

**40th Symposium on
Chemical Kinetics and Dynamics
Book of Abstracts**

**第40回化学反応討論会
講演要旨集**

June 4 (Wed.) – 6 (Fri.), 2025

Kobe University Centennial Hall

Hosted by
Local Organizing Committee of SCKD40

Co-hosted by
Graduate School of Science, Kobe University

Cooperated by
The Japanese Photochemistry Association
Japan Society for Molecular Science

Symposium Venue

**Kobe University
Centennial Hall**

1-1 Rokkodai-cho, Nada-ku, Kobe
(Tel.) 078-803-5695

Banquet

**Kobe University
Takigawa Memorial Hall**

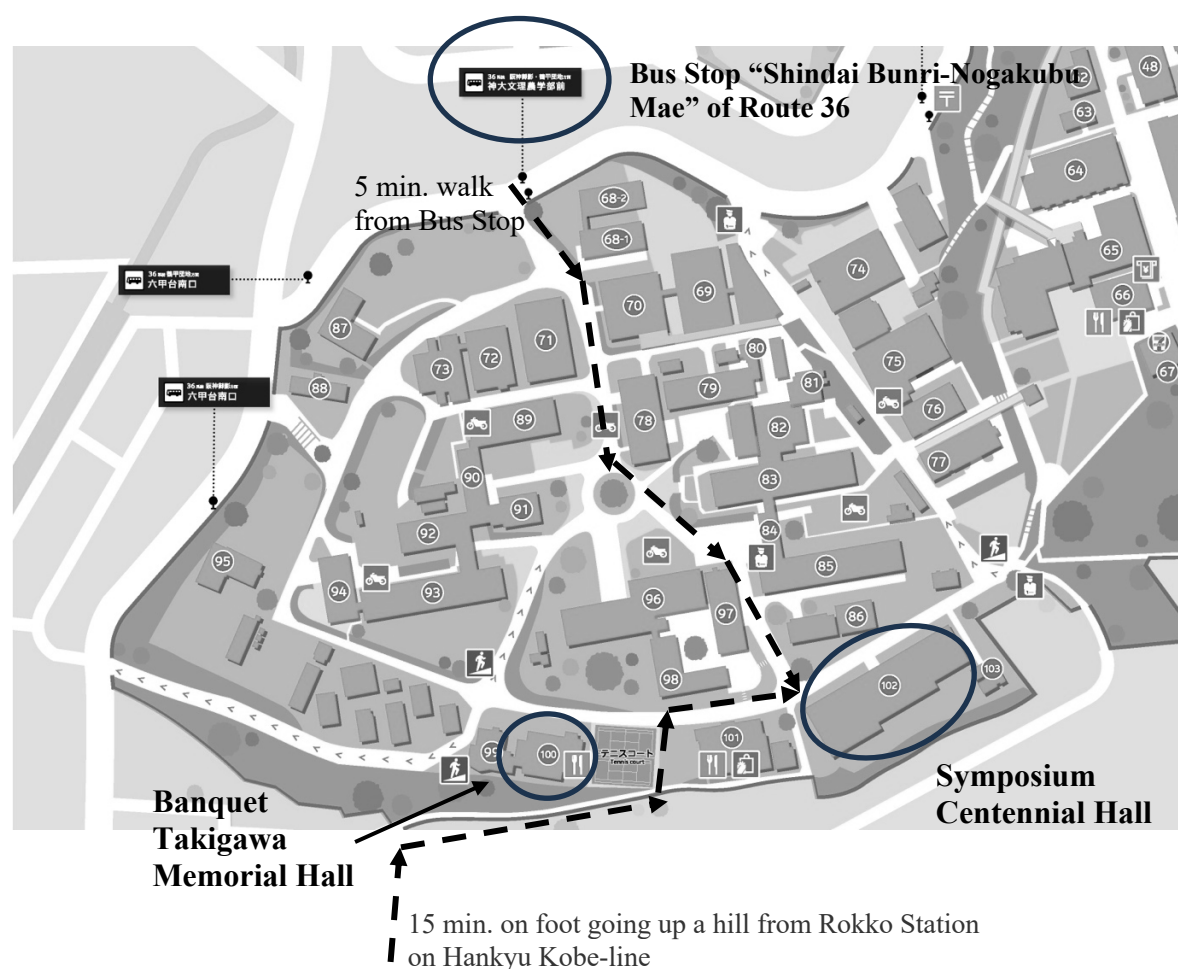
[Date & Time]

Thursday, 17:30-19:30 5th June 2025

Oral talks: Rokko Hall (2F)

Posters & Exhibitions: Foyer of Rokko Hall (2F)

Registration: Foyer of Rokko Hall (2F)



Recommended: Take Route "36 for Tsurukabutodanchi" of Kobe-Shi Bus from Rokko Station on Hankyu Kobe-line, JR Rokko-michi Station, or Mikage Station on Hanshin main-line, for about 10, 15, and 20 min, respectively, and get off at "Shindai Bunri Nogakubu-Mae" stop. Then, walk down the campus to Centennial Hall for 5 min. on foot.

From Rokko Station on Hankyu Kobe-line: 15 min. on foot going up a hill.

From JR Shin-Kobe Station: 15 min. by Taxi.

