

**41st Symposium on
Chemical Kinetics and Dynamics
Book of Abstracts**

第 41 回化学反応討論会
講演要旨集

June 2 (Tue.) – 4 (Thu.), 2026

Suzuki Akira Hall, Hokkaido University

Hosted by

ICReDD-Hokkaido University

Local Organizing Committee of SCKD41

Cooperated by

The Chemical Society of Japan
The Spectroscopical Society of Japan
Japan Society of Theoretical Chemistry
Japan Society for Molecular Science
The Atomic Collision Society of Japan

Timetable for SCKD41 in Sapporo

Day 1 June 2 (Tue.)		Day 2 June 3 (Wed.)	Day 3 June 4 (Thu.)
9:00	9:05-9:10 Opening Remarks		
	9:10-10:25		
10:00	Chair: Nanbu, Shinkoh 1A1 Suzuki, Toshinori 1A2 Nakagawa, Shoto 1A3 Wada, Sato	9:30-10:50 Chair: Hasegawa, Jun-ya IL3 Zhu, Chaoyuan IL4 Takahashi, Satoshi	9:30-11:00 Chair: Ishibashi, Atsuki IL6 Kawai, Akio 3A1 Majima, Takuya 3A2 Sie, Ni-En
	10:25-10:40 Coffee/Tea Break		
	10:40-12:00	10:50-11:05 Coffee/Tea Break	11:00-11:15 Coffee/Tea Break
11:00	Chair: Sekikawa, Taro IL1 Hishikawa, Akiyoshi IL2 Tiwari, Ashwani K.	11:05-11:55 Chair: Sumiya, Yosuke 2A1 Nagahata, Yutaka 2A2 Tsuoka, Kazuki	11:15-12:05 Chair: Hamada, Morihiko 3A3 Nakajima, Atsushi 3A4 Ohta, Nobuhiro
12:00	12:00-13:30 Lunch Break	11:55-14:00 Lunch Break	12:05-13:30 Group Photo Lunch Break
13:00	13:30-14:45		13:30-15:00 Poster Session 3
	Chair: Horio, Takuya 1A4 Yamada, Kana 1A5 Fushitani, Mizuho 1A6 Kumagai, Yoshiaki	14:00-15:30 Poster Session 2	
14:00	14:45-15:00 Break		
	15:00-16:30 Poster Session 1	15:30-15:45 Break	15:00-15:10 Break
16:00		15:45-17:15	15:10-16:40 Chair: Komatsuzaki, Tamiki IL7 Ishizaki, Akihito 3A5 Tsubouchi, Masaaki 3A6 Minato, Taketoshi
	16:30-16:45 Break	Chair: Kumagai, Yoshiaki IL5 Sims, Ian 2A3 Ardelia, Mellisa 2A4 Minemoto, Shinichiro	16:40-17:00 Poster Award Ceremony
	16:45-17:35		
17:00	Chair: Murakami, Tatsuhiro 1A7 Zhou, Zhiyi 1A8 Lu, Bateer		17:00-17:10 Closing
		17:30- Banquet	

41st Symposium on Chemical Kinetics and Dynamics

Invited Lectures:

IL1 "Tunnel-Electron Momentum Imaging of Gas-Phase Molecules in Intense Laser Fields"

Hishikawa, Akiyoshi (Nagoya University)

June 2, 10:40 - 11:20

IL2 "Dynamics of atoms and molecules under the influence of intense laser pulses"

Tiwari, Ashwani K. (Indian Institute of Science Education and Research, Kolkata)

June 2, 11:20 - 12:00

IL3 "Nuclear quantum effects in semiclassical and mixed quantum-classical nonadiabatic molecular dynamics"

Zhu, Chaoyuan (National Yang Ming Chiao Tung University)

June 3, 9:30 - 10:10

IL4 "Numerical analysis of the pathway selection in fully reversible chemical reaction networks"

Takahashi, Satoshi (The University of Tokyo)

June 3, 10:10 - 10:50

IL5 "Absolute rate constants and branching fractions for low temperature reactions and inelastic collisions of astrophysical interest"

Sims, Ian (University of Rennes)

June 3, 15:45 - 16:25

IL6 "Elementary reaction rate constants of organic free radicals in liquid phase as measured by the laser synchronized pulsed ESR method"

Kawai, Akio (Kanagawa University)

June 4, 9:30 - 10:10

IL7 "Exploring dynamics in molecular systems using quantum science and technology"

Ishizaki, Akihito (The University of Tokyo)

June 4, 15:10 - 15:50

Day 1: June 2 (Tue.)

9:05–9:10 Opening Remarks

9:10–10:25 Oral Presentations (Chair: Nanbu, Shinkoh)

1A1

Impact of C5 Methylation on Nonadiabatic Transition and Photohydration Damage of Nucleosides

Ghosh, Srijon¹; Obara, Yuki¹; Jaiswal, Vishal Kumar²; Taddei, Mario²; Nenov, Artur²; Conti, Irene²; Garavelli, Marco²; Suzuki, Toshinori¹

(¹Kyoto University, ²Universita degli Studi Bologna)

1A2

Solvent Effects on Ambimodal Diels-Alder/Dipolar Cycloadditions: Classical and Ring-Polymer Molecular Dynamics with Explicit Solvation

Nakagawa, Shoto¹; Matsubuchi, Hayato¹; Ota, Haruki¹; Takayanagi, Toshiyuki¹;

Murakami, Tatsuhiko²

(¹Saitama University, ²Tokyo Metropolitan University)

1A3

Solvent effects on the photoreaction dynamics of cis-stilbene: A QM/MM nonadiabatic molecular dynamics study

Wada, Sato¹; Minegishi, Yusuke¹; Tsutsumi, Takuro¹; Taketsugu, Tetsuya¹

(¹Hokkaido University)

10:25–10:40 Coffee/Tea Break

10:40–12:00 Oral Presentations (Chair: Sekikawa, Taro)

IL1

Tunnel-Electron Momentum Imaging of Gas-Phase Molecules in Intense Laser Fields

Hishikawa, Akiyoshi

(Nagoya University)

IL2

Dynamics of atoms and molecules under the influence of intense laser pulses

Tiwari, Ashwani K.

