Poster Session 1 (PA1-PA44)　20:00～ Monday May 20

PA1 New Methods in Mixed Electronic-Vibrational Coherent Multidimensional Spectroscopy: Triple Sum Frequency CMDS and Application

Erin S. Boyle, Andrei V. Pakoulev, and John C. Wright

PA2 Early steps in the uncaging reaction of NVOC protected puromycin

Jörg Kohl-Landgraf, Florian Buhr, Harald Schwalbe, and Josef Wachtveitl

PA3 Mutual Orientation of Reactants in Bimolecular Photoinduced Electron Transfer in Solution

Marius Koch and Eric Vauthey

PA4 UV-excited time-resolved HD-VSFG study of the photoionization dynamics of indole at the air/water interface: A vibrational signature of hydrated electrons at the interface

Korenobu Matsuzaki, Satoshi Nihonyanagi, Shoichi Yamaguchi, Takashi Nagata, and Tahei Tahara

PA5 New Methods to Measure Anharmonic Coupling using Femtosecond Stimulated Raman Spectroscopy

Barbara Dunlap, Peter Richter, and David W. McCamant

PA6 Conformational change of azobenzene-based photoswitchable OmPE-foldamer due to photoisomerization

Sabrina Steinwand, Chavdar Slavov, Zhilin Yu, Stefan Hecht, and Josef Wachtveitl

PA7 Raman-enhancement mechanism by a nearby plasmonic cluster: the coupling of plasmonic electron motion with vibrational modes of analyte

Tomokazu Yasuike and Katsuyuki Nobusada

PA8 Charge Dynamics in Novel Star-Shaped Conjugated Molecules

Oleg V. Kozlov, Vlad G. Pavelyev, Almis Serbenta, Yuriy N. Luponosov, Sergei A. Ponomarenko, Dmitry Yu. Paraschuk, Andreas Elschner, and Maxim S. Pshenichnikov

PA9 Femtosecond Time-Domain Raman Tracking of the Primary Photoreaction Process of Photoactive Yellow Protein

Hikaru Kuramochi, Satoshi Takeuchi, Hironari Kamikubo, Mikio Kataoka, and Tahei

Tahara

PA10 Real-Time Tracking of Two Phytochrome Isoforms During Pr Photoisomerization

Y. Yang, M. Linke, T. von Haimberger, J. Hahn, P. Schmieder, R. Matute, L. González, K. Heyne

PA11 Salt bridges function as nucleation sites for α-helix folding

Heleen Meuzelaar, Martijn Tros, Adriana Huerta Viga, Chris N. van Dijk, and Sander Woutersen

PA12 Towards Time-Resolved Host-Guest Chemistry: Charge Transfer Dynamics of Perylene-Macrocycle Complex

Ryan M. Young, Scott M. Dyar, Dick T. Co, and Michael R. Wasielewski

PA13 Structural transformations of liquid water under high pressure conditions: experimental and computational characterization

Andrea Lapini, Samuele Fanetti, Marco Pagliai, Mariangela di Donato, Margherita Citroni, Sandro Scandolo, Roberto Bini, and Roberto Righini

PA14 Mid-infrared spectroscopy by chirped pulse upconversion

Jingyi Zhu, Tilo Mathes, John T.M. Kennis, and Marie Louise Groot

PA15 Conformational dynamics of fish type III antifreeze protein studied with time-resolved vibrational spectroscopy

Stephan Lotze and Huib J. Bakker

PA16 Visible pump-IR probe Spectroscopy on Fluorenone and Water-soluble Fluorenone in Solutions

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

PA17 Laser-induced temperature-jump infrared-spectroscopy to study peptide folding dynamics with site-specific resolution

Karin Hauser, Alexander Popp, and Benjamin Heck

PA18 Transporting a proton with a molecular crane

Tibert H. vab der Loop, Freek Ruesink, Hans J. Sanders, Wybren J. Buma, and Sander Woutersen