シンポジウム会場

神戸大学百年記念館（神大会館）
神戸市灘区六甲台町1-1
(Tel) 078-803-5695

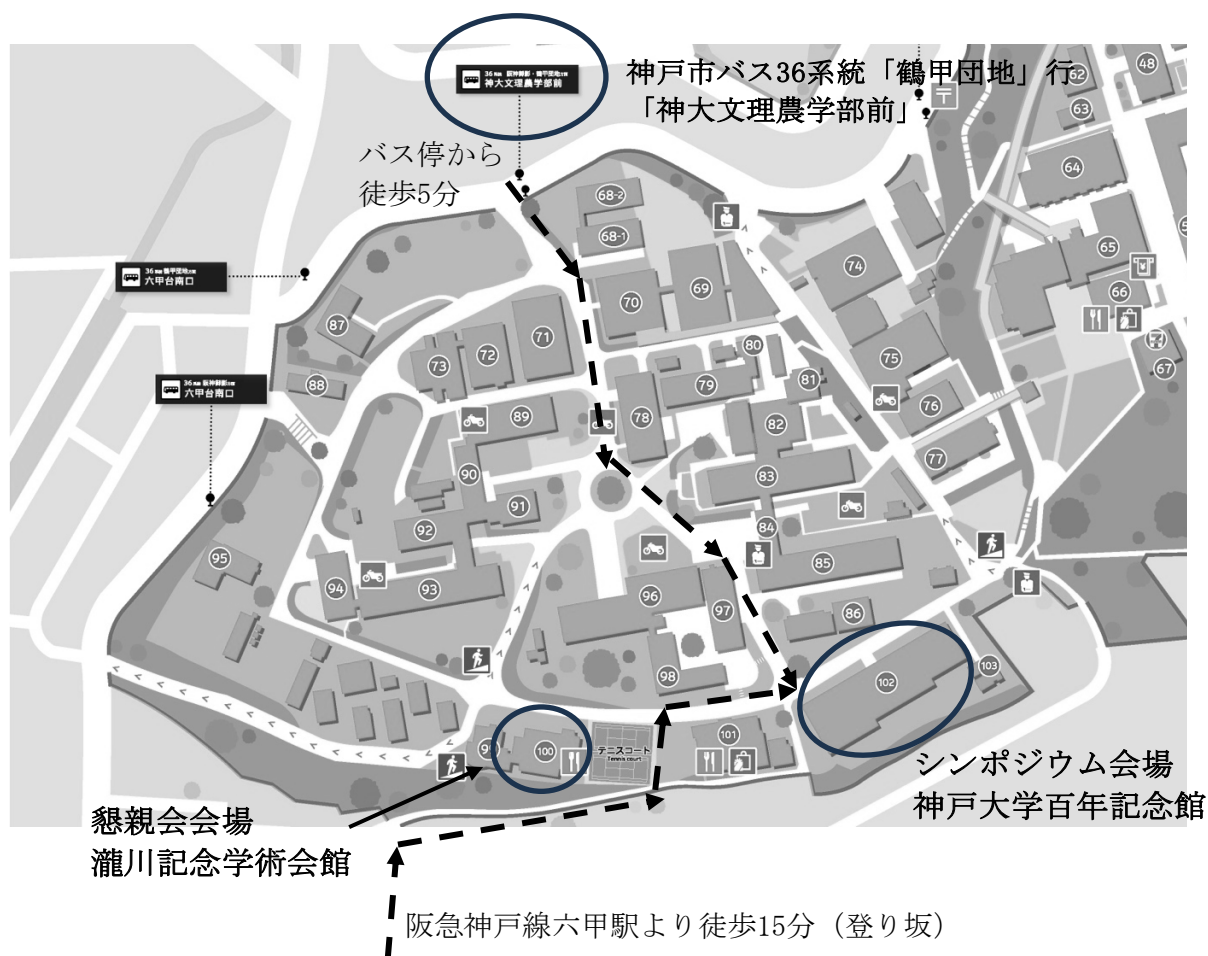
口頭発表： 六甲ホール(2F)

ポスター発表： 六甲ホールホワイエ(2F)

受付・企業展示： 六甲ホールホワイエ(2F)

懇親会会場

神戸大学瀧川記念学術交流会館
[日時] 2025年6月5日(木)
17:30-19:30



推奨: 阪急神戸線「六甲」駅、JR「六甲道」駅、又は阪神本線「御影」駅より市バス36系統「鶴甲団地」行きに乗車、「神大文・理・農学部前」下車。

- ・ 阪急六甲駅から約10分
 - ・ JR六甲道駅から約15分
 - ・ 阪神御影駅から約20分
- バス停より徒歩約5分

阪急神戸線「六甲」駅より（登り坂）徒歩約15分

新幹線「新神戸」駅から、タクシーで約15分。

Timetable for “SCKD40” in Kobe

Day 1, June 4 (Wed) 9:05~17:15	Day 2, June 5 (Thu) 9:30~17:15 17:30~19:30 Banquet	Day 3, June 6(Fri) 9:10~16:45
9:05~9:10 Opening remarks		
9:10~10:25 Chair: FUKAHORI, Shinichi 1A1 SOTOME, Hikaru 1A2 YAMAZAKI, Masakazu 1A2 ENDO, Tomoyuki	9:30~10:45 Chair: OHTSUKI, Yoshiyuki 2A1 KITANO, Tomoyuki 2A2 KAMBARA, Ryuto 2A3 MURAKAMI, Tatsuihiro	9:10~10:25 Chair: YAMAZAKI, Masakazu 3A1 KANAYA, Satoru 3A2 NONOSE, Shinji 3A3 ISHII, Nobuhisa
10:25~10:40 Break		10:25~10:40 Break
10:40~11:45 Chair: TOMINAGA, Keisuke IA4 GHOSH, Srijon IL1 LOH, Zhi-Heng	10:45~11:00 Break 11:00~11:40 Chair: TSUBOUCHI, Masaki IL3 TOMO, Tatsuya	10:40~11:45 Chair: KOHGUUCHI, Hiroshi 3A4 ODAGIRI, Takeshi IL5 OHSHIMA, Yasuhiro
11:45~13:00 Lunch Break	11:40~13:00 Lunch Break	11:45~13:00 Lunch Break
13:00~14:30 Poster Presentation 1	13:00~14:30 Poster Presentation 2	13:00~14:30 Poster Presentation 3
14:40~15:45 Chair: OHTA, Kaoru 1A5 MATSUZAKI, Korenobu IL2 YOSHIDA, Tatsuya	14:40~16:10 Chair: ONDA, Ken IL4 YAMAKATA, Akira 2A5 MIZUNO, Tomoya 2A6 PHUC, Nyuyen Thanh	14:40~15:30 Chair: ITAKURA, Ryuji 3A5 GUTIERREZ, Avram 3A6 KARAHIMA, Shutaro
15:45~16:00 Break		15:30~15:40 Break
16:00~17:15 Chair: MURAKAMI, Tatsuihiro 1A6 CHEN, Mingchen 1A7 NAGAHATA, Yutaka 1A8 WADA, Sato	16:10~16:25 Break 16:25~17:15 Chair: WADA, Akihide SL SHEN, Jian-Ren	15:40~16:30 Chair: KATSUKI, Hiroyuki 3A7 YAMADA, Kana 3A8 ONISHI, Hiroshi
	17:30~19:30 Banquet	16:30~16:45 Closing Remarks

40th Symposium on Chemical Kinetics and Dynamics

Special Lecture:

"Mechanism of Light-Induced Water Oxidation in Photosynthesis Revealed by XFEL"

Shen, Jian-Ren (Okayama University)

June 5, 16:25 - 17:15

Invited Lectures:

IL1 "Capturing Transient Species in Ionized Liquid Water"

Loh, Zhi-Heng (Nanyang Technological University)

June 4, 11:05 - 11:45

IL2 "Excited State Dynamics of Advanced Organic Light-Emitting Materials Tracked by Picosecond Time-Resolved Photoluminescence Techniques"

Tatsuya Yoshida (Kyushu University)

June 4, 15:05 - 15:45

IL3 "Diversity in Light Harvesting: Steady-State and Ultrafast Energy Transfer Dynamics Across Photosynthetic Lineages"

Tomo, Tatsuya (Tokyo University of Science)

June 5, 11:00 - 11:40

IL4 "Role of Heteroatom Doping in Modulating Charge Carrier Dynamics for Photocatalysis"

Yamakata, Akira (Okayama University)

June 5, 14:40 - 15:20

IL5 "Creating and Observing Coherently Rotating/Vibrating Molecular Ensembles"

Ohshima, Yasuhiro (Institute of Science Tokyo)

June 6, 11:05 - 11:45

Day 1: June 4 (Wed.)

