

Theoretical and Computational Molecular Science

- M. HIGASHI and S. SAITO**, “Quantitative Evaluation of Site Energies and Their Fluctuations of Pigments in the Fenna-Matthews-Olson Complex with an Efficient Method for Generating a Potential Energy Surface,” *J. Chem. Theory Comput.* **12**, 4128–4137 (2016).
- K. KOIZUMI, K. NOBUSADA and M. BOERO**, “The Absence of a Gap State and Enhancement of the Mars-van Krevelen Reaction on Oxygen Defective Cu/CeO₂ Surfaces,” *Phys. Chem. Chem. Phys.* **18**, 20708–20712 (2016).
- Y. NIHORI, M. EGURO, A. KATO, S. SHARMA, B. KUMAR, W. KURASHIGE, K. NOBUSADA and Y. NEGISHI**, “Improvements in the Ligand-Exchange Reactivity of Phenylethanethiolate-Protected Au₂₅ Nanocluster by Ag or Cu Incorporation,” *J. Phys. Chem. C* **120**, 14301–14309 (2016).
- K. IIDA and K. NOBUSADA**, “Electric Field Effects on the Electronic Properties of the Silicene–Amine Interface,” *Phys. Chem. Chem. Phys.* **18**, 15639–15644 (2016).
- M. YAMAGUCHI and K. NOBUSADA**, “Indirect Interband Transition Induced by Optical Near Fields with Large Wave Numbers,” *Phys. Rev. B* **93**, 195111 (9 pages) (2016).
- M. ZHOU, H. QIAN, M. Y. SFEIR, K. NOBUSADA and R. JIN**, “Effects of Single Atom Doping on the Ultrafast Electron Dynamics of M₁Au₂₄(SR)₁₈ (M = Pd, Pt) Nanoclusters,” *Nanoscale* **8**, 7163–7171 (2016).
- C. ZENG, Y. CHEN, K. IIDA, K. NOBUSADA, K. KIRSCHBAUM, K. J. LAMBRIGHT and R. JIN**, “Gold Quantum Boxes: On the Periodicities and the Quantum Confinement in the Au₂₈, Au₃₆, Au₄₄, and Au₅₂ Magic Series,” *J. Am. Chem. Soc.* **138**, 3950–3953 (2016).
- K. KOIZUMI, K. NOBUSADA and M. BOERO**, “Reducing the Cost and Preserving the Reactivity in Noble-Metal-Based Catalysts: Oxidation of CO by Pt and Al-Pt Alloy Clusters Supported on Graphene,” *Chem. –Eur. J.* **22**, 5181–5188 (2016).
- T. YATSUI, T. TSUBOI, M. YAMAGUCHI, K. NOBUSADA, S. TOJO, F. STEHLIN, O. SOPPERA and D. BLOCH**, “Optically Controlled Magnetic-Field Etching on the Nano-Scale,” *Light: Sci. Appl.* **5**, e16054 (7 pages) (2016).
- M. YAMAGUCHI and K. NOBUSADA**, “Photodissociation Path in H₂⁺ Induced by Nonuniform Optical Near Fields: Two-Step Excitation via Vibrationally Excited States,” *Phys. Rev. A* **93**, 023416 (5 pages) (2016).
- K. IIDA, M. NODA and K. NOBUSADA**, “Interface Electronic Properties between a Gold Core and Thiolate Ligands: Effects on an Optical Absorption Spectrum in Au₁₃₃(SPtBu)₅₂,” *J. Phys. Chem. C* **120**, 2753–2759 (2016).
- M. YAMAGUCHI, K. NOBUSADA and T. YATSUI**, “Nonlinear Optical Response Induced by A Second-Harmonic Electric-Field Component Concomitant with Optical Near-Field Excitation,” *Phys. Rev. A* **92**, 043809 (9 pages) (2015).
- C. ZENG, Y. CHEN, C. LIU, K. NOBUSADA, N. L. ROSI and R. JIN**, “Gold Tetrahedra Coil Up: Kekulé-Like and Double Helical Superstructures,” *Sci. Adv.* **1**, e1500425 (6 pages) (2015).
- C. LIU, T. LI, G. LI, K. NOBUSADA, C. ZENG, G. PANG, N. L. ROSI and R. JIN**, “Observation of Body-Centered Cubic Gold Nanocluster,” *Angew. Chem., Int. Ed.* **54**, 9826–9829 (2015).