PA19 Triplet Formation Mechanism in Cofacial Perylene Diimide Dimers Interrogated by Femtosecond Stimulated Raman Spectroscopy

Kristen E. Brown, Kelly M. Lefler, Walter A. Salamant, Dick T. Co, and Michael R. Wasielewski

PA20 S_2 Fluorescence Dynamics of *meso*-Aryl-substituted Subporphyrins

Jooyoung Sung, Pyosang Kim, Shun Saga, Atsuhiro Osuka, and Dongho Kim

PA21 Ultrafast dynamics of solvent coordination to organometallic photoproducts probed via solvent vibrational oscillators

Son C. Nguyen, Justin P. Lomont, Ben W. Caplins, and Charles B. Harris

PA22 Bimolecular Electron Transfer between Pyrene and 1,4-Dicyanobenzene as Studied by Nanosecond Time-Resolved Near/Mid-Infrared Spectroscopy

Sudhakar Narra and Shinsuke Shigeto

PA23 Two-dimensional broadband mid-IR spectroscopy

Mark Cheng, Anthony Reynolds, and **Munira Khalil**

PA24 Femtosecond OPA pumped by 1030 nm Yb:KGW laser

Valeri Kozich, M. Hartmann, and K. Heyne

PA25 Analyzing brominated Al-Corroles with Vis-pump and IR-, NIR- and VIS- probe experiments

Till Stensitzki, Yang Yang, T. von Haimberger, Atif Mahammed, Zeev Gross, and Karsten Heyne

PA26 Initial interfacial structure and dynamics of dye sensitizer under photo-excitation studied by ultrafast infrared spectroscopy

Hidenori Noguchi, Mikio Ito, and Kohei Uosaki

PA27 Elucidating the mechanism of a unidirectional molecular motor

Saeed Amirjalayer, Wesley R. Browne, Ben L. Feringa, Wybren J. Buma, and Sander Woutersen

PA28 Towards excited-state surface-enhanced femtosecond stimulated Raman spectroscopy

Natalie L. Gruenke, Renee R. Frontiera, and Richard P. Van Duyne

PA29 Folding of a light-switched β-hairpin peptide: Comparison of isomerization and temperature-jump induced peptide dynamics

Andreas Deeg, Michael Rampp, Alexander Popp, Bert Pilles, Tobias Schrader, Jose Pfizer, Luis Moroder, Karin Hauser, and Wolfgang Zinth

PA30 Links between Structure, Dynamics and Function in the Inhibition of Catalase by Nitric Oxide

Marco Candelaresi, Andrea Gumiero, **Katrin Adamczyk**, Kristy Robb, Cesar Bellota-Antón, Vartul Sangal, John Munnoch, Gregory M. Greetham, Michael Towrie, Paul A. Hoskisson, Anthony W. Parker, Nicholas P. Tucker, Martin A. Walsh, and Neil T. Hunt

PA31 Secondary and quaternary structural imaging of human hairs by using VSFG-detected IR super-resolution microscope

Makoto Sakai and Masaaki Fujii

PA32 Dynamics of two-photon isomerization of DTTCI observed by femtosecond pump-probe and two-pulse correlation measurements

Koich Furuta, Masanori Fuyuki, and **Akihide Wada**

PA33 Ultrafast hydrogen-bonding dynamics in the electronic excited state of photoactive yellow protein

Ryosuke Nakamura, Norio Hamada, Kenta Abe, and Masayuki Yoshizawa

PA34 Time-resolved IR spectroscopy of hydrogenase enzyme mimics: the effect of hydrogel encapsulation

Pim W.J.M. Frederix, Rafal Kania, Joseph A. Wright, Rein V. Ulijn, Christopher J. Pickett, and Neil T. Hunt

PA35 Real-time observation of destruction of hydration shells

Akira Yamakata and Masatoshi Osawa

PA36 Time-resolved FTIR study of a light-driven sodium pump rhodopsin

Hui-Fen Chen, Keiichi Inoue, and Kandori Hideki

PA37 Towards time-domain ultrafast vibrational spectroscopy of chemical reaction dynamics
Matz Liebel and Philipp Kukura