9:05 - 9:10 Opening Remarks

9:10 - 10:25 Oral Presentations (Chair: Fukahori, Shinichi)

1A1

Twisting impact of distant aryl groups on photocyclization reactivity of inverse-type diarylethenes
Sotome, Hikaru¹; Kitagawa, Daichi²; Hamatani, Shota²; Mittelheisser, Cédric³; Sliwa, Michel^{3,4};
Ito, Syoji¹; Miyasaka, Hiroshi¹; Kobatake, Seiya²
(¹Osaka Univ., ²Osaka Metropolitan Univ., ³Univ. of Lille, ⁴IP Paris)

1A2

Development of a highly-sensitive electron spectrometer for studying electronic and nuclear motion in a molecule
Yamazaki, Masakazu¹; Sakaguchi, Sota¹; Sato, Takumi¹; Kurosu, Akane¹; Kodama, Tomomasa¹;
Konishi, Hana¹; Hasegawa, Tatsushi¹; Takahashi, Masahiko²; Ohshima, Yasuhiro¹
(¹Institute of Science Tokyo, ²Tohoku University)

1A3

Electron recollisional excitation of OCS⁺ in phase-locked two-color laser fields
Endo, Tomoyuki; Otobe, Tomohito; Itakura, Ryuji
(Kansai Institute for Photon Science, QST)

10:25 - 10:40 Coffee/Tea Break

10:40 - 11:45 Oral Presentations (Chair: Tominaga, Keisuke)

1A4

Formation of Ground-State Intermediate during Electronic Relaxation of Pyrimidine Nucleobases
Obara, Yuki; Ghosh, Srijon; Humeniuk, Alexander; Kamibashira, Shota; Adachi, Shunsuke; and
Suzuki, Toshinori
(Kyoto University)

IL1

Capturing Transient Species in Ionized Liquid Water
Loh, Zhi-Heng
(Nanyang Technological University)

11:45 - 13:00 Lunch Break

13:00 - 14:30 Poster Presentations Session 1

14:40 - 15:45 Oral Presentations (Chair: Ohta, Kaoru)

1A5

Inhomogeneity of hydrated electrons elucidated by transient two-dimensional electronic spectroscopy

Matsuzaki, Korenobu¹; Kuramochi, Hikaru^{1,2}; Tahara, Tahei¹
(¹RIKEN, ²Osaka Univ.)

IL2

Excited State Dynamics of Advanced Organic Light-Emitting Materials Tracked by Picosecond Time-Resolved Photoluminescence Techniques

Yoshida, Tatsuya¹; Miyata, Kiyoshi¹; Kaya, Yusei²; Takeishi, Nobuhiro²; Adachi, Chihaya²; Onda, Ken¹
(¹Department of Chemistry, Kyushu University, ²OPERA, Kyushu University)

15:45 - 16:00 Coffee/Tea Break

16:00 - 17:15 Oral Presentations (Chair: Murakami, Tatsuhiko)

1A6

Nonadiabatic *ab initio* molecular dynamics for the photoisomerization pathway of 2*E*,4*E*-hexadiene on the electronically excited state, *S*₃

Chen, Mingchen, Nanbu, Shinkoh
(Sophia University)

1A7

An encompassed representation of timescale hierarchies in first-order reaction network

Nagahata, Yutaka²; Kobayashi, Masato^{1,2,3}; Toda, Mikito^{2,4,5}; Maeda, Satoshi^{1,3}; Taketsugu, Tetsuya^{1,3}; Komatsuzaki, Tamiki^{1,2,6,7}

(¹ICReDD, Hokkaido University, ²RIES, Hokkaido University, ³Faculty of Science, Hokkaido University, ⁴Faculty Division of Natural Sciences, Nara Women's University, ⁵Graduate School of Information Science, University of Hyogo, ⁶OTRI, Osaka University, ⁷SANKEN, Osaka University)

1A8

Non-adiabatic molecular dynamics and reaction space projector analysis of photo-induced reaction of *ortho*-nitrophenol

Wada, Sato¹; Tsutsumi, Takuro¹; Saita, Kenichiro²; Taketsugu, Tetsuya¹
(¹Hokkaido Univ., ²Yokohama City Univ.)

Day 2: June 5 (Thu.)

9:30 - 10:45 Oral Presentations (Chair: Ohtsuki, Yoshiyuki)

2A1

Multi-objective Blackbox Optimization of Reaction Conditions of Nucleophilic ^{211}At -astatination
Kitano, Tomoyuki¹; Mizuno, Yuta^{2,1}; Mukaimine, Akari¹; Hashiba, Shunnichi¹; Nakajima, Kohei¹;
Tabata, Koji¹; Ogawa, Mikako¹; Komatsuzaki, Tamiki¹

(¹Hokkaido University, ²National Institute of Advanced Industrial Science and Technology)

2A2

Theoretical study on photodissociation dynamics of OCS^{2+} and dynamically hidden reaction pathway

Kambara, Ryuto¹; Tsutsumi, Takuro¹; Furuya, Kenji²; Taketsugu, Tetsuya¹

(¹Hokkaido Univ., ²Kyushu Univ.)

2A3

Nuclear Quantum Effects in Proton Transfer within Hydrogen-Bond Networks: Application to the Ionic Dissociation of HCl in a Water Cluster

Murakami, Tatsuhiro^{1,2}; Ueno, Hinami¹; Kikuma, Yuya¹; Takayanagi, Toshiyuki¹

(¹Saitama Univ., ²Tokyo Metropolitan Univ.)

