydration Dynamics in Cationic Reverse and Regular Micelles Using 2D-IR

P89

Ved Prakash Roy, Kevin J. Kubarych

University of Michigan, ANN ARBOR, United States of America

We use thiocyanate ions to probe interfacial hydration dynamics in regular and reverse micelles using ultrafast 2D-IR. The affinity of the anion for the cationic interfaces enables examination of dynamics independent of surface curvature.

Comparison of Coherent Oscillations in 2DES studies of Bacterial Reaction Centers and Bacteriochlorophyll a

P91

Veronica Policht, Andrew Niedringhaus, Jennifer Ogilvie

University of Michigan, ANN ARBOR, United States of America

We use two-dimensional electronic spectroscopy to study the coherent dynamics of photosynthetic Bacterial Reaction Centers (BRC) and monomeric Bacteriochlorophyll a (BChl a), the most abundant pigment in BRCs. We find several coherent modes common to both systems and consider the origin of the coherent dynamics.

2D-IR Spectroscopy of Water Molecules in a Hydrated Lithium Nitrate Crystal

P93

Wilbert J. Smit, Huib J. Bakker

FOM Institute AMOLF, AMSTERDAM, The Netherlands

Water molecules in lithium nitrate trihydrate have a well-defined geometrical arrangement and contain three distinct hydrogen-bond strengths: strong, bifurcated, and weak. The vibrational relaxation dynamics of the three distinct OD stretch vibrations of dilute HDO molecules is studied using 2D IR pump-probe spectroscopy in the temperature range 22-295 K.

Vibrational Spectroscopy and Dynamics of $W(CO)_6$ in Solid Methane as a Probe of Lattice Properties

P95

Wutharath Chin[1], Raphaël Thon[2], Didier Chamma[3], Jean-Pierre Galaup[4], Claudine Crépin[1]

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[2]*CNRS DR4, GIF-SUR-YVETTE, France*

[3]*LAMPS Univ. de Perpignan, PERPIGNAN, France*

[4]*LAC CNRS-Univ. Paris Sud, ORSAY, France*

The phase transition of solid methane is observed through the vibrational spectroscopy of $W(CO)_6$ guest molecule and through its dynamics characterized by time-resolved four-wave mixing experiments. The specificities of the methane lattice are highlighted by surprising behaviors in the vibrational dynamics of the guest in the 5-35 K temperature range.

Direct Observation of Liquid-Liquid Transitions in Aqueous Solutions

P97

Sander Woutersen[1], Michiel Hilbers[1], Jeroen R. Bruijn[1], Tibert H. Van der Loop[1], C. Austen Angell[2]

[1]*University of Amsterdam, AMSTERDAM, The Netherlands*

[2]*School of Molecular Sciences, Arizona State University, TEMPE (AZ), United States of America*

We investigate structural changes during liquid-liquid transitions in supercooled aqueous solutions. In glycerol solution the transition involves nanoscopic phase separation, but in N_2H_5TFA solution both liquid states are homogeneous at the molecular level. The implied existence of two liquid phases in supercooled water provides a unified explanation for its anomalies.

Energy flow between spectral components in 2D broadband stimulated Raman spectroscopy

P99

G. Fumero[1], G. Batignani[1,2], S. Mukamel[3], T. Scopigno[1]

[1]*Dipartimento di Fisica, Sapienza, Università di Roma.*

[2]*Dipartimento di Scienze Fisiche e Chimiche, Università degli Studi dell'Aquila.*

[3]*Department of Chemistry, University of California, Irvine.*

We introduce a general theoretical description of non-resonant 2D broadband stimulated Raman spectroscopy in a multimode model. Upon impulsive excitation, coherences induced in the low frequency modes modulate the Raman signal in time. Monitoring the transmitted intensity, we elucidate the mechanism underlying the energy redistribution pathway between probe field modes.

Poster Session II (Even Numbers)

11:00 **Friday, July 1**

Vibrational-Coherence Measurement of Nonequilibrium Quantum Systems by Four-Wave Mixing

P02

Alexander Schubert[1], Cyril Falvo[2], Christoph Meier[3]
[1]*University of Michigan, ANN ARBOR, United States of America*
[2]*ISMO, Univ. Paris-Sud, Université Paris-Saclay, ORSAY, France*
[3]*LCAR, IRSAMC, Université Paul Sabatier, TOULOUSE, France*

Within a four wave mixing set up, coherences in non-equilibrium quantum systems are shown to lead to signal emission in directions opposite to the ones usually considered. Since this emission is generated uniquely by the coherences, a background-free measurement should be possible by placing the detectors in specific, unconventional directions.