- M. OKAMURA, M. KONDO, R. KUGA, Y. KURASHIGE, T. YANAI, S. HAYAMI, M. YOSHIDA, K. YONEDA, S. KAWATA and S. MASAOKA**, “A Pentanuclear Iron Catalyst Designed for Water Oxidation,” *Nature* **530**, 465–468 (2016).
- S. SHIRAI, Y. KURASHIGE and T. YANAI**, “Computational Evidence of Inversion of ¹L_a and ¹L_b Derived Excited States in Naphthalene Excimer Formation from *ab Initio* Multireference Theory with Large Active Space: DMRG-CASPT2 Study,” *J. Chem. Theory Comput.* **12**, 2366–2372 (2016).
- K.-W. SUN, Y. FUJIIHASHI, A. ISHIZAKI and Y. ZHAO**, “A Variational Master Equation Approach to Quantum Dynamics with Off-Diagonal Coupling in a Sub-Ohmic Environment,” *J. Chem. Phys.* **144**, 204106 (8 pages) (2016).
- Y. FUJIIHASHI and A. ISHIZAKI**, “Fluctuations in Electronic Energy Affecting Singlet Fission Dynamics and Mixing with Charge Transfer State: Quantum Dynamics Study,” *J. Phys. Chem. Lett.* **7**, 363–369 (2016).
- Y. FUJIIHASHI, G. R. FLEMING and A. ISHIZAKI**, “Influences of Quantum Mechanically Mixed Electronic and Vibrational Pigment States in 2D Electronic Spectra of Photosynthetic Systems: Strong Electronic Coupling Cases,” *J. Chin. Chem. Soc.* **63**, 49–56 (2016).
- S. KARANJIT, M. EHARA and H. SAKURAI**, “Mechanism of the Aerobic Homocoupling of Phenylboronic Acid on Au₂₀⁻: A DFT Study,” *Chem. –Asian J.* **10**, 2397–2403 (2015).
- S. RAI, M. EHARA and U. DEVA PRIYAKUMAR**, “Nucleobases Tagged to Gold Nanoclusters Cause a Mechanistic Crossover in the Oxidation of CO,” *Phys. Chem. Chem. Phys.* **17**, 24275–24281 (2015).
- R. N. DHITAL, M. EHARA and H. SAKURAI**, “Gold/Palladium Bimetallic Nanoparticles for C–X Bond Activations: A Unique Effect of Gold,” *J. Synth. Org. Chem., Jpn.* **73**(11), 1130–1140 (2015).
- T. SOMMERFELD and M. EHARA**, “Complex Absorbing Potential with Voronoi Isosurfaces Wrapping Perfectly around Molecules,” *J. Chem. Theory Comput.* **11**, 4627–4633 (2015).
- R. N. DHITAL, K. BOBUATONG, M. EHARA and H. SAKURAI**, “Gold/Palladium Alloy for Carbon–Halogen Bond Activation: An Unprecedented Halide Dependence,” *Chem. –Asian J.* **10**, 2669–2676 (2015).
- S. IMPENG, P. KHONGPRACHA, J. SIRIJARAENSRE, B. JANSANG, M. EHARA and J. LIMTRAKUL**, “Methane Activation on Fe- and FeO-Embedded Graphene and Boron Nitride Sheet: Role of Atomic Defects in Catalytic Activities,” *RSC Adv.* **5**, 97918–97927 (2015).
- S. NAMUANGRUK, S. JUNGSTIWIWONG, N. KUNGWAN, V. PROMARAK, T. SUDYOADSUK, B. JANSANG and M. EHARA**, “Coumarin-Based Donor- π -Acceptor Organic Dyes for a Dye-Sensitized Solar Cell: Photophysical Properties and Electron Injection Mechanism,” *Theor. Chem. Acc.* **135**, 14 (13 pages) (2015). (special issue on Health & Energy from the Sun: A Computational Perspective)
- M. EHARA, R. FUKUDA and T. SOMMERFELD**, “Projected CAP/SAC-CI Method with Smooth Voronoi Potential for Calculating Resonance States,” *J. Comput. Chem.* **37**, 242–249 (2016).