10:45 - 11:00 Coffee/Tea Break

11:00 - 11:40 Oral Presentations (Chair: Tsubouchi, Masaki)

IL3

Diversity in Light Harvesting: Steady-State and Ultrafast Energy Transfer Dynamics Across Photosynthetic Lineages

Tomo, Tatsuya¹; Akimoto, Seiji²

(¹Grad. Sch. Sci., Tokyo Univ. Sci., ²Grad. Sch. Sci., Kobe Univ.)

11:40 - 13:00 Lunch Break

13:00 - 14:30 Poster Presentations Session 2

14:40 - 16:10 Oral Presentations (Chair: Onda, Ken)

IL4

Role of Heteroatom Doping in Modulating Charge Carrier Dynamics for Photocatalysis

Yamakata, Akira

(Okayama University)

2A5

Observation of evanescent field induced harmonic generation in pre-ionized liquid ethanol and water

Mizuno, Tomoya; Tianqi, Yang; Kurihara, Takayuki; Kanai, Teruto; Itatani, Jiro

(The University of Tokyo)

2A6

Chiral-Induced Spin Selectivity in Photon-Coupled Achiral Matters

Phuc, Nguyen Thanh

(Kyoto University)

16:10 - 16:25 Coffee/Tea Break

16:25 - 17:15 Oral Presentations (Chair: Wada, Akihide)

SL

Mechanism of light-induced water oxidation in photosynthesis revealed by XFEL

Shen, Jian-Ren

(Okayama University)

17:30 - 19:30 Banquet

Day 3: June 6 (Fri.)

9:10 - 10:25 Oral Presentations (Chair: Yamazaki, Masakazu)

3A1

A joint experimental and theoretical study of inelastic electron backscattering by He
Kanaya, Satoru¹; Onitsuka, Yuuki¹; Houamer, Salim²; Chuluunbaatar, Ochbadrakh^{3,4,5}; Popov, Yuri V.^{3,6}; Fursa, Dmitry⁷; Bray, Igor⁷; Takahashi, Masahiko¹
(¹IMRAM, Tohoku Univ., ²LQPDS, Univ. Setif-1, ³Joint Institute for Nuclear Research,
⁴Mongolian Academy of Sciences, ⁵Mongolian Univ. of Science and Technology, ⁶SINP,
Lomonosov Moscow State Univ., ⁷Department of Physics and Astronomy, Curtin Univ.)

3A2

OPIG-DC-Resolved Proton Transfer Reactions of Biomolecular Ions
Nonose, Shinji; Sasano, Koki; Nagashima, Hiroshi; Kodaira, Reo; Sugiyama, Tomoya
(Yokohama City Univ.)

3A3

X-ray absorption near edge structure measurements using a laser-based soft x-ray light source
beyond the water window region
Ishii, Nobuhisa; Maruyama, Momoko; Itakura, Ryuji
(Kansai Institute for Photon Science, QST)

10:25 - 10:40 Coffee/Tea Break

10:40 - 11:45 Oral Presentations (Chair: Kohguchi, Hiroshi)

3A4

Dipolar photodissociation of water molecule
Odagiri, Takeshi¹; Oda, Akiko¹; Kamata, Haruka¹; Takamura, Asahi¹; Imamura, Hayato¹; Suzuki, Isao H^{1,2}
(¹Sophia University, ²KEK-IMSS-PF)

IL5

Creating and observing coherently rotating/vibrating molecular ensembles
Ohshima, Yasuhiro
(Institute of Science Tokyo)

11:45 - 13:00 Lunch Break

13:00 - 14:30 Poster Presentations Session 3

14:40 - 15:30 Oral Presentations (Chair: Itakura, Ryuji)

3A5

Ultrafast relaxation dynamics of NH_4SCN under vibrational strong coupling

Gutierrez, Avram; Kiyokawa, Masaki; Nishiuchi, Joel; Stemo, Garrek; Katsuki, Hiroyuki

(Nara Institute of Science and Technology)

3A6

Ultrafast Vibrational Coherences during the Electronic Relaxation of Pyrimidine Nucleobases and Nucleosides

Karashima, Shutaro; Suzuki, Toshinori

(Kyoto University)

15:30 - 15:40 Coffee/Tea Break

15:40 - 16:30 Oral Presentations (Chair: Katsuki Hiroyuki)

3A7

Real-time probing of early-stage nuclear dynamics of O_2^+ by pump-probe measurements with few-cycle near-infrared laser pulses and high-order harmonics

Yamada, Kana; Ando, Toshiaki; Iwasaki, Atsushi; Yamanouchi, Kaoru

(The University of Tokyo)

3A8

Time-lapse O_2 detection over semiconductor photocatalysts for liquid water splitting

Onishi, Hiroshi

(Kobe University and Institute for Molecular Science)

16:30 - 16:45 Closing Remarks

Poster Presentations

(*Candidates for the Best Poster Prize)

Session 1 (June 4, 13:00 - 14:30)

1P01

Carbon atom adsorption on solid CO

Tsuge, Masashi¹; Molpeceres, Germán ²; Watanabe, Naoki¹

(¹Hokkaido University; ²IFF-CSIC)

1P02*

Ultraviolet photodissociation spectroscopy of protonated adenosine in the gas phase and its application to D-amino acid analysis in solution

Nakanishi, Riyo; Fujihara, Akimasa

(Osaka Metropolitan University)

1P03*

Observation Ion-molecule Reactions using NO⁺ Collision Energy Control by Pulse Offset Voltage

MIYAKE, Hinata; SAKUDA, Taro; KOHGUCHI, Hiroshi

(Hiroshima University)

1P04*

Electron-atom Compton scattering from CH₄ and N₂: Towards atomic momentum spectroscopy study on elements heavier than hydrogen

Sakaguchi, Sota¹; Kodama, Tomomasa¹; Konishi, Hana¹; Takahashi, Masahiko² Ohshima, Yasuhiro¹; Yamazaki, Masakazu¹

(¹Institute of Science Tokyo; ²Tohoku University)

1P05*

UV photodissociation dynamics of O₄⁺ studied by mass-analyzed ion-imaging technique and theoretical calculation

Watabe, Yu; Koshiba, Takumi; Ito, Yuri; Kanno, Manabu; Ohshimo, Keijiro; Misaizu, Fuminori

(Graduate School of Science, Tohoku University)

1P06

Rotationally resolved REMPI spectroscopy of O₂⁺ created by ionization of O₂ in an intense femtosecond laser field

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)

1P07*

Inelastic electron rescattering of CO in intense laser fields by electron-ion coincidence momentum imaging

Yasui, Kyoichiro¹; Amaike, Shunsuke¹; Aso, Tatsuya¹; Ikeya, Daimu¹; Ishida, Yasushi²; Hasegawa, Hiroka²; Morishita, Toru²; Hishikawa, Akiyoshi^{1,3}

(¹Dep. Chem, Nagoya Univ.; ²Univ. Electro-Comm; ³RCMS, Nagoya Univ.)