(Indian Institute of Science Education and Research, Kolkata)

12:00–13:30 Lunch Break

13:30–14:45 Oral Presentations (Chair: Horio, Takuya)

1A4

Ultrafast state-selective dynamics of electronically excited N_2^+ by pump-probe measurements using few-cycle near-infrared laser pulses and high-order harmonics

Yamada, Kana¹; Ando, Toshiaki¹; Iwasaki, Atsushi¹; Yamanouchi, Kaoru¹

(¹The University of Tokyo)

1A5

Formation of I 4d double-core-hole states of CH_3I in strong EUV-FEL fields studied by electron-ion coincidence spectroscopy

Fushitani, Mizuho^{1,2}; Hikosaka, Yasumasa^{2,3}; Owada, Shigeki^{2,4}; Hishikawa, Akiyoshi^{1,2,5}

(¹Nagoya Univ., ²RIKEN SPring-8 Center, ³Univ. of Toyama, ⁴JASRI, ⁵RCMS, Nagoya Univ.)

1A6

Ultraviolet photodynamics in iodopropane isomers studied by time-resolved momentum imaging with extreme ultraviolet photoionization

Kumagai, Yoshiaki^{1,2}; Allum, Felix^{3,4,5}; Nagaya, Kiyonobu⁶; Harries, James R.⁷; Iwayama, Hiroshi^{8,9}; Britton, Mathew⁵; H. Bucksbaum, Philip⁴; Burt, Michael^{10,11}; Brouard, Mark¹⁰; Downes-Ward, Briony¹²; Driver, Taran⁵; Heathcote, David¹⁰; Hockett, Paul¹³; J. Howard, Andrew⁴; W. L. Lee, Jason³; Liu, Yusong⁴; Kukk, Edwin¹⁴; W. McManus, Joseph¹⁰; Milčević, Dennis¹⁰; S. Minns, Russell¹²; Niozu, Akinobu¹⁵; Niskanen, Johannes¹⁴; J. Orr-Ewing, Andrew¹⁶; Owada, Shigeki^{17,18}; Robertson, Patrick^{10,19}; Rolles, Daniel²⁰; Rudenko, Artem²⁰; Ueda, Kiyoshi²¹; Unwin, James¹⁰; Vallance, Claire¹⁰; Walmsley, Tiffany¹⁰; N. R. Ashfold, Michael¹⁶; Forbes, Ruaridh^{5,22}

(¹Nara Women's University, ²Tokyo University of Agriculture and Technology, ³Deutsches Elektronen-Synchrotron (DESY), ⁴Stanford PULSE Institute, SLAC, ⁵Linac Coherent Light Source, SLAC, ⁶Kyoto University, ⁷QST, ⁸Institute for Molecular Science, ⁹Sokendai, ¹⁰University of Oxford, ¹¹Trent University, ¹²University of Southampton, ¹³National Research Council of Canada, ¹⁴University of Turku, ¹⁵Hiroshima University, ¹⁶University of Bristol, ¹⁷RIKEN SPring-8 Center, ¹⁸Japan Synchrotron Radiation Research Institute, ¹⁹University of Nottingham, ²⁰Kansas State University, ²¹Tohoku University, ²²University of California, Davis)

14:45–15:00 Break (Proceed to the Poster Session Venue)

15:00–16:30 Poster Session 1

16:30–16:45 Break (Return to the Oral Session Venue)

16:45–17:35 Oral Presentations (Chair: Murakami, Tatsuhiro)

1A7

Ring-opening via conical intersections in thiophene revealed by extreme ultraviolet time-resolved photoelectron spectroscopy

Zhou, Zhiyi¹; Wada, Sato²; Arai, Yuto¹; Kambara, Ryuto³; Taketsugu, Tetsuya^{2,4}; Sekikawa, Taro¹

(¹Dept. of Applied Physics, Fac. of Eng., Hokkaido Univ., ²WPI-ICReDD, Hokkaido Univ., ³Grad. Sch. of Chem. Sci. & Eng., Hokkaido Univ., ⁴Dept. of Chemistry, Fac. of Sci., Hokkaido Univ.)

1A8

First observation of sequential photochemical and thermal ring-opening dynamics in 1,3-cyclohexadiene

Lu, Bateer¹; Sekikawa, Taro¹

(¹Hokkaido University)

Day 2: June 3 (Wed.)