PA38 Bimodal dynamics of DNA bubbles
Chris N. van Dijk, Heleen Meuzelaar Matthijs R. Panman, and Sander Woutersen

PA39 Determination of Huang-Rhys factors of multi-dimensional hyper-potential surfaces obtained by a few-cycle pulse laser
Takayoshi Kobayashi, Tsugumasa Iiyama, Kotaro Okamura, Juan Du, and Toshio Masuda

PA40 Ultrafast time-resolved pump/IR probe spectroscopy of [FeFe]-hydrogenase model compounds
Melissa Johnson, James Thuman, Christopher J. Stromberg, and **Edwin J. Heilweil**

PA41 Spectral diffusion of heavy water in presence of bromide and iodide ions at supercritical conditions: First principle molecular dynamics study
Anwesa Karmakar and Amalendu Chandra

PA42 Anomalous Blinking Characteristics in Single Molecule Surface-Enhanced Raman Spectroscopy (SMSERS)
Wen-Hsiang Yu and Chao-Yi Tai

PA43 Intermolecular vibrational energy transfer analyzed by ultrafast two-dimensional infrared spectroscopy
Albert A. Villaeys and **Kuo Kan Liang**

PA44 Electronic transitions and heterogeneity of the phytochrome Pr absorption band: An angle balanced polarization resolved femtosecond VIS pump – IR probe study
Martin Linke, Y. Yang, B. Zienicke, M.A.S. Hammam, T. von Haimberger, A. Zacarias, K. Inomata, T. Lamparter, and K. Heyne

Poster Session 2 (PB1-PB43) 20:00~ Tuesday May 21

PB1 Anharmonic and solvent effects on Franck-Condon factors with application to molecular electronic spectroscopy

Chaoyuan Zhu and Sheng Hsien Lin

PB2 Ultrafast isomerization dynamics of a substituted azobenzene driving a cyclodextrin shuttle
Matthew M. Sartin, Masahisa Osawa, and Tahei Tahara

PB3 Femtosecond stimulated Raman spectroscopy of a BLUF protein PapB from the purple bacterium *Rhodopseudomonas palustris*
Tomotsumi Fujisawa, Satoshi Takeuchi, Shinji Masuda, and Tahei Tahara

PB4 Two-dimensional heterodyne-detected vibrational sum frequency generation spectroscopy of water at a charged interface with excess salt
Prashant C. Singh, Satoshi Nihonyanagi, Shoichi Yamaguchi, and Tahei Tahara

PB5 Fullerene Excitons Reveal Morphology of Polymer: Fullerene Blends
Almis Serbenta, Vlad G. Pavelyev, Jan C. Hummelen, Paul H.M. van Loosdrecht, and Maxim S. Pshenichnikov

PB6 Three dimensional infrared spectroscopy of ice Ih
Fivos Perakis, Joanna Borek, and Peter Hamm

PB7 Parallel Relaxation Pathways of Malachite Green Revealed by Ultrafast Pump-Dump-Probe Spectroscopy
Zhengrong Wei, Satoshi Takeuchi, and Tahei Tahara

PB8 *In situ* monitoring of a protein folding process on the artificial lipid bilayer by Surface Enhanced Infrared Absorption Spectroscopy
Kenichi Ataka, Axel Baumann, Silke Kerruth, Ramona Schlesinger, Jörg Fitter, and Joachim Heberle

PB9 Chemical exchange between phenol and phenol-benzene complex observed by 3D IR spectroscopy
Joanna A. Borek, Fivos Perakis, and Peter Hamm

PB10 Ligand Binding Studied by 2D IR Spectroscopy Using the Azidohomoalanine Label
Robbert Bloem, **Klemens Koziol**, Steven A. Waldauer, Brigitte Buchli, Reto Walser, Brighton Samatanga, Ilian Jelesarov, and Peter Hamm