1P08*

Tuning and Stabilization of Vibrational Polaritons Based on a Semiconductor Distance Sensor
Nishiuchi, Joel; Stemo, Garrek; Gutierrez, Avram; Katsuki, Hiroyuki
(Graduate School of Science and Technology, NAIST)

1P09

Dynamics of photo-excited light-harvesting chromoproteins revealed by artificial gene synthesis and two-dimensional electronic spectroscopy
Tsubouchi, Masaaki; Fujita, Takatoshi; Adachi, Motoyasu; Itakura, Ryuji
(QST)

1P10*

Exciton Dynamics in Indole-fused zinc porphyrin-C₆₀ Fullerene System Studied by Time-Resolved Electron Paramagnetic Resonance
Tanaka, Hidetoshi¹; Kobori, Yasuhiro^{1,2}; D'Souza, Francis³; Wang, Hong³
(¹Graduate School of Science, Kobe University; ²Molecular Photoscience Research Center, Kobe University; ³Department of Chemistry, University of North Texas)

1P11*

Exploring charge and structural dynamics of organic–inorganic perovskites under dynamic equilibrium by single-particle spectroscopy
Takeuchi, Aito¹; Kumabe, Yoshitaka^{1,2}; Tachikawa, Takashi^{1,2}
(¹Graduate School of Science, Kobe University; ²Molecular Photoscience Research Center, Kobe University)

1P12*

Single-Particle Photoluminescence Observation of Charge Carrier Dynamics in BaZrS₃ Perovskites
Iwata, Aki¹; Kumabe, Yoshitaka^{1,2}; Tachikawa, Takashi^{1,2}
(¹Graduate School of Science, Kobe University; ²Molecular Photoscience Research Center, Kobe University)

1P13*

Machine learning-guided identification of reaction-relevant descriptors in multi-element-doped hematite photoelectrodes
Nishimura, Takuma¹; Kumabe, Yoshitaka^{1,2}; Harashima, Yosuke^{3,4}; Fujii, Mikiya^{3,4}; Tachikawa, Takashi^{1,2};
(¹Graduate School of Science, Kobe University; ²Molecular Photoscience Research Center, Kobe University; ³MS, NAIST; ⁴DSC, NAIST)

1P14*

Sonication Effect on hydroxyflavone derivatives in DMSO
Aso, Tetsuya; Inada, Taeko
(Kitasato University)

1P15*

Luminol Reaction without utilizing hydrogen peroxide: repeated chemiluminescence by shaking
Ie, Kanon; Suzuki, Takahiro; Inoue, Masayuki
(Tokyo University of Science)

1P16*

Exciton delocalization in π -conjugated cycloparaphenylene and aggregated perylenetetracarboxylicdiimide using electroabsorption and Stark fluorescence spectroscopy
Rahman, Md. Bulu; Kono, Sho; Islam, Ahatashamul; Iimori, Toshifumi
(Muroran Institute of Technology)

1P17

Drawing Patterns in Solution with Light Using a Reversible Photochemical Redox Reaction: Mechanistic and Kinetic Studies
Suzuki, Takahiro; Ie, Kanon; Inoue, Masayuki
(Tokyo University of Science)

1P18*

Adaptation of energy transfer in red alga *Porphyridium aerugineum* to light qualities
Kurachi, Hidetaka¹; Aikawa, Shimpei²; Akimoto, Seiji¹
(¹Grad. Sch. Sci., Kobe Univ.; ²JIRCAS)

1P19*

Minor Red-Shifted Chlorophyll a Serves as a Key Light-Harvesting Pigment Enabling Growth Under Far-Red Light Conditions in Green Algae
Wang, Fei¹; Akimoto, Seiji²; Miyashita, Hideaki¹
(¹Kyoto University; ²Kobe University)

1P20*

Repartition of excitation energy and electron flow in the diatom *Chaetoceros gracilis* with a truncated PSI-LHCI supercomplex
Xing, Jian¹; Kumazawa, Minoru¹; Akimoto, Seiji²; Tsuji, Shoko¹; Ishikawa, Noriko¹; Ifuku, Kentaro¹
(¹Graduate School of Agriculture, Kyoto University; ²Graduate School of Science, Kobe University)

1P21*

Spectroscopic analysis of heme transport in ABC transporter
Nakagawa, Kaito¹; Shiro, Yoshitsugu²; Sugimoto, Hiroshi^{2,3}; Kimura, Tetsunari^{1,4}
(¹Graduate School of Science, Kobe University; ²Graduate School of Science, University of Hyogo; ³SPRING-8 Center, RIKEN; ⁴Molecular Photonics Science Center, Kobe University)

1P22*

Collision branching dynamics in the interstellar $\text{H}_3^+ + \text{HNCO}$ system on the machine-learning full-dimensional potential energy surface
Murakami, Tatsuhiko²; Nakagawa, Shoto¹; Ota, Haruki¹; Takayanagi, Toshiyuki¹
(¹Saitama University; ²Tokyo Metropolitan University)

1P23

Machine learning for predicting full quantum-control landscape maps: Three-dimensional molecular alignment with pairs of linearly polarized laser pulses
Namba, Tomotaro; Ohtsuki, Yukiyo¹
(Tohoku University)

1P24*

The global area search approach for finding reaction pathways using repulsive interactions among walkers

Kikkawa, Takechika¹; Kawakami, Takashi¹; Yamanaka, Shusuke¹; Shoji, Mitsuo²; Okumura, Mitsutaka¹

(¹Graduate School of Science, Osaka University; ²Center for Computational Sciences, University of Tsukuba)

1P25*

Theoretical analysis of reaction path network: kinetics simulation and ab initio molecular dynamics

Soei Takizawa; Takuro Tsutsumi; Yuriko Ono; Kazuki Sada; Tetsuya Taketsugu

(Hokkaido University)

1P26*

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

Kobayashi, Yuto¹; Minegishi, Yusuke¹; Saita, Kenichiro²; Taketsugu, Tetsuya¹

(¹Hokkaido University; ²Yokohama City University)

1P27*

In silico design utilizing reaction path search method: Application to synthesis of organic fluorine compounds

Nagano, Ayana; Kawamoto, Takuji; Sumiya, Yosuke

(Yamaguchi University)

