

Conference Program

Monday May 20

8:30 *Opening Remark*

Chairperson: Peter Hamm (University of Zurich, Switzerland)

- 8:40 PL1 Ultrafast 2D infrared spectroscopy of phosphate-water interactions and water dynamics in phospholipid reverse micelles
René Costard, Ismael A. Heisler, Christian Greve, and **Thomas Elsaesser**

Chairperson: Keisuke Tominaga (Kobe University, Japan)

- 9:20 IT1 The role of high frequency vibrations in ultrafast metal-to-metal charge transfer transitions in mixed valence complexes
Michael S. Lynch, Karla M. Slenkamp, Benjamin E. Van Kuiken, Mark Cheng, Stephanie L. Daifuku, Caitlin Bannan, and **Munira Khalil**

- 9:50 CT1 A hydrogen-bond “flip-flop” through a Bjerrum-type defect
Martin Olschewski, Jörg Lindner, and **Peter Vöhringer**

- 10:10 CT2 Nanosecond tautomerization dynamics of aromatic heterocycles studied by temperature-jump transient 2D IR spectroscopy: application to an anti-HIV drug
Chunte Sam Peng, Carlos R. Baiz, Mike Reppert, Vipender Singh, Deyu Li, Tiffany J. Amariuta, John M. Essigmann, and Andrei Tokmakoff

10:30 *Coffee Break*

Chairperson: Erik T.J. Nibbering (Max Born Institute, Germany)

- 11:10 IT2 Water Friction Dominates Dynamics of a Photoswitchable Allosteric Protein
Brigitte Buchli, Steven A. Waldauer, Reto Walser, Rolf Pfister, Oliver Zerbe, and **Peter Hamm**

- 11:40 CT3 Accessing solute-solvent interactions and solvation dynamics with small ionic probes: Ultrafast infrared spectroscopic study
Kaoru Ohta, Kyoko Aikawa, and Keisuke Tominaga

- 12:00 CT4 Ultrafast Vis-Pump/IR-Probe and Transient 2D-IR Investigation of the Excited State Dynamics of trans- β -apo-8'-carotenal
Mariangela Di Donato, Andrea Lapini, Manuela Lima, Roberto Righini, Chiara Cappelli, Fabrizio Santoro, Mireia Segado, and Francisco Jose Avila Ferrer

12:20 CT5 Band merger and intensity bias in 1D and 2D vibrational spectra arising from coupling between different isotopic species

Hajime Torii, Maria Grazia Giorgini, and Maurizio Musso

12:40 Lunch

Chairperson: Cather Simpson (The University of Auckland, New Zealand)

14:00 IT3 Real-time wavepacket dynamics through a conical intersection

Giulio Cerullo, Dario Polli, Marco Garavelli, and Richard Mathies

14:30 CT6 Time-resolved spectroscopy of J-aggregates with sub-10-fs resolution

Takayoshi Kobayashi, Daisuke Hasegawa, Kazuaki Nakata, Eiji Tokunaga, Okamura Kotaro, and Du Juan

14:50 CT7 Excited state intramolecular proton transfer dynamics of hydroxyanthraquinones in solution by impulsive excitation of vibrations

Myeongkee Park, Jaehyun Ryu, and **Taiha Joo**

15:10 IT4 Following excited state evolution with impulsive vibrational spectroscopy

A. Wand and **Sanford Ruhman**

15:40 Coffee Break

Chairperson: Shoichi Yamaguchi (RIKEN, Japan)

16:20 IT5 Water migration dynamics studied by picosecond time-resolved IR spectroscopy

Masaaki Fujii

16:50 CT8 Study on photoisomerization of PYP chromophore by picosecond time-resolved pump-probe spectroscopy in the gas phase

Takayuki Ebata, Yasunori Miyazaki, Daiki Shimada, Yoshiya Inokuchi, and Masahiro Ehara

17:10 CT9 Effects of Hydrogen Bonding on Internal Conversion of GFP-like Chromophores

Chi-Wen Cheng, Guan-Jhih Huang, Hung-Yu Hsu, Ch. Prabhakar, Eric Wei-Guang Diao, Jye-Shane Yang, and **Yuan-Pern Lee**

17:30 CT10 Excited-state multiple proton transfer in solvated 7-azaindole clusters

Kenji Sakota, Yuto Ikegami, and **Hiroshi Sekiya**

18:00 Dinner

20:00 *Poster Session 1 (PA1-PA44)*

Tuesday May 21

Chairperson: Tahei Tahara (RIKEN, Japan)

8:50 PL2 Studies of Organic Monolayers at Water interfaces
 Shuai Zha, Shanshan Yang, Yu-Chieh Wen, Chuanshan Tian, and **Y. Ron Shen**

Chairperson: Hidenori Noguchi (National Institute for Materials Science, Japan)

9:30 CT11 2D Heterodyne-Detected VSFG Spectroscopy of Water at Aqueous Interfaces
 Satoshi Nihonyanagi, Prashant C. Singh, Shoichi Yamaguchi, and Tahei Tahara