9:30–10:50 Oral Presentations (Chair: Hasegawa, Jun-ya)

IL3

Nuclear quantum effects in semiclassical and mixed quantum-classical nonadiabatic molecular dynamics

Zhu, Chaoyuan

(National Yang Ming Chiao Tung University)

IL4

Numerical analysis of the pathway selection in fully reversible chemical reaction networks

Takahashi, Satoshi

(The University of Tokyo)

10:50–11:05 Coffee/Tea Break

11:05–11:55 Oral Presentations (Chair: Sumiya, Yosuke)

2A1

An efficient approximation of the timescale hierarchies in a large-scale first-order kinetics

Nagahata, Yutaka¹; Toda, Mikito^{1,2,3}; Komatsuzaki, Tamiki^{1,4,5,6}

(¹RIES, Hokkaido University, ²Research Institute for Engineering, Kanagawa University, ³Graduate School of Information Science, University of Hyogo, ⁴WPI-ICReDD, Hokkaido University, ⁵Department of Chemistry, Faculty of Science, Hokkaido University, ⁶OTRI, Osaka University)

2A2

Exploration of chemical reaction pathways by quantum walk

Tsuoka, Kazuki¹; Nishi, Takanori^{1,2}; Kaoru, Yamanouchi^{1,2}

(¹School of Science, The Univ. of Tokyo, ²Institute for Attosecond Laser Facility, The Univ. of Tokyo)

11:55–14:00 Lunch Break

14:00–15:30 Poster Session 2

15:45–17:15 Oral Presentations (Chair: Kumagai, Yoshiaki)

IL5

Absolute rate constants and branching fractions for low temperature reactions and inelastic collisions of astrophysical interest

Sims, Ian

(University of Rennes)

2A3

Observation of Rabi oscillation between the inversion splitting doubling in ammonia

Ardelia, Mellisa¹; Ueno, Kazuki¹; Saida, Ryota¹; Nakamura, Masaaki¹; Ohshima, Yasuhiro¹

(¹Graduate School of Science, Institute of Science Tokyo)

2A4

Hydrogen momentum spectroscopy of small hydrocarbon molecules

Minemoto, Shinichirou¹; Kanaya, Satoru¹; Sugai, Takuma¹; Jones, Darryl²; Takahashi, Masahiko¹

(¹IMRAM, Tohoku University, ²Flinders University)

17:30– Banquet

Day 3: June 4 (Thu.)

9:30–11:00 Oral Presentations (Chair: Ishibashi, Atsuki)

IL6

Elementary reaction rate constants of organic free radicals in liquid phase as measured by the laser synchronized pulsed ESR method

Kawai, Akio

(Kanagawa University)

3A1

Combined experimental and computational study of ionization-induced reactions on propanol ice surfaces

Majima, Takuya¹; Otsuka, Sota¹; Jifuku, Shuntaro¹; Murakami, Tatsuhiko²; Tsuchida, Hidetsugu¹; Saito, Manabu¹

(¹Kyoto University, ²Tokyo Metropolitan University)

3A2

Photodesorption of hydroxyl radical on ice induced by visible light

Sie, Ni-En¹; Tsuge, Masashi^{1,2}; Nakai, Yoichi³; Watanabe, Naoki¹

(¹Hokkaido University, ²Hiroshima University, ³RIKEN Nishina Center for Accelerator-based Science)

11:00–11:15 Coffee/Tea Break

11:15–12:05 Oral Presentations (Chair: Hamada, Morihiko)

3A3

Oxygen reactivity of surface-supported pure and boron-doped aluminum superatoms

Inoue, Tomoya¹; Nakajima, Atsushi¹

(¹Keio University)

3A4

Effects of nanosecond pulsed electric field on brain and pancreatic cells and fluorescence microscopy with particular attention to the difference between cancerous and normal cells

Ohta, Nobuhiro¹; Awasthi, Kamlesh¹; Bai, Dong-Jie¹; Wei, Chun-Yen¹; Hsu, Hsin-Yun¹

(¹National Yang Ming Chiao Tung University (NYCU))

12:05–13:30 Lunch Break

13:30–15:00 Poster Session 3

15:10–16:40 Oral Presentations (Chair: Komatsuzaki, Tamiki)

IL7

Exploring dynamics in molecular systems using quantum science and technology

Ishizaki, Akihito

(The University of Tokyo)

3A5

Two-dimensional electronic spectroscopy of light-harvesting phycobiliproteins synthesized by recombinant DNA techniques

Tsubouchi, Masaaki^{1,2}; Fujita, Takatoshi²; Adachi, Motoyasu²; Itakura, Ryuji¹

(¹Kansai Institute for Photon Science, QST, ²Institute for Quantum Life Science, QST)

3A6

Reaction of fluoride ions at the electrode–electrolyte interface for high energy density batteries

Minato, Taketoshi^{1,2}; Tabtimtong, Nicha^{1,3}; Kaisook, Pattanapon^{1,3}; Tenailon Johan, 1⁴;

Athikaphan Pakpoom^{5,1}; Imai, Yumiko¹; Ueda, Tadashi¹; Nakamoto, Kei-ichi^{1,6};

Neramittagapong, Arthit³; Neramittagapong, Sutasinee³

(¹Institute for Molecular Science, ²Spin-L, ³Khon Kaen Univ., ⁴Chimie-ParisTech ENSCP, ⁵National Institutes of Natural Science, ⁶NAIST)

16:40–17:00 Poster Award Ceremony

17:00–17:10 Closing Remarks

Poster Presentations

(*Candidates for the Best Poster Prize)

Session 1 (June 2, 15:00–16:30)