1P28*

Quantum Monte Carlo and Vibronic Analysis accurately reproduce ionization energy and electron affinity of Al₁₃

Meliton R. Chiong III¹; Yoshitada Morikawa¹; Atsushi Nakajima²

(¹Graduate School of Engineering, The University of Osaka; ²Keio Institute of Pure and Applied Sciences, Keio University)

Session 2 (June 13, 15:05 - 16:35)

2P01

Radical–radical reactions on cold ice surfaces

Iguchi, Arisa; Hidaka, Hiroshi; Oba, Yasuhiro; Tsuge, Masashi; Watanabe, Naoki
(Hokkaido University)

2P02*

Precise control of an optical cavity to observe gas-phase vibrational polaritons

Mistukawa, Eiyu¹; Oyaide, Yuma¹; Furukawa, Taiki¹; Miyashita, Kaichi¹; Matsumoto, Yoshiteru²
(¹Grad. Sch. Integr. Sci. Technol., Shizuoka Univ.; ²Dept. Chem., Fac. Sci., Shizuoka Univ.)

2P03*

Observation of highly vibrational excited HCO photodissociated from *N,N*-dimethylformamide

Karino, Momiji; Shinohara, Ryo; Inoue, Kosuke; Yamasaki, Katsuyoshi; Kohguchi, Hiroshi
(Hiroshima University)

2P04*

A New Method for Chiral Recognition Using Molecular Orientation and Coulomb Explosion Imaging

Kataoka, Shunsuke; Nakamura, Masaaki; Ohshima, Yasuhiro
(Institute of Science Tokyo)

2P05*

Anomalous shortfall of elastic electron backscattering from H revisited

Kanaya, Satoru; Onitsuka, Yuuki; Takahashi, Masahiko
(IMRAM, Tohoku University)

2P06

Estimation of bond angles in H₂O using photoelectron angular distributions undergoing femtosecond-scale X-ray-induced structural dynamics

Mitsui, Satoshi¹; Kobayashi, Daichi¹; Abe, Shigeru¹; Tamura, Yoshiaki¹; Hatada, Keisuke¹; Ueda, Kiyoshi²; Jahnke, Till³; Inhester, Ludger⁴; Santra, Robin^{4,5};
(¹Dep. Phys., Univ. Toyama; ²Grad. Sch. of Sci., Tohoku Univ.; ³EuXFEL; ⁴DESY; ⁵Dep. Phys., Univ. Hamburg)

2P07*

Tunnel electron circular dichroism of methyloxirane studied by electron-ion coincidence momentum imaging

Kuroda, Runa¹; Uchida, Tomohide¹; Nishimura, Koya¹; Matsuda, Akitaka¹; Hishikawa, Akiyoshi^{1,2};
(¹Grad. Sc. Sci, Nagoya Univ.; ²RCMS, Nagoya Univ.)

2P08*

Probing the Effect of Phonons in Charge Transport Characteristics of All Inorganic and Hybrid Perovskite Nanocrystals

Singha, Prajit^{1,2}; Ohta, Kaoru¹; Kumar, Ankit²; Datta, Anindya²; Tominaga, Keisuke¹
(¹Kobe University; ²Indian Institute of Technology Bombay)

2P09*

Real-space visualization of exciton diffusion dynamics of a thermally activated delayed fluorescence material using time-resolved imaging

Yoneda, Hidenori¹; Sotome, Hikaru¹; Yasuda, Yuka²; Okumura, Ryosuke²; Ito, Syoji¹; Kaji, Hironori²; Miyasaka, Hiroshi¹

(¹Osaka University; ²Kyoto University)

2P10*

Spectral analysis of steady-state spectra based on Marcus theory for intramolecular charge transfer reaction

Takamoto, Kazuya¹; Ueno, Yoshifumi²; Ohta, Kaoru³; Hayashi, Michitoshi⁴; Akimoto, Seiji¹; Matsubara, Ryosuke¹; Tominaga, Keisuke^{1,3}

(¹Grad. Sch. of Sci., Kobe University; ²Tokyo University of Science; ³Molecular Photoscience Research Center, Kobe University; ⁴National Taiwan University)

2P11*

Single-Particle Fluorescence Imaging of Enzyme-Mediated PET Degradation

Mouri, Asuka¹; Kimura, Tetsunari^{1,2}; Nakagawa, Yuto¹; Murakami, Suguru¹; Kumabe, Yoshitaka²; Matsubara, Ryosuke¹; Tachikawa, Takashi^{1,2}

(¹Grad. Sch. of Sci., Kobe Univ.; ²Mol. Photosci. Res. Center, Kobe Univ.)

2P12*

Relationship between phase transition and photocatalytic activity of cesium lead bromide

Nishimoto, Akari¹; Kumabe, Yoshitaka²; Tachikawa, Takashi^{1,2}

(¹Grad. Sch. of Sci., Kobe Univ.; ²Mol. Photosci. Res. Center, Kobe Univ.)

2P13*

Elucidation of the Reaction Mechanism of Photocatalytic Decarboxylation Using Time-Resolved EPR Method

Daiki, Tomiya¹; Takeshi, Inoue²; Masaaki, Fuki¹; Tsubasa, Okamoto¹; Harunobu, Mitsunuma²; Motomu, Kanai²; Yasuhiro, Kobori¹

(¹Kobe University; ²The University of Tokyo)

2P14*

Effect of molecular motion on electron spin polarization in the photo-excited chromophore radical systems of molecular spin-qubit candidates

Kokado, Yuya¹; Kopp, Kevin Lars²; Olav, Schiemann²; Kobori, Yasuhiro¹

(¹Kobe University; ²University of Bonn)

2P15

Kinetic analysis for the photochemical reaction of anthracene with CCl₄ in various solvents

Watanabe, Akihiro; Hamada, Yutaka

(Kobe City College of Technology)

2P16*

Kinetics of photoinduced electron transfer sensitized by germanium porphyrin derivatives

Inoue, Maika; Shiragami, Tsutomu

(University of Miyazaki)

2P17

Kinetic Analysis of Oxygen Reduction Reaction on Sodium Tantalate Photocatalysts

Saijo, Naoki¹; Hirata, Kaito²; Kawabe, Yusuke²; Takahashi, Yasuhumi²; Onishi, Hiroshi^{1,3}

(¹Kobe University; ²Nagoya University; ³Institute for molecular Science)

2P18*

Response of *Halomicronema hongdechloris* acclimated to one light quality to another light quality:
Far-red-light-adapted cells