9:50 CT12 Vibrational dynamics of adsorbates on metal surfaces studied by time-resolved
 sum-frequency generation
 Kazuya Watanabe, Ken-ichi Inoue, Yoshiki Miyamoto, Toshiki Sugimoto, and
 Yoshiyasu Matsumoto

10:10 IT6 Probing Organometallic Photochemistry in Conventional and supercritical Fluids
 using time-resolved IR
 Michael George

10:40 *Coffee Break*

Chairperson: Klaus Gerwert (Ruhr-University Bochum, Germany)

11:20 CT13 Heme cyanide photodissociation in myoglobin and horseradish peroxidase
 Weiqiao Zeng, Yuhua Sun, Abdelkrim Benabbas, and **Paul M. Champion**

11:40 CT14 Allosteric dynamics of hemoglobin revealed by time-resolved resonance Raman
 spectroscopy
 Yasuhisa Mizutani, Kenta Yamada, Haruto Ishikawa, and Misao Mizuno

12:00 CT15 Proteins in Action: Time Resolved Infra-red Study of a Photoactive Flavoprotein
 from Femtoseconds to Milliseconds
 Richard Brust, Andras Lukacs, Allison Haigney, Kiri Addison, Agnieszka Zieba,
 Michael Towrie, Gregory M. Greetham, Peter J. Tonge, and **Stephen R. Meech**

12:20 CT16 Proton transfer and photoswitching in Fluorescent Proteins
 Jasper J. van Thor, Marius Kaucikas, Paul Champion, and J. Timothy Sage

12:40 *Lunch*

Chairperson: Satoshi Takeuchi (RIKEN, Japan)

- 14:00 IT7 Femtosecond stimulated Raman scattering of S₁ *trans*- and *cis* stilbene
Sergey A. Kovalenko, Alexander L. Dobryakov, and **Nikolaus P. Ernsting**
- 14:30 CT17 Vibrational Relaxation of Guanosine Following Ultraviolet Photoexcitation
David W. McCamant, J. Reddy Challa, Joohyun Lee, and Yong Du
- 14:50 CT18 Sub-ps photoinduced dynamics in Heme-proteins studied by Femtosecond Stimulated Resonance Raman Scattering
Emanuele Pontecorvo, Carino Ferrante, and **Tullio Scopigno**
- 15:10 CT19 Difference of the carotenoid S* state between light harvesting complex and solution revealed by femtosecond stimulated Raman spectroscopy
Masayuki Yoshizawa, Orihiro Yoshimatsu, Kenta Abe, Shunsuke Sakai, Tomoko Horibe, Ritsuko Fujii, Mamoru Nango, and Hideki Hashimoto

15:30 *Coffee Break*

Chairperson: Shaul Mukamel (University of California, Irvine, USA)

- 16:10 CT20 Femtosecond near-IR multiplex stimulated Raman gain and loss spectroscopy of β -carotene in 1.0 – 1.6 μ m region
Tomohisa Takaya and Koichi Iwata
- 16:30 CT21 New insights into the reactivity, ordering, and structure of the low-lying excited triplet states of aromatic compounds as provided by time-resolved near/mid-IR spectroscopy
Sohshi Yabumoto, Sudhakar Narra, Hiro-o Hamaguchi, and **Shinsuke Shigeto**
- 16:50 CT22 Electronic and vibrational coherence during the initial charge separation in Photosynthesis
Sighart F. Fischer, Philipp O. J. Scherer, and Wolfgang Dietz
- 17:10 CT23 Water Potential for Vibrational Spectroscopy
Yoshitaka Tanimura, Taisuke Hasegawa, and Hironobu Ito
- 17:30 CT24 Anharmonic vibrational structure calculations from the first-principles
Kiyoshi Yagi

18:00 *Dinner*

20:00 *Poster Session 2 (PB1-PB43)*

Wednesday May 22

Chairperson: Paul Champion (Northeastern University, U.S.A.)

8:50 IT8 Exciton Delocalization Processes of Various π -Expanded Oligothiophenes

Dongho Kim

9:20 CT25 Vibrational energy transport through molecules

Christopher M. Berg, Brant Pein, Yuxiao Sun, and Dana D. Dlott

9:40 *Coffee Break*

~Robin M. Hochstrasser's Memorial Session~

Chairperson: Edwin Heilweil (National Institute of Standards & Technology, U.S.A.)

10:10 IT9 Quantifying transition dipole strengths to identify molecular structures

Martin T. Zanni

10:40 IT10 Monitoring excited-state vibrational dynamics by broadband infrared or Raman probes; A unified picture based on loop diagrams

Konstantin E. Dorman, Benjamin P. Fingerhut, and **Shaul Mukamel**

11:10 CT26 Structure and dynamics of a drug bound to its allosteric pocket in HIV-1 reverse transcriptase

Daniel Kuroda, J. Reddy Challa, Thomas Troxler, Joseph D. Bauman, Disha Patel, Kalyan Das, Eddy Arnold, and Robin M. Hochstrasser

Thursday May 23

Chairperson: Thomas Elsaesser (Max born Institute, Germany)

8:50 IT11 Light-triggered peptides – a new tool for the investigation of ultrafast folding dynamics