1P01*

Floquet-theory-based nonadiabatic ab initio molecular dynamics for analyzing chemical reactions in strong laser fields

Kambara, Ryuto¹; Tsutsumi, Takuro¹; Taketsugu, Tetsuya¹

(¹Hokkaido University)

1P02

Femtosecond laser filament reaction in gaseous hexane studied by time-of-flight mass spectrometry with velocity screening

Matsuda, Akitaka¹; Okumura, Yuya¹; Hashigaya, Kasumi¹; Hishikawa, Akiyoshi¹

(¹Nagoya University)

1P03*

Nonadiabatic internal conversion of S₂ and isomerization dynamics of silabenzene

Sato, Hazuki¹; Kimura, Mizuki¹; Nanbu, Shinkoh²

(¹Graduate School of Science and Technology, Sophia University, ²Faculty of Science and Technology, Sophia University)

1P04

Photofragment imaging of oriented methyl/ethyl bromide (CH₃Br, C₂H₅Br) for the assessment of their transition dipole moments

Kawamata, Hiroshi¹; Nakamura, Masaaki²; Che, Dock-Chil³

(¹Hokkaido University, ²Institute of Science Tokyo, ³Osaka University)

1P05*

Suppression of twisted intermediate formation in uracil by C6 methylation

Aki, Yoshino¹; Ghosh, Srijon¹; Obara, Yuki¹; Suzuki, Toshinori¹

(¹Kyoto University)

1P06*

Theoretical study on C5 substituent effects on the excited-state relaxation dynamics of pyrimidine bases

Kobayashi, Yuto¹; Kambara, Ryuto¹; Minegishi, Yusuke¹; Wada, Satoi¹; Taketsugu, Tetsuya¹

(¹Hokkaido University)

1P07

Observations of vibrational wavepackets of N₂ and N₂⁺ generated in air plasma
Endo, Tomoyuki¹; Mashiko, Hiroki²; Sako, Tokuei³; Oguri, Katsuya²; Itakura, Ryuji¹
(¹QST, KPSI, ²NTT BRL, ³Nihon University)

1P08*

Photoelectron circular dichroism of epichlorohydrin in near-infrared intense laser fields studied by electron-ion coincidence momentum imaging
Ogawa, Kazumi¹; Kuroda, Runa¹; Matsuda, Akitaka¹; Hishikawa, Akiyoshi^{1,2}
(¹Grad. Sc. Sci, Nagoya U., ²RCMS, Nagoya U.)

1P09*

Multimodal Energy Landscape Underlying Adhesive Interface Peeling
Kubo, Koki¹; Sumiya, Yosuke¹
(¹Yamaguchi University)

1P10*

Predicting Product Branching in Post-Transition State Bifurcation Reactions via Molecular Dynamics Simulations
Okamoto, Daichi¹; Yamaki, Keita¹; Hayashi, Daiki¹; Nakagawa, Shota¹; Matsubuchi, Hayato¹; Sasaki, Yuki¹; Takayanagi, Toshiyuki¹; Murakami, Tatsuhiko²
(¹Saitama University, ²Tokyo Metropolitan University)

1P11

Robust High-Order Derivative Evaluation for Phase-Space Reaction Dynamics Using Chebyshev Polynomial-Based Spectral Differentiation
Umer, Umair¹; Li, Jizhou²; Komatsuzaki, Tamki^{1,2}; Staub, Ruben¹; Taketsugu, Tetsuya¹; Yagi, Kiyoshi³
(¹ICReDD, Hokkaido University, ²RIES, Hokkaido University, ³Department of Chemistry, University of Tsukuba)

1P12*

Development of a fluctuation-assisted molecular dynamics method for the efficient sampling of chemical reactions
Tsukamura, Sei¹; Nishimura, Yoshifumi²; Nakai, Hiromi^{1,2}
(¹Grad. Sch. Adv. Sci. Eng., Waseda University, ²WISE, Waseda University)

1P13*

Dynamical Effects Beyond Kinetic Analysis Based on Reaction Path Networks: An Ab Initio Molecular Dynamics Study
Takizawa, Soei¹; Tsutsumi, Takuro¹; Ono, Yuriko¹; Sada, Kazuki¹; Taketsugu, Tetsuya¹
(¹Hokkaido University)

1P14

A Reusable Explicit Chemical Ontology-Based Method to Expedite Reaction Path Searches

Nath, Pinku¹; (¹WPI-ICReDD, Hokkaido University)

1P15*

Analysis of the Product Branching Boundary Determining Reaction-Path Bifurcation
Suzuki, Jidai¹; Nakanishi, Tatsuhiro¹; Kambara, Ryuto¹; Ono, Yuriko^{2,3}; Taketsugu, Tetsuya^{2,4}

(¹Grad. School Chem. Sci. Eng., Hokkaido Univ., ²Fac. Sci., Hokkaido Univ., ³Institute for Quantum Chemical Exploration, ⁴WPI-ICReDD, Hokkaido Univ.)

1P16

Merged-beam experiment on a low-energy ion-neutral reaction study

Dhongade, Siddhant¹; Tamaru, Hiroya¹; Ota, Rin¹; Bllantyne, Lucius Thaine¹; Matsuzaki, Taichi¹; Yabuki, Sorato¹; Nakayama, Akifumi²; Nakano, Yuji¹

(¹Department of Physics, Rikkyo University, ²Earth-Life Science Institute, Institute of Science Tokyo)

1P17*

Entropic advantage and induction-mediated polarization in the adsorption of cyclic oligomers on fullerene surfaces

Arima, Sota¹; Yamamoto, Takuya²; Sato, Shin-ichiro²

(¹Grad. School Chem. Sci. Eng., Hokkaido Univ., ²Div. Appl. Chem., Fac. Eng., Hokkaido Univ.)