Coherent Vibrational Coupling in Singly Fused Diporphyrins

P04

Andre Al Haddad[1], Lars Mewes[1], Jesse Bergkamp[2], Silvio Decurtins[2], Majed Chergui[1]
[1]*EPFL, LAUSANNE, Switzerland*
[2]*University of Bern, BERN, Switzerland*

Electronic and vibrational dynamics of singly-fused diporphyrins with different metal centers are studied by 2D visible spectroscopy and ultrafast transient absorption spectroscopy. By investigating the timescales between 10 fs and 7 ps, we witness the rise of the coupling between the Q bands.

Structural Transformations and Hydrogen Bond Reorganization of Liquid Water Under High-Pressure Conditions

P06

Andrea Lapini[1], Chiara Calvagna[1], Samuele Fanetti[1], Marco Pagliai[2], Margherita Citroni[1], Mariangela di Donato[1], Sandro Scandolo[3], Roberto Righini[1], Roberto Bini[1]
[1]*University of Florence, SESTO FIORENTINO (FIRENZE), Italy*
[2]*Scuola Normale Superiore di Pisa, PISA, Italy*
[3]*International Centre for Theoretical Physics, TRIESTE, Italy*

We used Non-linear Infrared Spectroscopy (pump-probe and 2D-IR) to study the structural modification and the hydrogen bond reorganization in pure water and in aqueous ionic solution as a function of pressure and temperature.

Time-Frequency Methods for Coherent Spectroscopy

P08

Andrea Volpato, Elisabetta Collini

University of Padova, PADOVA, Italy

Time-frequency decomposition techniques, borrowed from the signal-processing field, are adapted and applied to the analysis of 2D oscillating signals. Synthetic signals are used to optimize and benchmark the performances of several time-frequency approaches. The methods are applied on sample 2D electronic spectroscopy data of a common dye.

Are Cataracts an Amyloid Disease? 2D IR Spectra Say YES!

P10

Ariel M. Alperstein, Tianqi O. Zhang, Martin T. Zanni

University of Wisconsin-Madison, MADISON, WISCONSIN, United States of America

Cataracts are caused by the aggregation of proteins in the eye lens. Many *in vitro* experiments result in amyloid fibrils, but no fibrils have been found in the lens tissue. We measure cataractous lens tissue using 2D IR spectroscopy and observe the cross peak signature of amyloid fibril formation.

Photoluminescence Anisotropy in Organic Semiconducting Single Crystals

P12

Artur Mannanov[1], Maxim S. Kazantsev[2], Oleg V. Borshchev[3], Sergey A. Ponomarenko[3], Dmitry Yu. Paraschuk[4], Maxim S. Pshenichnikov[1]

[1]*University of Groningen, GRONINGEN, Netherlands*

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Time-resolved photoluminescence (PL) anisotropy is studied in novel thiophene-phenylene co-oligomers single crystals. PL is mainly polarized along the molecular backbones regardless of the excitation polarization. PL induced by orthogonal polarizations, has very different time signatures. The origin of such PL behavior is discussed in relation to the molecular packing.

Observation of Long-Lived Coherence in the Metalorganic System Cobalt/Alq3

P14

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The hybrid metalorganic interface Co/Alq3 is investigated with kinetic-energy-resolved coherent 2D photoemission spectroscopy. Long-lived coherent excited states of the adsorbate are probed via coupling to the substrate in a single-photon photoemission process.

Molecular Origin of the Extensibility of Fibrin

P16

Biplab Dutta, Yves Rezus

AMOLF, AMSTERDAM, The Netherlands

We report on the design and construction of a novel shear cell for performing in-situ 2DIR spectroscopy on protein gels under mechanical shear. The shear cell will be used to study the molecular origin of the extensibility of fibrin.

Species-selective photochemistry of coumarin-cages by VIPER 2D-IR

P18

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Johann Wolfgang Goethe-Universität, FRANKFURT/MAIN, Germany

We demonstrate the species-selective spectroscopy of a mixture of isotopomers of a photocage. In order to select an isotopomer and monitor its photochemistry, the VIPER 2D-IR pulse sequence is used, employing resonant vibrational pre-excitation followed by an off-resonant visible-pump pulse.