PB11 Quantum decoherence in vibrational nonadiabatic transitions of water studied by quantum-classical molecular dynamics simulations

Tatsuya Joutsuka, Ward H. Thompson, and Damien Laage

PB12 Two-Dimensional Raman-THz Spectroscopy of Water

Janne Savolainen, Saima Ahmed, and Peter Hamm

PB13 Ultrafast dynamics of excited state DNA probed by femtosecond stimulated Raman spectroscopy

Joohyun Lee, J. Reddy Challa, Yong Du, and David W. McCamant

PB14 Excited state dynamics for thymine by using sub-10 femtosecond deep ultraviolet pump and probe pulses

Bing Xue, Takayoshi Kobayashi, Juan Du, and Yongliang Jiang

PB15 Picosecond protein response to the chromophore isomerization in microbial rhodopsins

Misao Mizuno, Seisuke Inada, Yumi Shimoo, Hideki Kandori, Yuki Sudo, and Yasuhisa Mizutani

PB16 Chromophore structures of photocycle intermediates in *Gloeobacter* rhodopsin: a resonance Raman study

Ayumi Nakajima, Misao Mizuno, Hideki Kandori, and Yasuhisa Mizutani

PB17 Ultrafast structural dynamics of membrane-bound water molecules revealed by two-dimensional surface-specific vibrational spectroscopy

Ellen H.G. Backus, Zhen Zhang, Lukasz Piatkowski, Huib J. Bakker, and Mischa Bonn

PB18 Vibrational-Excitation Induced Proton Transfer in Nafion Nano-Channels

Liyuan Liu, **Artem Bakulin**, and Huib J. Bakker

PB19 Towards unraveling the mechanism of an anti-tuberculosis drug target

Daniel J. Shaw, Katrin Adamczyk, Niall Simpson, Kirsty Robb, Marco Candelaresi, Pim W.J.M. Frederix, Gregory M Greetham, Michael Towrie Anthony W. Parker, Paul Hoskisson, and Neil T. Hunt

PB20 Theoretical study on frequency fluctuation and energy relaxation of HOH bend in liquid water

Sho Imoto and Shinji Saito

PB21 Thermochemical solar energy capture via photoisomerization of dimetallic fulvalene complexes

Justin Lomont, Son Nguyen, Zongrui Hou, Michael R. Harpham, Jeffrey C. Grossman, Yosuke Kanai, Michael W. Mara, Andrew B. Stickrath, Alexie M. Kolpak, Donghwa Lee, Di-Jia Liu, Kasper Moth-Poulsen, Nickolai Vinokurov, Lin X. Chen, K. Peter C. Vollhardt, and Charles B. Harris

PB22 Exciton Delocalization and Dynamics in Helical π-stacks of Self-assembled Perylene Bisimides

Jong Min Lim, Pyosang Kim, Frank Würthner, and Dongho Kim,

PB23 Relationship Between Exciton Delocalization and Excited-State Conformational Dynamics in Linear and Cyclic π-Conjugated Oligothiophenes

Pyosang Kim, Jaesung Yang, Masahiko Iyoda, and Dongho Kim

PB24 Vibrational Relaxation in RNA Nucleotides following Electronic Excitation

Jakob B. Nielsen, Jan Thøgersen, Svend K. Jensen, and Søren R. Keiding

PB25 Vibronic relaxation dynamics in multiphoton reactions of indocyanine green in ethanol

Masanori Fuyuki and Akihide Wada

PB26 The influence of hybrid orbital reconstruction on the mechanism of proton transfer in protonated benzene

Ayaka Kuroki, Hiroshi Ushiyama, and Koichi Yamashita

PB27 Water migration around peptide linkage in Acetanilide-(water) 1:1 cluster studied by time-resolved IR spectroscopy

Martin Weiler, Mitsuhiko Miyazaki, Hiroshi Sekiya, Otto Dopfer, and Masaaki Fujii