1P18

Surface reactions of sulfur-bearing molecules with hydrogen atoms on amor-phous solid water

Nguyen, Thanh^{1,2}; Oba, Yasuhiro¹; Sameera, W. M. C.^{1,3}; Molpeceres, German⁴; Watanabe, Naoki¹

(¹Hokkaido University, ²Present address: Leiden University, ³University of Gothenburg, ⁴Institute de Fisica Fundamental (IFF-CSIC))

1P19*

Towards the Observation of Gas-Phase Vibrational Polaritons via Cavity Transmission Spectroscopy

Miyashita, Kaichi¹; Mitsukawa, Eiyu¹; Matsumoto, Yoshiteru²

(¹Grad. Sch. Integr. Sci. Technol., Shizuoka Univ., ²Dept. Chem., Fac. Sci., Shizuoka Univ.)

1P20

Physical Adsorption and Conformational Changes of Figure-Eight Poly(ethylene glycol) on Gold Nanosheet Surfaces: A Molecular Dynamics Study

Kobayashi, Takuto¹; Arima, Souta¹; Yamamoto, Takuya¹; Sato, Shin-ichiro¹

(¹Hokkaido University)

1P21*

Molecular Dynamics Simulation of the Rotational Relaxation Time of an Aptamer-Based Fluorescent Molecular Sensor in Aqueous Solution

Hashimoto, Kohei¹; Arima, Sota¹; Tokeshi, Manabu¹; Yamamoto, Takuya¹; Sato, Shinichiro¹

(¹Hokkaido University)

1P23*

Theoretical prediction of atomic diffusion energy at the ice surface under cryogenic conditions using the kinetic MC method.

Taniguchi, Riko¹; Nakatani, Naoki¹; Nakatani, Kaho¹

(¹Tokyo Metropolitan University)

1P24

Conformational Constraints in Ni Complexes for Tuning H₂ Production and Oxidation: A DFT-Based Ligand Design Study

Hadsadee, S.¹; Ratanasak, M.¹; Naweephattana, P.¹; Morita, S.¹; Miyazaki, R.¹; Iida, K.¹; Nakayama, A.¹; Jungsuttiwong, S.²; Hasegawa, J.¹

(¹Hokkaido University, ²Ubonrachatani University)

1P25*

Electron Momentum Spectroscopy Study of the Intramolecular Hydrogen Bond in Acetylacetone

Mohri, Fumiya¹; Sato, Takumi¹; Takahashi, Masahiko²; Ohshima, Yasuhiro¹; Yamazaki, Masakazu^{1,3}

(¹Institute of Science Tokyo, ²Tohoku University, ³Keio University)

1P26

Electrochemical Behavior of BiF₃-Based Electrodes in Liquid Electrolyte for Fluoride Shuttle Batteries

Athikaphan, Pakpoom¹; Tabtimtong, Nicha²; Kaisook, Pattanapon²; Imai, Yumiko¹; Ueda, Tadashi¹; Neramittagapong, Arthit^{2,3}; Sutasinee Neramittagapong, ^{2,3}; Minato, Taketoshi^{1,4}

(¹Institute for Molecular Science, National Institutes of Natural Sciences, ²Department of Chemical Engineering, Faculty of Engineering, Khon Kaen University, ³Research Center for Environmental and Hazardous Substance Management, Khon Kaen University, ⁴Core for Spin Life Sciences, Okazaki Collaborative Platform, National Institutes of Natural Sciences)

1P27*

Polar-molecule trajectory simulations for cluster isolation using a Stark deflector

Miwa, Yutaro¹; Ardelia, Mellisa¹; Nakamura, Masaaki¹; Ohshima, Yasuhiro¹

(¹Institute of Science Tokyo)

1P28

Photochemical Reaction of Methylene Blue and Ascorbic Acid

Suzuki, Takahiro¹; Ie, Kanon¹; Kimura, Takayoshi¹; Inoue, Masayuki¹

(¹Tokyo University of Science)

Session 2 (June 3, 14:00–15:30)

2P01*

Photodissociation dynamics of *N,N*-dimethylformamide: Generation of highly vibrational excited HCO

Karino, Momiji¹; Shinohara, Ryo¹; Inoue, Kosuke¹; Yamasaki, Katsuyoshi¹; Kohguchi, Hiroshi¹

(¹Hiroshima University)

2P02

High-Resolution Laser Spectroscopy of the S₁←S₀ transition of Fluorene: Perturbation analysis in the S₁ state

Kasahara, Shunji¹; Minik, Luke¹; Kuroda, Shinji¹

(¹Kobe University)

2P03*

Photoelectron Circular Dichroism in chiral molecules using 21.7eV HHG light

Matano, Shuhei¹; Oshima, Ryunosuke¹; Minemoto, Shinichiro²; Sekikawa, Taro¹

(¹Department of Applied Physics, Hokkaido University, ²IMRAM, Tohoku University)

2P04

Unimolecular decomposition of highly excited C₂H₄: Trajectory calculations of product branching

Matsugi, Akira¹; Matsui, Hiroyuki²

(¹AIST, ²NYCU)