Analytical Solutions to the Bloch Model for Multidimensional Coherent Spectroscopy with Gaussian Pulse Envelopes

P20 Christopher L. Smallwood[1], Travis M. Autry[2], Steven T. Cundiff[3]

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[2]*University of Colorado / NIST, BOULDER, United States of America*

[3]*University of Michigan, ANN ARBOR, United States of America*

We present third-order analytical solutions to the optical Bloch equations under the assumption of perturbative laser pulses with Gaussian envelopes. The treatment shows that off-resonant interactions can affect both signal amplitude and phase.

2D-Photon Echo on Chlorophyll a: Relaxation Dynamics of the Q_y band

P22 Cristina Leonardo, Elena Meneghin, Elisabetta Collini

University of Padova, PADOVA, Italy

2D-PhotonEcho is particularly suitable in the analysis of coherent relaxation dynamics in complex systems. The use of different laser bandwidths, carefully tuned to sweep specific energy ranges, enables the characterization of dynamics in Chl a involving different vibrational coherences and their description beyond the simplified model of the displaced oscillator.

2D Lineshape of a Fano Model

P24 Daniel Finkelstein-Shapiro[1], Felipe Poulsen[2], Tõnu Pullerits[1], Thorsten Hansen[2]

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We present the analytical expressionof the 2D lineshape of a Fano system coupled to a Markovian bath. We discuss its most prominent features as well asthe physical parameters of the system that can be accessed.

Structure and Dynamics in Non-canonically H-Bonded RNAs

P26 David A. Price, Zachary J. Kartje, Tayler D. Hill, Gisela Cairó Baza, Keith T. Gagnon, Sean D. Moran

Southern Illinois University Carbondale, CARBONDALE, IL, United States of America

We are investigating effects of salt conditions on structure in G-rich nucleic acids that are implicated in neurodegenerative diseases. We have observed frequency shifts using FTIR and confirmed structure change in short G-repeat sequences. Using 2D IR spectroscopy, we will examine vibrational coupling and ultrafast dynamics in these RNA complexes.

Two-Dimensional Electronic Spectroscopy of Biomimetic Light-Harvesting Antennas

P28

Elena Meneghin, Marina Gobbo, Andrea Volpato, Luca Bolzonello, Francesca Biscaglia, Elisabetta Collini

University of Padova, PADOVA, Italy

The structural features that could support quantum phenomena in photosynthesis are quite difficult to unravel in complex biological light-harvesting systems. We designed self-assembling chromophore-peptide conjugates in order to mimic natural antennas and we followed their excitonic states dynamics with two-dimensional electronic spectroscopy.

Isolation and Characterization of Individual Interfacial Quantum Dots Using 2D Coherent Spectroscopy

P30

Eric W. Martin, Steven T. Cundiff

University of Michigan, ANN ARBOR, United States of America

Via an original collinear multidimensional coherent spectroscopy (MDCS) technique, we resolve and measure individual oscillators in a layer of interfacial quantum dots. Only a few oscillators are excited by focusing tightly, which is possible in a fully collinear geometry. Unfolding the signal spectrum in 2D further isolates the emitters.

Quantum Beats in the Fenna-Matthews-Olson Complex

P32

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Long- and short-lived quantum beats observed in the ultrafast dynamics of the FMO complex are studied at cryogenic temperature by polarization-controlled 2D electronic spectroscopy. The observed response can be explained with a straight-forward vibronic model that does not require correlated bath interactions.

Intramolecular Vibrations in 2D Electronic Spectroscopy (2D-ES) under Different Excitation Conditions

P34

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2D-ES is ideally suited to study electronic or vibrational molecular couplings. However, unravelling the origin of the ensuing coherences can prove challenging, as similar features arise from distinct physical processes. Vibrations coupled to electronic transitions are ubiquitous and here we explore their signatures in 2D spectra under different excitation conditions.

Finite Pulse Effects in 2D Electronic Spectroscopies

P36

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When modelling experimental 2D spectra, the effects of finite pulse durations are usually neglected to optimize computational costs. We present analytic treatment of finite pulse duration effects on electronic 2D spectra. While k_i and k_{ii} signals are rather robust, the double quantum signal k_{iii} shows unexpected but readily interpreted dependencies.