Wang, Yipeng¹; Wang, Zhe¹; Shinoda, Toshiyoki²; Tomo, Tatsuya²; Akimoto, Seiji¹

(¹Kobe University; ²Tokyo University of Science)

2P19*

Response of *Halomicronema hongdechloris* acclimated to one light quality to another light quality:
White-light-adapted cells

Wang, Zhe¹; Shinoda, Toshiyoki²; Tomo, Tatsuya²; Akimoto, Seiji¹

(¹Kobe University; ²Tokyo University of Science)

2P20

Characterization of light-harvesting complexes from extremely Halophilic purple sulfur bacteria

Kimura, Yukihiro¹; Tani, Kazutoshi^{2,3}; Nagashima, Kenji V.P.⁴; Kojima, Risa⁵; Kondo, Masaharu⁶; Kanno, Ryo⁷; Satoh, Issei⁸; Kawakami, Mai⁸; Hiwatashi, Naho⁸; Nakata, Kazuna¹; Nagashima, Sakiko⁴; Inoue, Kazuhito^{4,9}; Isawa, Yugo⁵; Morishita, Ryoga⁶; Takaichi, Shinichi¹⁰; Purba, Endang R.¹¹; Hall, Malgorzata¹¹; Yu, Long-Jiang¹²; Madigan, Michael T.¹³; Mizoguchi, Akira³; Humbel, Bruno M.^{14,15}; Nagasawa, Yutaka⁵; Dewa, Takehisa⁶; Wang-Otomo, Zheng-Yu⁸

(¹Graduate School of Agriculture, Kobe University; ²Center for Computational Sciences, University of Tsukuba; ³Graduate School of Medicine, Mie University; ⁴Research Institute for Integrated Science, Kanagawa University; ⁵College of Life Sciences, Ritsumeikan University; ⁶Graduate School of Engineering, Nagoya Institute of Technology; ⁷Quantum Wave Microscopy Unit, OIST; ⁸Faculty of Science, Ibaraki University; ⁹Faculty of Chemistry and Biochemistry, Kanagawa University; ¹⁰Faculty of Life Science, Tokyo University of Agriculture; ¹¹Scientific Imaging Section, OIST; ¹²Photosynthesis Research Center, Institute of Botany, Chinese Academy of Sciences; ¹³Department of Microbiology, Southern Illinois University; ¹⁴Provost Office, OIST; ¹⁵Graduate School of Medicine, Juntendo University)

2P21*

Adaptive changes in FCP composition in response to light and CO₂ conditions in *Chaetoceros gracilis*

Nakamura, Midori¹; Kumazawa, Minoru²; Nagao, Ryo³; Tsuji, Shoko¹; Suzuki, Takehiro⁴; Ishikawa, Noriko¹; Dohmae, Naoshi⁴; Akimoto, Seiji⁵; Ifuku, Kentaro¹

(¹Grad. Sch. Agri., Kyoto Univ.; ²ILTS, Hokkaido Univ.; ³Fac. Agri., Shizuoka Univ.; ⁴RIKEN CSRS; ⁵Grad. Sch. Sci., Kobe Univ.)

2P22*

Nonadiabatic Photodissociation of morpholine in gas phase

Araiso, Hiroyo¹; Nanbu, Shinkoh²

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

2P23

Quantum chemical study on monomethylhydrazine/nitrous acid clusters

Kanno, Nozomu

(Meijo University)

2P24*

Solvent effects on excited state dynamics of cyanine dye 1122C

MINEGISHI, Yusuke¹; SAITA, Kenichiro²; TSUTSUMI, Takuro¹; TAKETSUGU, Tetsuya¹

(¹Hokkaido University; ²Yokohama City University)

2P25*

Structural Changes in Alcohol Molecules and Water Clusters Induced by Positron Attachment: A Theoretical Study Using the CPP Method

Yamaki, Keita¹; Yamada, Hayato¹; Yoshida, Daisuke²; Takayanagi, Toshiyuki¹

(¹Saitama University; ²Tohoku University)

2P26

Exciton quantum dynamics calculations for molecular design of the quantum logic gates

Yonetani, Yoshiteru

(QST)

2P27*

A model electronic Hamiltonian to study electronic states and electronic absorption spectra of [Ni(phen)₃]²⁺

Sugimura, Leo¹; Iuchi, Satoru²; Hirofumi, Sato^{1,3}

(¹Kyoto University; ²Nagoya University; ³Fukui Institute for Fundamental Chemistry)

2P28*

Low-energy uphill energy transfer in the light-harvesting 1 reaction center complexes from psychrophilic purple bacteria

Inada, Kazuki¹; Akimoto, Seiji²; Takenaka, Shinji¹; Madigan, Michael T.³; Wang-Otomo, Zheng-Yu⁴; Kimura, Yukihiro¹

(¹Graduate School of Agriculture, Kobe University; ²Graduate School of Science, Kobe University;

³Program in Microbiology, Southern Illinois University; ⁴Faculty of Science, Ibaraki University)

Session 3 (June 14, 10:40 - 12:10)

3P01

Reaction dynamics of the interstellar $\text{CH}_3\text{OH} + \text{H}_3^+ \rightarrow \text{CH}_3\text{OH}_2^+ + \text{H}_2 / \text{CH}_2\text{OH}^+ + 2\text{H}_2$ reaction using the Δ -Machine Learning Potential Energy Surface

Sasaki, Yuki

(Saitama University)

3P02*

Analysis of High-Resolution spectra $S_1 \leftarrow S_0$ transition of chloronaphthalenes

Shimizu, Akira¹; Yamamoto, Ryo¹; Kanzawa, Kenichiro¹; Kasahara, Shunji^{1,2}

(¹Grad. Sch. Sci., Kobe Univ.; ²MPRC, Kobe Univ.)

3P03*

IR Spectroscopy of Protonated Water – Acetonitrile Cluster: Comparison of Condensed phase and Gas phase

Chiba, Kohei; Asuka, Fujii

(Tohoku University)

3P04*

State-Selected REMPI-PECD Study of (-)-Fenchone

Xiao, Yuxiao; Karino, Momiji; Kohguchi Hiroshi

(Grad. Sch. of Adv. Sci. & Eng., Hiroshima Univ.)