2P05*

Simulation of post-ionization population inversion in CO₂⁺ in an ultrashort intense laser pulse

Huang, Siwei¹; Lötstedt, Erik^{1,2}; Yamanouchi, Kaoru^{1,3}

(¹School of Science, The University of Tokyo, ²iTHEMS, RIKEN, ³I-ALFA, The University of Tokyo)

2P06

Relaxation dynamics via the S₁ state of Ag₃⁻ probed by time-resolved photoelectron imaging

Kusaba, Yuri¹; Aoki, Yuma¹; Suzuki, Yuta¹; Ushiki, Yuta¹; Shimizu, Misaki¹; Toyama, Yuki¹; Terasaki, Akira¹; Horio, Takuya¹

(¹Kyushu University)

2P07*

Microsolvation effects on photodissociation dynamics of the hemibonded (H₂S)₂⁺ ioncore

Shioura, Mitsuaki¹; Koshiba, Takumi¹; Kanno, Manabu¹; Misaizu, Fuminori¹; Fujii, Asuka¹

(¹Tohoku University)

2P08

High-resolution laser spectroscopy of the A-X transition of ¹⁴NO₂ radical

Tada, Kohei¹; Misono, Masatoshi¹; Yoshizawa, Takumi²; Kishigami, Ko²; Kasahara, Shunji³

(¹Faculty of Science, Fukuoka University, ²Faculty of Science, Kobe University, ³Center for Life Photonic Innovation, Kobe University)

2P09*

An analysis of charge migration in the McLafferty rearrangement utilizing natural reaction orbital method

Nakanishi, Tatsuhiro¹; Takayama, Mitsuo²; Taketsugu, Tetsuya^{3,4}

(¹Grad. Sch. Chem. Sci. Eng., Hokkaido Univ., ²Grad. Nanobio., Yokohama City Univ., ³Dep. Chem., Fac. Sci., Hokkaido Univ., ⁴WPI-ICReDD, Hokkaido Univ.)

2P10*

Theoretical Design of Unactivated Arene Conversion Reactions Using Triazene Compounds

Nagano, Ayana¹; Kokubu, Shusuke²; Yamakawa, Kazuhito²; Haraguchi, Ryosuke²; Sumiya, Yosuke¹

(¹Yamaguchi University, ²Chiba Institute of Technology)

2P11

Theoretical study on the thermal dissociation reaction of 3-methylaminopropylamine

Kanno, Nozomu¹

(¹Meijo University)

2P12*

What Underlies the Woodward-Hoffmann rules? A Reaction Analysis Based on Orbital Energies

Tsuruta, Masaya¹; Mita, Tsuyoshi²; Taketsugu, Tetsuya^{2,3}; Tsuneda, Takao^{2,4}

(¹Grad. Sch. Chem. Sci. Eng., Hokkaido Univ., ²WPI-ICReDD, Hokkaido Univ., ³Fac. Sci., Hokkaido Univ., ⁴Grad. Sch. System Informatics, Kobe Univ.)

2P13*

Quantifying the Contribution of Nonreactive Modes to Reaction Dynamics in Phase Space: Analytical Prediction of the Passage Time τ near a Saddle Point

Kurahashi, Ryo¹; Li, Jizhou¹; Tanaka, Ryoichi¹; Umer, Umair¹; Nagahata, Yutaka¹; Mizuno, Yuta²; Komatsuzaki, Tamiki¹
(¹Hokkaido University, ²AIST)

2P14*

Development of a quadratic convergence two-point search algorithm using the Dynamical NEB method

Kanazawa, Ryosuke¹; Nakatani, Naoki¹; Nakatani, Kaho¹
(¹Tokyo Metropolitan University)

2P15*

Electronic Driving Factors in Outer-Sphere Electron Transfer Reactions: A Reactive Orbital Energy Theory Analysis

Yamada, Daisuke¹; Tsuruta, Masaya¹; Taketsugu, Tetsuya^{2,3}; Tsuneda, Takao^{3,4}
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2P16

Heavy atom tunneling reactions on interstellar icy grain analogs

Tsuge, Masashi^{1,2}; Molpeceres, Germán³; Sie, Ni-En¹; Watanabe, Naoki¹
(¹Hokkaido University, ²Hiroshima University, ³IFF CSIC)

2P17*

Molecular orbital signatures in photoelectron circular dichroism of oxirane derivatives studied by a tunnel ionization theory

Kuroda, Runa¹; Ogawa, Kazumi¹; Uchida, Tomohide¹; Nishimura, Koya¹; Matsuda, Akitaka¹; Hishikawa, Akiyoshi^{1,2}
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2P18*

Experimental determination of N-atom surface diffusion activation energy based on the decay of surface number density due to diffusive recombination reactions

Endo, Tamaki^{1,2}; Tsuge, Masashi^{2,3}; Watanabe, Naoki²
(¹Cosmosciences-Graduate School of Science, Hokkaido Univ., ²Institute of Low Temperature Science, Hokkaido Univ., ³ADSE, Hiroshima University)

2P19

Dynamical electronic structure change of metal oxide surface with oxygen defects under electric current revealed by first-principles computational method

Toyama, Shunsuke¹; Iida, Kenji¹; Hasegawa, Jun-ya¹

(¹Institute for Catalysis, Hokkaido University)

2P20*

Comparison of HCl dissociation behaviors on hexagonal (I_h) and amorphous ice clusters accounting for nuclear quantum effects