Probing the Molecular Origin of the Viscosity of Hyaluronic Acid Solutions by 2D-IR Spectroscopy

P38

Giulia Giubertoni, Biplab Dutta

FOM Institute Amolf, AMSTERDAM, The Netherlands

We use 2D-IR spectroscopy to study the spectral diffusion dynamics of the carbonyl vibrations of hyaluronic acid in highly viscous solutions. These measurements will provide insight into the molecular origin of the viscosity of these solutions.

Fully Coherent 2D Electronic Spectrometer With Polarization Shaping Capabilities

P40

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[2]*Fastlite, VALBONNE, France*

We present a 2D spectrometer for visible spectroscopy based on two acousto-optic pulse shapers arranged in a Mach-Zehnder geometry. The setup enables the production of fully coherent, polarization-shaped pulse trains. Ultimately this feature will be exploited to observe multi-quantum coherences in molecules and colloidal nanostructures.

Two-dimensional Electronic Spectroscopy of Fenna-Matthews-Olson Complex at Ambient Temperature

P42

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[1]*Max-Planck Institute, HAMBURG, Germany*
[2]*University of Glasgow, GLASGOW, United Kingdom*
[3]*University of Hamburg, HAMBURG, Germany*

We have performed the 2D electronic spectroscopy of the Fenna-Matthews-Olson (FMO) complex using a broadband laser source with transform-limited 16-fs pulses. No clear oscillations were observed in a series of 2D spectra at ambient temperature.

Coherent Two-Dimensional Terahertz-Terahertz-Raman Spectroscopy Of Liquids

P44

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We demonstrate 2D-THz-THz-Raman spectroscopy to investigate the dynamics of liquids. By varying the timing between two intense terahertz pulses, we control the orientation of molecules in the liquid and excite nonlinear vibrational coherences. We have sufficient sensitivity to observe non-rephasing and rephasing nonlinear signals.

A Novel Conformation of PYP Caused by a Vibrational Marker

P46 Jianping Wang, Pengyun Yu, Fan Yang

Institute of Chemistry, the Chinese Academy of Sciences, BEIJING, China

Upon the binding of a ruthenium carbonyl complex to photoactive yellow protein, large conformation of the protein occurred, as evidenced by several steady-state spectroscopic methods. Ultrafast local structural dynamics of the newly formed conformation were characterized by ultrafast 2D IR spectroscopy.

Delocalised Terahertz Phonon-Like Modes In Biomolecules

Klaas Wynne[1], Mario González-Jiménez[1], Gopakumar Ramakrishnan[1], Thomas Harwood[2], Adrian Lapthorn[1], Hans Martin Senn[1], Sharon Kelly[3], Elizabeth Ellis[2]

P48

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Ultrafast optical Kerr-effect experiments have been carried out on proteins, DNA, and other biomolecules demonstrating the presence of coherent delocalised vibrational modes at physiologically relevant conditions as well as dramatically slowed down (20x) solvation-water dynamics.

Two-Phonon Quantum Coherences in InSb Observed by Two-Dimensional Three-Pulse THz Spectroscopy

P50 Carmine Somma, Giulia Folpini, Klaus Reimann, Michael Woerner, Thomas Elsaesser

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Two-phonon quantum coherences are observed in the narrow-gap semiconductor InSb by two-dimensional terahertz spectroscopy using three nonresonant THz pulses. The two-phonon signals originate from impulsive excitation in the nonperturbative regime of light-matter interaction mediated by the large interband dipole moment.

Investigation of MoS_2 Exciton Dynamics Using State-Selective Multidimensional Spectroscopy

P52

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University of Wisconsin-Madison, MADISON, United States of America

The A and B excitonic states of MoS_2 thin films were investigated using state-selective multidimensional spectroscopy. Interband electron transfer and intraband carrier relaxation is observed on a sub-70 fs timescale, while A and B excitons are observed to decay on a ~680 fs timescale.

Mapping Exciton Localization in Linear TDBC Aggregates by Two-Dimensional Electronic Spectroscopy

P54

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Exciton dephasing and relaxation is observed by two-dimensional electronic spectroscopy (2DES) in linear aggregates of TDBC molecules. Combining global analysis with quantum mechanical simulations, we distinguish dephasing from exciton relaxation and quantify the dynamics of exciton localization on specific low energy segments.