3P05*

Recoil frame photoelectron angular distributions in the above threshold ionization of CH_4 and CF_4

Kimura, Taiki; Hirabayashi, Naoto; Ohshima, Yasuhiro; Yamazaki, Masakazu

(Institute of Science Tokyo)

3P06*

Direct Observation of the Orientational Distribution of State-selected Iodomethane Molecules

Ohama, Keito; Kataoka, Shunsuke; Ardelia, Mellisa; Kondo, Ryo; Nakamura, Masaaki; Yasuhiro, Ohshima

(Institute of Science Tokyo)

3P07

Photofragment imaging of oriented methyl/ethyl bromide (CH_3Br , $\text{C}_2\text{H}_5\text{Br}$) for discovering their transition dipole moments

KAWAMATA, Hiroshi¹; NAKAMURA, Masaaki²; CHE, Dock-Chil³

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

3P08*

Laser tunnel ionization imaging of spin-orbit state resolved CH_3I using auxiliary dissociation pulse

Yazawa, Joe¹; Yoshino, Takato¹; Uchida, Tomohide¹; Hishikawa, Akiyoshi^{1,2}

(¹Grad. Sc. Sci, Nagoya Univ.; ²RCMS, Nagoya Univ.)

3P09*

Asymmetric Coulomb Explosion of Acetonitrile in $\omega-2\omega$ Intense Laser Fields Studied by Coincidence Momentum Imaging

Miyasaka, Sato¹; Ono, Yuki¹; Hasegawa, Hiroka¹; Matsuda, Akitaka¹; Hishikawa, Akiyoshi^{1,2}
(¹Grad. Sc. Sci, Nagoya Univ.; ²RCMS, Nagoya Univ.)

3P10

Transient 2-dimensional electronic spectroscopy (tr-2DES) on a photoswitch: inhomogeneity in the excited state and subsequent spectral evolution

Borter, Jan-Hendrik; Matsuzaki, Korenobu; Tahara, Tahei
(RIKEN)

3P11

Development of an electron energy spectrometer for an attosecond electron beam line at 30 keV

Tachibana, Yuichi; Morimoto, Yuya
(RIKEN)

3P12*

Analysis of Intramolecular Singlet Fission Mechanism by Time-Resolved EPR

Tanaka, Masahiro¹; Fuki, Masaaki¹; Nakamura, Shunta²; Sakai, Hayato²; Hasobe, Taku²; Kobori, Yasuhiro¹
(¹Kobe University; ²Keio University)

3P13

Photoinduced Charge Separation in CdSe/ZnS Quantum Dots and PC₆₁BM

Hamada, Morihiko¹; Kawanaka, Shota¹; Fuki, Masaaki²; Kobori, Yasuhiro²
(¹Applied Chemistry, Kobe City College of Technology; ²Molecular Photoscience Research Center, Kobe University)

3P14*

Evaluation of exciton-polariton lasing in π -conjugated molecular aggregates under cavity strong coupling

Arakawa, Yutaka¹; Sotome, Hikaru¹; Hirai, Kenji²; Uji-i, Hiroshi²; Ito, Syoji¹
(¹Osaka University; ²Hokkaido University)

3P15*

Kinetic study of multicolor multilevel reaction system using Sudan red 7B

Nabetani, Takuma¹; Sakai Ayaka; Yamamoto Masaaki; Wada Akihide
(Kobe University)

3P16*

Electron transfer dynamics in microbe-photocatalyst hybrid systems

Itoh, Masaru¹; Kamasaka, Kouhei²; Kumabe, Yoshitaka³; Hasunuma, Tomohisa²; Tachikawa, Takashi^{1,3}
(¹Graduate School of Science, Kobe University; ²Engineering Biology Research Center, Kobe University; ³Molecular Photoscience Research Center, Kobe University)

3P17*

Development of operando FTIR measurement system for photoelectrochemical reactions

Yoshida, Hisaki¹; Kumabe, Yoshitaka²; Tachikawa, Takashi^{1,2}

(¹Graduate School of Science, Kobe University; ²Molecular Photoscience Research Center, Kobe University)

3P18*

Chemical kinetics for the reactions of OH with methyl or ethyl substituted terminal alkenes

Fushimi, Ryota; Oguchi, Tatsuo

(Toyohashi University of Technology)

3P19*

Theoretical Analysis of the Reaction Mechanism of Benzene Oxide Photoisomerization via S2 State Excitation

Cui, Shirui¹; Nanbu, Shinkoh²

(¹Graduate School of Science and Technology, Sophia Univ.; ²Faculty of Science and Technology, Sophia Univ.)

3P20*

Theoretical investigation of allyl alcohol isomerization over La₂O₃, NiO and LaNiO₃-supported Au catalysts

Ishimaru, Yuhki¹; Ishida, Tamao²; Makoto, Tokunaga³; Mitsutaka, Okumura¹

(¹Osaka University; ²Tokyo Metropolitan University; ³Kyushu University)

3P21*

PME-ONIOM Molecular Dynamics Simulation for Organic Electrolytes

Watanabe, Tomoya¹; Nanbu, Shinkoh²

(¹Graduate School of Science and Technology, Sophia Univ.; ²Faculty of Science and Technology, Sophia Univ.)

3P22*

Theoretical investigation on the switching of CO oxidation mechanism over Au catalyst supported on polyoxometalate

Yonemori, Tomohisa¹; Hamada, Yasutaka¹; Ishida, Tamao²; Murayama, Toru³; Kawakami, Takashi¹; Yamanaka, Shusuke¹; Okumura, Mitsutaka¹

(¹Osaka University; ²Tokyo Metropolitan University; ³Hokkaido University)

3P23*

Theoretical study of solvent effects on post-transition state bifurcation reaction with explicit water molecules

Matsubuchi, Hayato

(Saitama University)

3P24*

Theoretical study on aggregation-suppressed branching reaction in photoexcited N-salicylideneaniline

KOMURO, Hiroto¹; SAITA, Kenichiro²; TSUTSUMI, Takuro¹; TAKETSUGU, Tetsuya¹

(¹Hokkaido University; ²Yokohama City University)

3P25*

Crystal-face dependence of solid-liquid interfacial reactions by potassium tantalate single crystals

Endo, Kanako¹; Hirata, Kaito²; Kawabe, Yusuke²; Takahashi, Yasufumi²; Onishi, Hiroshi^{1,3}

(¹Kobe University; ²Nagoya University; ³Institute for Molecular Science)

3P26

Unravelling the Influence of Major Seawater Salt Ions on the Photogenerated Charge Carriers in a Sr-Doped NaTaO₃ Photocatalyst via ATR-FTIR

Chew, Yi-Hao¹; Saijo, Naoki²; Kumabe, Yoshitaka²; Tachikawa, Takashi²; Onishi, Hiroshi^{2,3}

(¹Okayama University; ²Kobe University; ³Institute for Molecular Science)

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