Sasaki, Yuki¹; Ueno, Hinami¹; Takayanagi, Toshiyuki¹; Murakami, Tatsuhiro²

(¹Saitama University, ²Tokyo Metropolitan University)

2P21

Reactions between low-energy CH_3^+ ions and a methanol solid surface at low temperatures

Nakai, Yoichi¹; Hidaka, Hiroshi²; Watanabe, Naoki²

(¹RIKEN Nishina Center, ²ILTS, Hokkaido University)

2P22*

Development of a new apparatus for atomic momentum spectroscopy at the world's highest incident electron energy

Kanaya, Satoru¹; Minemoto, Shinichirou¹; Jagutzki, Ottmar^{2,3}; Takahashi, Masahiko¹

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2P23

Methanol formation via $\text{CH}_3 + \text{OH}$ reactions with transient diffusion on amorphous solid water at low temperatures

Hidaka, Hiroshi¹; Iguchi, Arisa²; Ishibashi, Atsuki³; Tsuge, Masashi⁴; Oba, Yasuhiro¹;

Watanabe, Naoki¹

(¹Hokkaido University, ²The University of Electro-Communications, ³The University of Tokyo, ⁴Hiroshima University)

2P24*

Kinetic analysis of luminol chemiluminescence in dimethyl sulfoxide driven by dissolved oxygen under a nitrogen atmosphere

Ie, Kanon¹; Suzuki, Takahiro²; Inoue, Masayuki²

(¹Graduate School of Science, Tokyo University of Science, ²Tokyo University of Science)

2P25

Development and Application of a Conformational Analysis Method Combining MD Simulation and Ion Mobility Mass Spectrometry

Tashiro, Keisuke¹; Ide, Yuki²; Taketsugu, Tetsuya^{1,2}; Ohara, Kazuaki³; Yamaguchi, Kentaro³; Kobayashi, Masato^{1,2}; Inokuma, Yasuhide^{2,4}

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2P26*

Development of Fourier Transform Three-Color Excitation Action Spectroscopy for Model-Free Analysis of Photo-Stationary States

Yamashita, Sayaka¹; Inoue, Rinka¹; Fukuda, Kai¹; Wada, Akihide¹

(¹Kobe University)

2P27

Vibrational states and transition intensities based on variational vibrational theory

Sunaga, Ayaki^{1,2}

(¹Hokkaido University, ²Eötvös Loránd University)

Session 3 (June 4, 13:30–15:00)

3P01*

Substituent Effects on Electrocyclic Reactions: Ultrafast Ring-Opening of α -Phellandrene Stimulated by Impulsively Excited Molecular Vibrations

Zhou, Zhiyi¹; Saita, Kenichiro²; Minegishi, Yusuke³; Taketsugu, Tetsuya^{4,5}; Sekikawa, Taro¹

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3P02

Photochemical reaction of pyrene with CCl₄ in alcohols

Watanabe, Akihiro¹; Kanemura, Sakura¹; Naruo, Nanami¹

(¹Kobe City College of Technology)

3P03*

Ion pair dissociation of carbon dioxide following absorption of a vacuum ultraviolet photon

Oda, Akiko¹; Suzuki, Isao H.¹; Odagiri, Takeshi¹

(¹Sophia University)

3P04

Rotational excitation of NO in an intense femtosecond laser field carrying orbital angular momentum

Fukahori, Shinichi^{1,2}; Hasegawa, Hirokazu^{1,2}

(¹Graduate School of Arts and Sciences, The Univ. of Tokyo, ²Komaba Institute for Science, The Univ. of Tokyo)

3P05*

Photodissociation pathways of O₄⁺ leading to singlet oxygen O₂(a ¹Δ_g) and O₂(b ¹Σ_g⁺) studied by mass-analyzed ion imaging

Watabe, Yu¹; Koshiba, Takumi¹; Ito, Yuri¹; Kanno, Manabu¹; Ohshimo, Keijiro²; Misaizu, Fuminori¹

(¹Graduate School of Science, Tohoku Univ., ²Hokkaido University of Education)

3P06

Mechanism of the delayed fragmentation of ethanol molecules upon VUV photoionization

Nakao, Tomohiko¹; Kaneyasu, Tatsuo^{2,3}; Yanagawaya, Takuma¹; Iwayama, Hiroshi²; Majima, Takuya¹

(¹Kyoto University, ²Institute for Molecular Science, ³Sokendai)

3P07*

The relationship between photon energy and two translational energy components of the CH₃ fragment in photodissociation of Zn(CH₃)₂

Morimoto, Takumi¹; Okuda, Yuuka¹; Haze, Misato¹; Kohguchi, Hiroshi¹
(¹Hiroshima University)

3P08

Solvent effects on the ground and first excited states of aniline

Ohashi, Kazuhiko¹
(¹Kyushu University)

3P09*

Mechanochemical Reaction Path Analysis of Polymer Chain Cleavage

Mori, Itsuki¹; Sumiya, Yosuke¹
(¹Yamaguchi Univ.)