Recycling of Singlet Excitons in Organic Bilayers

P56

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Exciton dynamics are studied in C_{60}/Rubrene bilayers with 2D time-resolved photoluminescence. Triplet energy transfer from C_{60} to rubrene, triplet upconversion in rubrene, and back singlet energy transfer from rubrene to C_{60} are demonstrated, which leads to repopulation of the C_{60} singlets pool and increasing C_{60} fluorescence lifetime.

Preferential Solvation: Spectral Dynamic Slowdown of a Rhenium Photocatalyst

P58

Laura Kiefer, Kevin J. Kubarych

University of Michigan, ANN ARBOR, MI, United States of America

Equilibrium 2D IR spectroscopy was used to measure spectral diffusion of the photocatalyst $Re(bpy)(CO)_3Cl$ in multiple TEOA/solvent mixtures. The slowest spectral diffusion time was observed in the 20%/80% TEOA/solvent (v/v) mixture, indicating occurrence of preferential solvation.

2DIR Spectroscopy Study of Oxidation - From Biomarker Quantification to Spectral Imaging of Tissue Sections

P60

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[1]*Imperial College London, LONDON, United Kingdom*

Electron-Vibration-Vibration two-dimensional infrared spectroscopy is used here to study oxidation biomarkers, such as 3-nitrotyrosine. We aim to demonstrate how the spectral information obtained through this technique could be used to generate 2DIR images able to map the localisation of biomarkers across healthy and diseased human tissue sections.

Can Solvent Vibrational Modes Generate Coherent Oscillation in Excited Organic Dye?

P62

Luca Bolzonello, Elisabetta Collini

University of Padua, PADOVA, Italy

The coherent excited state dynamics of a charged organic molecule in different solvents have been studied with 2DES. The data demonstrated an unexpected enhancement of a specific vibrational mode of the molecule promoted by the coupling with a resonant mode of the solvent.

Background-Free Fourth-Order Optical Spectroscopy of Interfaces

P64

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Max-Planck Institute for Polymer Research, MAINZ, Germany

Recent development of the two-dimensional sum-frequency generation spectroscopy has enabled an insight into the molecular vibrational dynamics at interfaces. Its implementation, however, has so far remained limited to the pump-probe geometry, with its inherent restrictions. Here, we report proof-of-concept background-free measurements of the fourth-order susceptibility using non-collinear optical layout.

A broadband Femtosecond Time-Resolved Circular Dichroism Spectrometer in The Near-UV

P66

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Laboratory for Ultrafast Spectroscopy, LAUSANNE, Switzerland

A femtosecond time-resolved circular dichroism setup operating at 20 kHz in the near-UV spectral range is presented. The spectrometer employs broadband probe (260 - 360 nm) and tunable narrowband pump pulses (1.5 nm FWHM) over the same spectral range.

Influence of H-aggregate Formation on The Photophysics of a Push-Pull Phtalocyanine

P68

Sandra Doria, Nicolò Azzaroli, Andrea Lapini, Alessandro Iagatti, Paolo Foggi, Roberto Righini, Mariangela Di Donato
LENS-University of Florence, SESTO FIORENTINO, Italy

The relaxation dynamics of a push-pull Zn-phtalocyanine has been investigated by means of two-dimensional electronic spectroscopy and narrow-band transient absorption spectroscopy. The photophysics of monomer solution and H-aggregates have been compared on a time scale spanning from a few tens of femtoseconds up to 1.5 nanoseconds.

Three-Pulse Photon Echo Spectra at Conical Intersections: Model Dissipative Quantum Dynamical Studies

P70

Matthieu Sala, Dassia Egorova
Institute of Physical Chemistry, KIEL, Germany

Three-pulse photon echo signals for two model systems exhibiting strong vibronic interactions mediated by conical intersections are simulated using the equation-of-motion phase-matching approach combined with a dissipative treatment of the quantum dynamics.

Can We Throw Away Our OPA? Two-Dimensional White Light Spectroscopy at 100 kHz

P72

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We report on a two-dimensional white light spectrometer using a 100 kHz Spirit laser, pulse shaper, and supercontinuua for both pump and probe. We show that high repetitions rates coupled with shot-to-shot delay scanning gives sufficient signal-to-noise such that spectra can be collected rapidly on a variety of interesting systems.