LIST OF PUBLICATIONS

- R. ZHAO, Y. GUO, P. ZHAO, M. EHARA, S. NAGASE and X. ZHAO**, “Warning to Theoretical Structure Elucidation of Endohedral Metallofullerenes,” *J. Phys. Chem. C* **120**, 1275–1283 (2016).
- Y. KANAZAWA, M. EHARA and T. SOMMERFELD**, “Low-Lying π^* Resonances of Standard and Rare DNA or RNA Bases Studied by the Projected CAP/SAC-CI Method,” *J. Phys. Chem. A* **120**, 1545–1553 (2016).
- S. GURTU, S. RAI, M. EHARA and U. DEVA PRIYAKUMAR**, “Ability of Density Functional Theory Methods to Accurately Model the Reaction Energy Pathways of the Oxidation of CO on Gold Cluster: A Benchmark Study,” *Theor. Chem. Acc.* **135**, 93 (12 pages) (2016).
- R. FUKUDA and M. EHARA**, “Electronic Excitation and Ionization Behavior of N-hydroxypyridine-2(1H)-thione and its Deprotonated Anion in a Polarizable Medium Studied Using Quantum Chemical Computations,” *Theor. Chem. Acc.* **135**, 105 (9 pages) (2016).
- J. MEEPRASERT, S. NAMUANGRUK, B. BOEKFA, R. N. DHITAL, H. SAKURAI and M. EHARA**, “Mechanism of Ullmann Coupling Reaction of Chloroarene on Au/Pd Alloy Nanocluster: A DFT Study,” *Organometallics* **35**, 1192–1201 (2016).
- A. GUPTA, B. BOEKFA, H. SAKURAI, M. EHARA and U. DEVA PRIYAKUMAR**, “Structure, Interaction and Dynamics of Au/Pd Bimetallic Nanoalloys Dispersed in Ethylpyrrolidone, Monomeric Moiety of Polyvinylpyrrolidone (PVP),” *J. Phys. Chem. C* **120**, 17454–17464 (2016).
- W.-J. GUAN, P. ZHAO, Q.-Z. LI, S. NAGASE, M. EHARA and X. ZHAO**, “ $\text{Sc}_3\text{N}@C_8(39715)-C_{82}$: A Missing Isomer Linked to $\text{Sc}_3\text{N}@C_{2v}(39718)-C_{82}$ by a Single Step Stone-Wales Transformation,” *RSC Adv.* **6**, 75588–75593 (2016).
- P. ZHAO, X. ZHAO and M. EHARA**, “Regioselectivity of $\text{Sc}_2\text{C}_2@C_{3v}(8)-C_{82}$: Role of the Sumanene-Type Hexagon in Diels–Alder Reaction,” *J. Org. Chem.* **81**, 8169–8174 (2016).
- S. G. ITOH and H. OKUMURA**, “Oligomer Formation of Amyloid- β (29-42) from Its Monomers Using the Hamiltonian Replica-Permutation Molecular Dynamics Simulation,” *J. Phys. Chem. B* **120**, 6555–6561 (2016).
- W. KHUNTAWE, T. RUNGROTMONGKOL, P. WOLSCHANN, P. PONGSAWASDI, N. KUNGWAN, H. OKUMURA and S. HANNONGBUA**, “Conformation Study of ϵ -Cyclodextrin: Replica-Exchange Molecular Dynamics Simulations,” *Carbohydr. Polym.* **141**, 99–105 (2016).
- Y. MORI and H. OKUMURA**, “Simulated Tempering Based on Global Balance or Detailed Balance Conditions: Suwa-Todo, Heat Bath, and Metropolis Algorithms,” *J. Comput. Chem.* **36**, 2344–2349 (2015).
- T. FUJITA, S. ATAHAN-EVRENK, N. P. D. SAWAYA and A. ASPURU-GUZI, K.** “Coherent Dynamics of Mixed Frenkel and Charge Transfer Excitons in Dinaphtho[2,3-*b*:2'3'-*f*]thieno[3,2-*b*]thiophene Thin Films: The Importance of Hole Delocalization,” *J. Phys. Chem. Lett.* **7**, 1374–1380 (2016).
- N. P. D. SAWAYA, J. HUH, S. K. SAIKIN, T. FUJITA and A. ASPURU-GUZI, K.** “Fast Delocalization Leads to Robust Long-Range Excitonic Transfer in a Large Quantum Chlorosome Model,” *Nano Lett.* **15**, 1722–1729 (2015).
- W. NAITO, N. YASUDA, T. MORIMOTO, Y. SHIGETA, H. TAKAYA, I. HISAKI and H. MAEDA**, “Doubly N-Methylated Porphyrinoids,” *Org. Lett.* **18**, 3006–3009 (2016).
- W. TANAKA, M. SHOJI, F. TOMOIKE, Y. UJIIE, K. HANAOKA, R. HARADA, M. KAYANUMA, K. KAMIYA, T. ISHIDA, R. MASUI, S. KURAMITSU and Y. SHIGETA**, “Molecular Mechanisms of Substrate Specificities of Uridine-Cytidine Kinase,” *Biophys. Physicobiol.* **13**, 77–82 (2016).
- R. HARADA, Y. TAKANO and Y. SHIGETA**, “TaBoo SeArch (TBSA) Algorithm with a Modified Inverse Histogram for Reproducing Biologically Relevant Rare-Events of Proteins,” *J. Chem. Theory Comput.* **12**, 2436–2445(2016).
- M. KAYANUMA, M. SHOJI, M. YODA, M. ODAKA and Y. SHIGETA**, “Catalytic Mechanism of Nitrile Hydratase Subsequent to Cyclic Intermediate Formation: A QM/MM Study,” *J. Phys. Chem. B* **120**, 3259–3266 (2016).
- S. MAEKAWA, R. SATO, K. HIRAO and Y. SHIGETA**, “Solvent Effects on Excited-State Electron-Transfer Rate of Pyrene-Labeled Deoxyuridine: A Theoretical Study,” *Chem. Phys. Lett.* **644**, 25–30 (2016).
- R. HARADA, T. NAKAMURA and Y. SHIGETA**, “Sparsity-Weighted Outlier FLOODing (OFLOOD) Method: Efficient Rare Event Sampling Method Using Sparsity of Distribution,” *J. Comput. Chem.* **37**, 724–738(2016).