3P10

Elucidation of the Mechanism of Bifurcation Control in Enzymatic Reactions Based on the Reaction Space Projector Method

Qu, Lihao¹; Tsutsumi, Takuro¹; Ono, Yuriko¹; Taketsugu, Tetsuya¹
(¹Hokkaido University)

3P11*

Accelerating the Mechanistic Study of Triarylborane Catalysts through Virtual Borane

Hirose, Ken¹; Maeda, Satoshi^{1,2}; Matsuoka, Wataru^{1,2}
(¹Hokkaido University, ²WPI-ICReDD)

3P12*

Mechanistic Study on the Degradation of Aliphatic Amines for CO₂ Capture Using Systematic Reaction Path Exploration

Toma, Shunta¹; Sumiya, Yosuke¹
(¹Yamaguchi Univ)

3P13*

Machine-learning extraction of reaction coordinates and transition states in phase space

Noda, Takuto¹; Md. Al Mehedi, Hasan²; Li, Jizhou²; Komatsuzaki, Tamiki^{1,2,3}
(¹CSE, Hokkaido University, ²RIES, Hokkaido University, ³WPI-ICReDD, Hokkaido University)

3P14*

Exploring Valley-Ridge Inflection Regions in Post-Transition State Bifurcation Reactions

Yamaki, Keita¹; Okamoto, Daichi¹; Hayashi, Daiki¹; Nakagawa, Shoto¹; Matsubuchi, Hayato¹; Sasaki, Yuki¹; Takayanagi, Toshiyuki¹; Murakami, Tatsuhiro²
(¹Saitama University, ²Tokyo Metropolitan University)

3P15*

Machine Learning-based Multi-objective Optimization of reaction condition of ²¹¹At Astatination Reactions

Kitano, Tomoyuki¹; Hashiba, Shunnichi¹; Ando, Masaya¹; Iida, Keita¹; Mukaimine, Akari¹; Mizuno, Yuta^{2,1}; Tabata, Koji¹; Nakajima, Kohei¹; Komatsuzaki, Tamiki¹; Ogawa, Mikako¹
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3P16*

Can Reactive Species Be Spontaneously Formed at the Air – Water Interface of Microdroplets? A Spray Ionization Mass Spectrometry Investigation

Kurokawa, Kei¹; Enami, Shinichi¹; Numadate, Naoki¹
(¹Tsukuba University)

3P17

Transient diffusion of radicals induced by surface reactions at 10 K

Ishibashi, Atsuki^{1,2}; Hidaka, Hiroshi²; Iguchi, Arisa²; Watanabe, Naoki²
(¹The University of Tokyo, ²Hokkaido University)

3P18*

Theoretical investigation of the structure and electronic properties of N₂O adsorbed on an Ir₂₀ cluster.

Uchiyama, Nino¹; Taketsugu, Tetsuya¹; Hinokuma, Satoshi²; Iwasa, Takeshi¹
(¹Hokkaido University, ²AIST)

3P19

A near-edge x-ray absorption fine structure study of products in ice film by monochromic soft x-ray irradiation

Nakagawa, Seiko¹; Obata, Yui²; Baba, Yuji³; Yokoya, Akinari^{2,4}
(¹Tokyo Metropolitan Industrial Technology Research Institute, ²Ibaraki University, ³Japan Atomic Energy Agency, ⁴National Institutes for Quantum Science and Technology)

3P20*

Nonlinear photocurrent generation in SiO₂ device by ω -2 ω asymmetric strong laser fields

Kinoshita, Hiroshi¹; Matsumoto, Ryutarō¹; Fushitani, Mizuho¹; Hishikawa, Akiyoshi¹
(¹Nagoya University)

3P21

Syntheses and evaluation of photocatalytic activities of the composites of antimony halide perovskites and graphitic carbon nitride

Akiyama, Sogo¹; Iitaka, Fumiaki¹; Kadota, Yusuke¹; Mitsuke, Koichiro^{1,2}; Ogata, Hironori^{1,2}

(¹Hosei University, ²Hosei Univ. Res. Cntr. Micro-Nano Technol.)

3P22*

Electron momentum spectroscopy of aniline: Towards molecular orbital imaging of the excited triplet state

Sato, Takumi¹; Mori, Yutori¹; Takahashi, Masahiko²; Ohshima, Yasuhiro¹; Yamazaki, Masakazu^{1,3}

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3P23

Toward Time-Resolved Core-Level Spectroscopy Beyond Oxygen K-edge Using an Ultrashort Soft X-ray Light Source

Ishii, Nobuhisa¹; Sun, Hung-Wei¹; Maruyama, Momoko¹; Itakura, Ryuji¹

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3P24*

Distribution of ions at the air-water interface investigated by spray ionization mass spectrometry

Kosugi, Kento¹; Numadate, Naoki¹; Enami, Shinichi¹

(¹University of Tsukuba)

3P25

Synthesis and Optical Property of Eu doped Carbon Dots

Hamada, Morihiko¹; Tanaka, Misaki¹; Fuki, Masaaki²; Kobori, Yasuhiro²

(¹Kobe City College of Technology, ²Kobe University)

3P26*

A Systematic Exploration of Nonradiative Decay Paths in Carbo[n]Helicenes(n=5-12):
Role of Cyclization Paths

Kondo, Itsuki¹; Harabuchi, Yu^{2,3}; Akiyama, Seiji⁴; Nagata, Yuuya^{2,3,5}; Maeda,
Satoshi^{2,3,6}

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ICReDD, Hokkaido University, ³JST, ERATO, ⁴RIKEN, ⁵NIMS, ⁶Graduate School of
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3P27

The rate rules for the reactions of Alkenes with OH

Fushimi, Ryota^{1,2}; Oguchi, Tatsuo¹

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College)

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