100 kHz Tunable Mid-IR Source for 2D-IR Spectroscopy

P74

Raman Maksimenka, Alexandre Thai, Clément Ferchaud, Nicolas Thiré, Nicolas Forget

Fastlite, VALBONNE, France

We present a 100-kHz parametric source delivering 40-fs pulses with an average output power of ~1 W. This source is tunable from 2.5 to 4.0 µm and delivers idler pulses in the 1.4-1.75 µm spectral range.

Signaling Transduction Pathway of AsLOV2 Revealed by Time-Resolved Vibrational Spectroscopy

P76

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VU University Amsterdam, AMSTERDAM, The Netherlands

Transient vibrational spectroscopy was used to investigate the photoactivation mechanism of LOV2 from *Avena sativa* (AsLOV2). Ultrafast relaxation reveals singlet to triplet conversion of the flavin chromophore. Slower microsecond components represent formation of the cysteinyl-flavin adduct and unfolding of the Jα helix.

Coherent Dynamics of Phosphate Ions in Bulk H_2O

P78

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We investigate dynamics of phosphate stretching vibrations of the ion $H_2PO_4^-$ dissolved in H_2O combining 2D-IR spectroscopy with mixed quantum-classical simulations. Dominantly homogeneously broadened lines are caused by ultrafast librational motions of hydration shell water. Cross peak dynamics reveal vibrational quantum beats with a lifetime of a few hundred femtoseconds.

In Silico Characterization of Polymer-Fullerene Organic Photovoltaic Bulk Heterojunctions

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P80

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In organic photovoltaic materials an ultrafast electron transfer starts the (eventual) charge separation process. The morphology of the active layer impacts the different pathways which this first step can lead to. This is investigated via a range of computational techniques, which allows to consider the relevant length and time scales.

Self-Compressed Visible Supercontinuum from 100 fs Pulses Using a Hollow-Core Fiber

P82

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We report the generation of visible supercontinuum from 100 fs Ti:Sapphire output in a single stage using a 2.57 m long hollow-core fiber in Ar. The impact of input energy and gas pressure on the output pulse are studied. This source exhibits self-compression, high transmission and good long-time stability.

Rapid-Scan 2D Fluorescence Spectroscopy

P84

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We implement liquid-phase 2D spectroscopy with collinear four-pulse excitation and fluorescence detection. Pulse-sequence parameters are varied on a shot-to-shot basis using a fast pulse shaper. A complete set of all third-order signals (photon echo, double-quantum coherence, etc.) is acquired via 27-fold phase cycling in just 6 s plus averaging.

Detection and Assignment of Inhibitor-Protein Interactions from EVV 2DIR Data

P86

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Electron-vibration-vibration (EVV) 2DIR spectroscopy is used to investigate inhibitor binding to mammalian and plant proteins. We demonstrate the ability to detect inhibitor binding, and suggest potential applications in label-free screening and identification of previously unknown binding sites.

Evidence for Intramolecular Antiparallel β-Sheet Structure in α-Synuclein Fibrils Aggregated Under Physiological Conditions

P88

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The aggregation of a-synuclein into fibrils in the presence of varying NaCl concentrations is studied with AFM and 2D-IR spectroscopy, and complemented with spectral calculations to assign the spectra. We find different fibril structures depending on whether the protein is aggregated in <25 mM or >25 mM NaCl buffer solution.

Comparing Active Site Dynamics and Catalytic Activity in a Thermophilic Enzyme

P90

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Enzyme-substrate dynamics under changing reaction conditions in a hyperthermophilic enzyme are studied with FTIR and 2D IR spectroscopy. The labeling scheme exploits the enzyme's promiscuity, allowing a cyanylated N-phenylmaleimide to probe the local electric field of the enzyme's active site and an analogous covalent substrate allows for single-turnover kinetics studies.

2D Electronic Spectra of Electron Transfer

P92

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We use non-equilibrium Green's functions to describe 2D spectra of Marcus electron transfer.

Transient Non-Equilibrium Ground State Signals in 2D Spectra due to Energy Transfer

P94

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Spectral features of energy transferring photosynthetic pigments are studied theoretically. We identify electronic ground state signals due to non-equilibrium state of nuclear vibrations resulting from de-excitation of pigments as the excitation passes through. We find characteristic long lived signals with unusual amplitude dependences on energy transfer rates and energetic disorder.