Photo-Molecular Science

- Y. NISHIYAMA, K. IMURA and H. OKAMOTO**, “Observation of Plasmon Wave Packet Motions via Femtosecond Time-Resolved Near-Field Imaging Techniques,” *Nano Lett.* **15**, 7657–7665 (2015).
- T. NARUSHIMA, S. HASHIYADA and H. OKAMOTO**, “Optical Activity Governed by Local Chiral Structures in Two-Dimensional Curved Metallic Nanostructures,” *Chirality* **28**, 540–544 (2016).
- C. SOMMER, G. PUPILLO, N. TAKEI, S. TAKEDA, A. TANAKA, K. OHMORI and C. GENES**, “Time Domain Ramsey Interferometry with Interacting Rydberg Atoms,” *arXiv:1604.02314* (2016).
- T. FRANSSON, Y. HARADA, N. KOSUGI, N. A. BESLEY, B. WINTER, J. J. REHR, L. G. M. PETERSSON and A. NILSSON**, “X-Ray and Electron Spectroscopy of Water,” *Chem. Rev.* **116**, 7551–7569 (2016).
- I. SONG, J. S. GOH, S. H. LEE, S. W. JUNG, J. S. SHIN, H. YAMANE, N. KOSUGI and H. W. YEOM**, “Realization of a Strained Atomic Wire Super lattice,” *ACS Nano* **9**, 10621–10627 (2015).
- Y. F. WANG, S. B. SINGH, M. V. LIMAYE, Y. C. SHAO, S. H. HSIEH, L. Y. CHEN, H. C. HSUEH, H. T. WANG, J. W. CHIOU, Y. C. YEH, C. W. CHEN, C. H. CHEN, S. C. RAY, J. WANG, W. F. PONG, Y. TAKAGI, T. OHGASHI, T. YOKOYAMA and N. KOSUGI**, “Visualizing Chemical States and Defects Induced Magnetism of Graphene Oxide by Spatially-Resolved-X-Ray Microscopy and Spectroscopy,” *Sci. Rep.* **5**, 15439 (2015).

H. YAMANE and N. KOSUGI, “Systematic Study on Intermolecular Valence-Band Dispersion in Molecular Crystalline Films,” *J. Electron Spectrosc. Relat. Phenom.* **204**, 61–67 (2015).

J. P. YANG, W. Q. WANG, L. W. CHENG, Y. Q. LI, J. X. TANG, S. KERA and N. UENO, “Mechanism for Doping Induced p Type C₆₀ Using Thermally Evaporated Molybdenum Trioxide (MoO₃) as a Dopant,” *J. Phys.: Condens. Matter* **28**, 185502 (6 pages) (2016).