PB28 Dispersed three pulse vibrational photon echoes of N_2O in water and octanol: Model systems for phospholipids

Jeffrey T. Shattuck, Shyam Erramilli, and Lawrence D. Ziegler

PB29 Molecular dynamics simulation for fast dielectric relaxation of hydrated ion

Yoji Kubota, Akira Yoshimori, Nobuyuki Matsubayashi, Makoto Suzuki, and Ryo

Akiyama

PB30 VIPER 2D-IR: chemical exchange beyond the vibrational lifetime and sub-ensemble selective photochemistry

Luuk J.G.W. van Wilderen, Andreas T. Messmer, and Jens Bredenbeck

PB31 Time resolved IR spectroscopy on the excited state decay in single stranded DNA

Dominik B. Bucher, Bert Pilles, and Wolfgang Zinth

PB32 Determining in situ protein conformation and orientation from the amide-I sum-frequency generation spectrum: theory and experiment

Steven J. Roeters, Mischa Bonn, and Sander Woutersen

PB33 Effect of specific interaction on C=O vibrational dynamics of the excited state 4-Aminopthalimide

Minako Kondo, Kaoru Ohta, and Keisuke Tominaga

PB34 Comparison of vibrational dynamics between hydrophobic probe and ionic probe in water studied by two-dimensional infrared spectroscopy

Masaki Okuda, Kaoru Ohta, and Keisuke Tominaga

PB35 Structure and Dynamics of Aqueous Hydroxides Studied Using Ultrafast Broadband Infrared Spectroscopy

Aritra Mandal, Krupa Ramasesha, Luigi De Marco, and Andrei Tokmakoff

PB36 Ultrafast two-dimensional phase-resolved vibrational sum frequency spectroscopy of aqueous interfaces

Masanari Okuno, Cho-Shuen Hsieh, Ellen H.G. Backus, and Mischa Bonn

PB37 *Ab Initio* Study of $S_3 \rightarrow S_2$ and $S_2 \rightarrow S_1$ internal conversion of PRODAN molecule

Tomotaka Kunisada, Hiroshi Ushiyama, and Koichi Yamashita

PB38 Electrocyclization reaction of a photocromic molecular switch and excited state dynamics of the molecular constituents studied by Femtosecond Stimulated Resonance Raman Scattering

Emanuele Pontecorvo, Carino Ferrante, Christopher G. Elles, and Tullio Scopigno

PB39 2D IR spectroscopy with a phase-locked pulse pair delayed by a birefringent delay line

Julien Réhault, Margherita Maiuri, Daniele Brida, Cristian Manzoni, Jan Helbing, and Giulio Cerullo

PB40 Structural change and ligand discrimination of oxygen sensor protein FixL studied by ultraviolet resonance Raman spectroscopy

Takeo Yamawaki, Shinji Yano, Haruto Ishikawa, Misao Mizuno, Hiro Nakamura, Yoshitsugu Shiro, and Yasuhisa Mizutani

PB41 N-H Stretching Excitations in Adenosine-Thymidine Base Pairs in Solution: Pair Geometries, Infrared Line Shapes, and Ultrafast Vibrational Dynamics

C. Greve, N.K. Preketes, B. Koeppe, H. Fidder, R. Costard, I.A. Heisler, P.M. Tolstoy, F. Temps, S. Mukamel, T. Elsaesser, and **Erik.T.J. Nibbering**

PB42 Molecular dynamics of proteins in solutions studied by ultrafast Optical Kerr effect (OKE) spectroscopy

David Turton, Thomas Harwood, Hans Senn, Adrian Lapthorn, Elizabeth M. Ellis, and **Klaas Wynne**

PB43 Vibrational relaxation dynamics of the pseudohalide (PS) complexes $Ru(bpy)_2(PS)_2$, PS=CN, NCS and N_3

Ryan Compton Helen K. Gerardi, Daniel Weidinger, Douglas J. Brown, Walter J. Dressick, **Edwin J. Heilweil**, and Jeffrey C. Owrutsky