Broadband 2D Electronic Spectroscopy by Hollow-Fiber Compression

P96

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We demonstrate broadband diffractive-optic-based 2D electronic spectroscopy (500-700 nm). Pulses are generated in an argon-filled hollow fiber pumped by a Ti:Sa laser and compressed to sub-7-fs duration at the sample position using dispersive mirrors. The fiber provides a clean spatial profile and thus avoids problems arising from spatial chirp.

Molecular Dynamics on Microbial Rhodopsins Probed by Time-resolved Vibrational Spectroscopy

P98

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Microbial rhodopsins are light-driven proteins having various functions such as proton pump, ion channel and cation pump. For many microbial rhodopsins, the molecular dynamics in between picoseconds and microseconds after photon absorption is unclear. We apply time-resolved stimulated Raman and two-dimensional infrared spectroscopies to elucidate transient reactions in microbial rhodopsins.

Resolving Structural Dynamics In Blue-Light Photoreceptors Through 2D IR Spectroscopy

P100 Jörn Weißenborn[1], Patrick Konold[1], John T.M. Kennis[1], Jennifer Mehlhorn[2], Peter Hegemann[2], Tilo Mathes[1]
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BLUF domains constitute a class of blue-light photoreceptors that show light-induced conformational changes ranging from ultrafast sidechain fluctuations to large scale changes in secondary structure. Here, we present results from 2D IR spectroscopy on an isotopically labelled BLUF domain to investigate its photoswitching mechanism.

State-resolved Dynamics in Structurally Precise Monolayer-Protected Gold Clusters Using Two-Dimensional Electronic Spectroscopy

P102 Kenneth L. Knappenberger Jr.[1], Giulio Cerullo[2], Tatjana Stoll[2], Patrick J. Herbert[1], Jeremy W. Jarrett[1]
[1]*Florida State University, TALLAHASSEE, United States of America*
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Superatom state-resolved electron relaxation dynamics of structurally precise $Au_{25}(SC_8H_9)_{18}^-$ nanoclusters were studied using Two-Dimensional Electronic Spectroscopy. The 2-D data allowed for for hot electron and hot hole carrier dynamics occuring in the < 300 fs time scale to be distinguished.

Exciton Delocalization in the Amide I Band of a Protein-Like Liquid

P104 Ana V. Cunha[1], Evgeniia Salamatova[1], Robbert Bloem[2], Steven J. Roeters[2], Sander Woutersen[2], Maxim S. Pshenichnikov[1], Thomas L.C. Jansen[1]
[1]*University of Groningen, GRONINGEN, The Netherlands*
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The exciton delocalization in the amide I band of neat N-methylacetamide is studied with 2D IR spectroscopy. The spectra consist of a diagonally elongated peak and a narrower shoulder assigned to delocalized excitons. According to the inverse participation ratio, the excitons are delocalized over tens of amide I oscillators.

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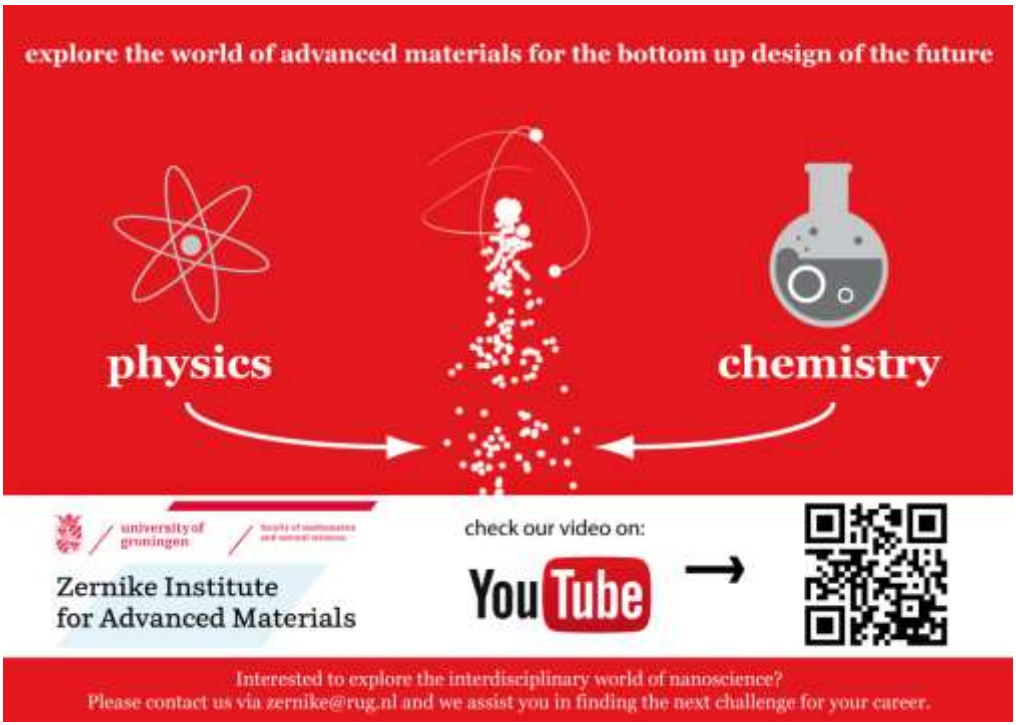