Y. NAKAYAMA, Y. URAGAMI, M. YAMAMOTO, K. YONEZAWA, K. MASE, S. KERA, H. ISHII and N. UENO, “High-Resolution Core-Level Photoemission Measurements on the Pentacene Single Crystal Surface Assisted by Photoconduction,” *J. Phys.: Condens. Matter* **28**, 094001 (8 pages) (2016).

T. UEBA, J. PARK, R. TERAWAKI, Y. WATANABE, T. YAMADA and T. MUNAKATA, “Unoccupied Electronic Structure and Molecular Orientation of Rubrene; from Evaporated Films to Single Crystals,” *Surf. Sci.* **649**, 7–13 (2016).

T. HOSOKAI, A. HINDERHOFER, F. BUSSOLOTTI, K. YONEZAWA, C. LORCH, T. WATANABE, A. VOROBIEV, Y. HASEGAWA, Y. YAMADA, Y. KUBOZONO, A. GERLACH, S. KERA, F. SCREIBER and N. UENO, “Thickness and Substrate Dependent Thin Films Growth of Picene and Impact to the Electronic Structure,” *J. Phys. Chem. C* **119**, 29027–29037 (2015).

F. BUSSOLOTTI, J. P. YANG, M. HIRAMOTO, T. KAJI, S. KERA and N. UENO, “Direct Detection of Density of Gap States in C₆₀ Single Crystal by Photoemission Spectroscopy,” *Phys. Rev. B* **92**, 115012 (7 pages) (2015).

J. P. YANG, F. BUSSOLOTTI, Y. Q. LI, X. H. ZENG, S. KERA, J. X. TANG and N. UENO, “The Role of Gap States on Energy Level Alignment at an α -NPD/HAT(CN)₆ Charge Generation Interface,” *Org. Electron.* **24**, 120–124 (2015).

S. KERA and N. UENO, “Photoelectron Spectroscopy on the Charge Reorganization Energy and Small Polaron Binding Energy of Molecular Film,” *J. Electron Spectrosc. Relat. Phenom.* **204**, 2–11 (2015).

H. ZEN, Y. TAIRA, T. KONOMI, T. HAYAKAWA, T. SHIZUMA, J. YAMAZAKI, T. KII, H. TOYOKAWA, M. KATOH and H. OHGAKI, “Generation of High Energy Gamma-Ray by Laser Compton Scattering of 1.94- μ m Fiber Laser in UVSOR-III Electron Storage Ring,” *Energy Procedia* **89**, 335–345 (2016).

E. TSUDA, Y. MITSUMOTO, K. TAKAKURA, N. SUNAGA, T. AKITSU, T. KONOMI and M. KATOH, “Electrochemical Tuning by Polarized UV Light Induced Molecular Orientation of Chiral Salen-Type Mn(II) and Co(II) Complexes in an Albumin Matrix,” *J. Chem. Chem. Eng.* **2**, 53–59 (2016).

J. OKABAYASHI, S. MIYASAKA, K. HEMMI, K. TANAKA, S. TAJIMA, H. WADATI, A. TANAKA, Y. TAKAGI and T. YOKOYAMA, “Investigating Orbital Magnetic Moments in Spinel-Type MnV₂O₄ Using X-Ray Magnetic Circular Dichroism,” *J. Phys. Soc. Jpn.* **84**, 104703 (5 pages) (2015).

M. NAKAYAMA, T. KONDO, Z. TIAN, J. J. ISHIKAWA, M. HALIM, C. BAREILLE, W. MALAEB, K. KURODA, T. TOMITA, S. IDETA, K. TANAKA, M. MATSUNAMI, S. KIMURA, N. INAMI, K. ONO, H. KUMIGASHIRA, L. BALENTS, S. NAKATSUJI and S. SHIN, “Slater to Mott Crossover in the Metal to Insulator Transition of Nd₂Ir₂O₇,” *Phys. Rev. Lett.* **117**, 056403 (6 pages) (2016).

K. HAGIWARA, Y. OHTSUBO, M. MATSUNAMI, S. IDETA, K. TANAKA, H. MIYAZAKI, J. E. RAULT, P. LE FÈVRE, F. BERTRAN, A. TALEB-IBRAHIMI, R. YUKAWA, M. KOBAYASHI, K. HORIBA, H. KUMIGASHIRA, K. SUMIDA, T. OKUDA, F. IGA and S. KIMURA, “Surface Kondo Effect and Non-Trivial Metallic State of the Kondo Insulator YbB₁₂,” *Nat. Commun.* **7**, 12690 (2016).