Wolfgang Zinth(TRVS2013 awardee), Andreas Deeg, Michael Rampp, and Bert Pilles

9:20 IT12 Improving signal generation and collection in Femtosecond Stimulated Raman Spectroscopy

John T.M. Kennis and Miroslav Klotz

9:50 CT27 Revealing excited state nuclear coherence in the photoisomerisation of bacteriorhodopsin by population assisted impulsive Raman

Matz Liebel and **Philipp Kukura**

10:10 CT28 Time-resolved IR spectroscopy of cyclopentane-1,3-diyl biradicals

Taka-aki Ishibashi, Akihiro Maeda, Takahide Oshita, and Manabu Abe

10:30 *Coffee Break*

Chairperson: Hajime Torii (Shizuoka University, Japan)

11:10 CT29 Probing Dimerization of 7-Azaindole in Solutions by Femtosecond Raman-Induced Kerr Effect Spectroscopy

Hideaki Shirota, Takao Fukuda, and Tatsuya Kato

11:30 CT30 Like-charge ion pairing in aqueous guanidinium chloride solution addressed by ultrafast optical Kerr-effect (OKE) spectroscopy

David Turton and **Klaas Wynne**

11:50 IT13 When do ions accelerate or retard water dynamics?

Guillaume Stirnemann, Erik Wernersson, Pavel Jungwirth, and **Damien Laage**

12:20 CT31 Hydrogen bond dynamics in supercooled water: Frequency dependent specific heat and emergence of correlated dynamics

Shinji Saito, Iwao Ohmine, and Biman Bagchi

12:40 *Lunch*

Chairperson: Yasuhisa Mizutani (Osaka University, Japan)

14:00 IT14 Mechanism of photosynthetic water oxidation as studied by flash-induced FTIR difference and time-resolved IR spectroscopies

Takumi Noguchi

14:30 CT32 Mechanism of light-driven sodium ion pump

Hideki Kandori, Hui-Fen Chen, and Keiichi Inoue

14:50 IT15 Proton transfer reactions and structural changes of the optogenetic protein channelrhodopsin-2 traced by time-resolved step-scan FTIR spectroscopy

V.A. Lórenz-Fonfría, T. Resler, N. Krause, M. Nack, M. Gossing, G. Fischer von Mollard, C. Bamann, E. Bamberg, R. Schlesinger, **Joachim Heberle**

15:20 *Coffee Break*

Chairperson: Stephen Meech (University of East Anglia, UK)

15:50 IT16 Catalysis of small GTPases by their G-Activating Proteins (GAPs) analyzed by time-resolved FTIR spectroscopy

Klaus Gerwert

16:20 CT33 Ultrafast Dynamics of Specific Interactions in Photoacid-Base Complexes
M. Prémont-Schwarz, D. Xiao, S. Keinan, D. Pines, D. Huppert, E. Pines, V.S. Batista, and **Erik T.J. Nibbering**

16:40 CT34 Ultrafast Charge Generation in Novel Push –Pull Polymers
Vlad G. Pavelyev, Almis Serbenta, Stoichko D. Dimitrov, James R. Durrant, Paul H.M. van Loosdrecht, and **Maxim S. Pshenichnikov**

17:00 *Presentation of Poster Award*

Friday May 24

Chairperson: Masayuki Yoshizawa (Tohoku University, Japan)

8:50 IT17 “Making the Molecular Movie”: Direct Observation of Atomic Motions Involved in Mode Coupling Along Reaction Coordinates

R.J. Dwayne Miller

9:20 CT35 Energy transfer in phosphatidylcholine lipid bilayer membranes examined by picosecond time-resolved Raman spectroscopy
Yuki Nojima, Tomohisa Takaya, and **Koichi Iwata**

9:40 CT36 Dynamics of molecular systems probed by IR-induced conductivity
Artem A. Bakulin, Akshay Rao, Robert Lovrincic, Maxim S. Pshenichnikov, Huib J. Bakker, David Cahen, and Richard H. Friend

10:00 CT37 Control of multipath interference in vibrational excitations for anharmonically coupled oscillator systems
Satoshi Ashihara and Jumpei Tayama

10:20 *Coffee Break*

Chairperson: Klaas Wynne (University of Glasgow, UK)

11:00 CT38 Vibrational dynamics in the electronically excited state in hydrogen bonding solvents

Yuki Fukui, Minako Kondo, Kaoru Ohta, and **Keisuke Tominaga**

11:20 CT39 Ultrafast photoisomerization of Pfr phytochrome studied by time-resolved infrared and Raman spectroscopy

Karsten Heyne, Yang Yang, Peter Schmieder, Clark Lagarias, Richard A. Mathies, and Jyothisman Dasgupta

11:40 CT40 Inter-molecular Coherent Vibration in Oligomers of Gold(I) complex

Munetaka Iwamura, Koichi Nozaki, Satoshi Takeuchi, and Tahei Tahara

12:00 CT41 Semiquantal wave packet molecular dynamics simulation of hydrogen-bond dynamics in water

Koji Ando, Junichi Ono, and Kim Hyeon-Deuk

12:20 *Closing Remark*