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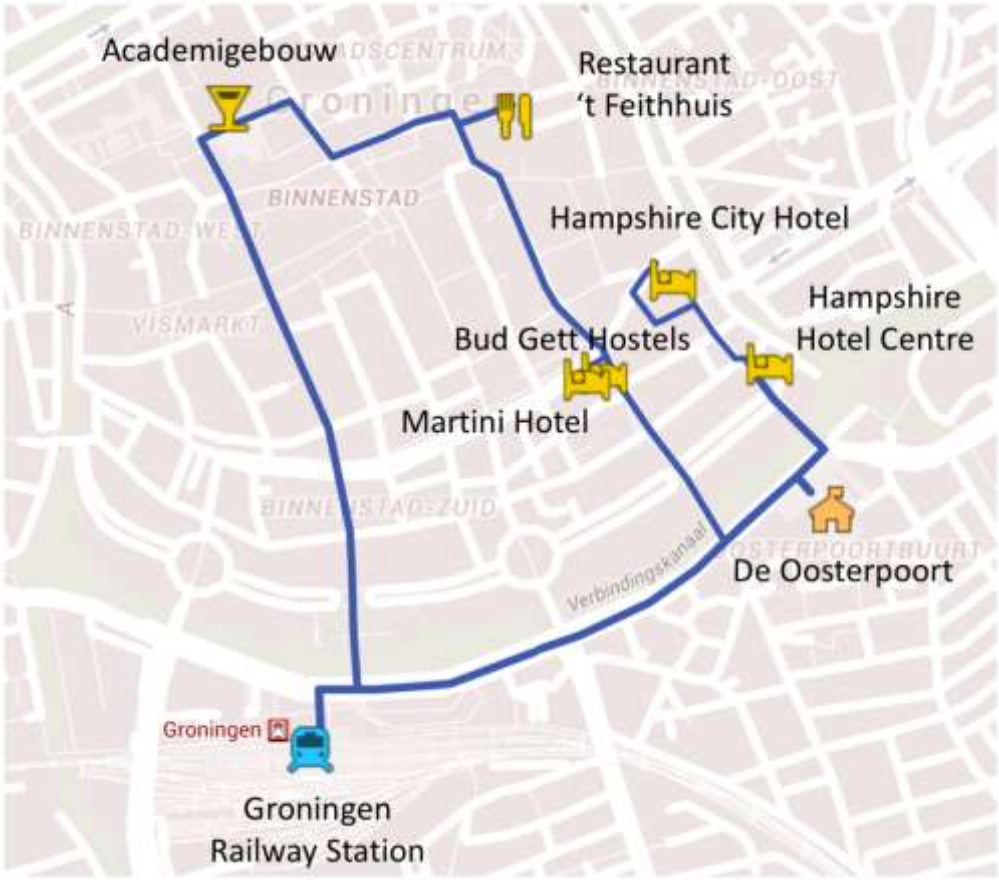

Registration
Tuesday 28 June 15:30-18:00
Wednesday 29 June 8:00
Address: "De Oosterpoort", Trompsingel 27

Reception
Tuesday 28 June 18:00-19:00
Address: Academigebouw, Broerstraat 5

Excursion
Thursday 30 June 17:00-18:00
Address: Departure from "De Oosterpoort", Trompsingel 27

Conference dinner
Thursday 30 June 19:00
Address: 't Feithhuis, Martinikerkhof 10

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