Y. HIKOSAKA, T. KANEYASU, P. LABLANQUIE, F. PENENT, E. SHIGEMASA and K. ITO, “Multiple Auger Decay of the Neon 1s-Core-Hole State Studied by Multielectron Coincidence Spectroscopy,” *Phys. Rev. A* **92**, 033413 (6 pages) (2015).

C. OHAE, J. R. HARRIES, H. IWAYAMA, K. KAWAGUCHI, S. KUMA, Y. MIYAMOTO, M. NAGASONO, K. NAKAJIMA, I. NAKANO, E. SHIGEMASA, N. SASAO, S. UETAKE, T. WAKABAYASHI, A. YOSHIMI, K. YOSHIMURA and M. YOSHIMURA, “Simultaneous Measurements of Superradiance at Multiple Wavelength from Helium Excited States: II. Analysis,” *J. Phys. Soc. Jpn.* **85**, 034301 (10 pages) (2016).

O. TRAVNIKOVA, T. MARCHENKO, G. GOLDSZTEJN, K. JÄNKÄLÄ, N. SISOURAT, S. CARNIATO, R. GUILLEMIN, L. JOURNAL, D. CÉOLIN, R. PÜTTNER, H. IWAYAMA, E. SHIGEMASA, M. N. PIANCASTELLI and M. SIMON, “Hard-X-Ray-Induced Multistep Ultrafast Dissociation,” *Phys. Rev. Lett.* **116**, 213001 (5 pages) (2016).

H. IWAYAMA, T. KANEYASU, Y. HIKOSAKA and E. SHIGEMASA, “Stability and Dissociation Dynamics of N₂⁺⁺ Ions Following Core Ionization Studied by an Auger-Electron-Photoion Coincidence Method,” *J. Chem. Phys.* **145**, 034305 (8 pages) (2016).

S. C. KUMAR, J. WEI, J. DEBRAY, V. KEMLIN, B. BOULANGER, H. ISHIZUKI, T. TAIRA and M. EBRAHIM-ZADEH, “High-Power, Widely Tunable, Room-Temperature Picosecond Optical Parametric Oscillator Based on Cylindrical 5%MgO:PPLN,” *Opt. Lett.* **40**, 3897–3900 (2015).

W. KONG, M. TSUNEKANE and T. TAIRA, “Diode Edge-Pumped Passively Q-Switched Microchip Laser,” *Opt. Eng.* **54**, 090501 (3 pages) (2015).

H. ISHIZUKI and T. TAIRA, “High-Gain Mid-Infrared Optical-Parametric Generation Pumped by Microchip Laser,” *Opt. Express* **24**, 1046–1052 (2016).

A. KAUSAS and T. TAIRA, “Giant-Pulse Nd:YVO₄ Microchip Laser with MW-Level Peak Power by Emission Cross-Sectional Control,” *Opt. Express* **24**, 3137–3149 (2016).

K. GALLO, Y. JEONG, T. TAIRA, S. JIANG and F. ILDAY, “Focus Issue Introduction: Advanced Solid State Lasers (ASSL) 2015,” *Opt. Express* **24**, 5674–5682 (2016).

M. TSUNEKANE and T. TAIRA, “Direct Measurement of Temporal Transmission Distribution of a Saturable Absorber in a Passively Q-Switched Laser,” *IEEE J. Quantum Electron.* **52**, 5200107 (7 pages) (2016).

T. GOTO, R. MORIMOTO, J. W. PRITCHARD, M. MINA, H. TAKAGI, Y. NAKAMURA, P. B. LIM, T. TAIRA and M. INOUE, “Magneto-Optical Q-Switching Using Magnetic Garnet Film with Micromagnetic Domains,” *Opt. Express* **24**, 17635–17643 (2016).

LIST OF PUBLICATIONS

- T. FUJI, H. SHIRAI and Y. NOMURA**, “Ultrabroadband Mid-Infrared Spectroscopy with Four-Wave Difference Frequency Generation,” *J. Opt.* **17**, 094004 (9 pages) (2015).
- T. OHIGASHI, M. NAGASAKA, T. HORIGOME, N. KOSUGI, S. M. ROSENDAHL and A. P. HITCHCOCK**, “Development of In-Situ Sample Cells for Scanning Transmission X-Ray Microscopy,” *AIP Conf. Proc.* **1741**, 050002 (2016).
- M.-W. LIN, K.-C. WANG, J.-H. WANG, M.-H. LI, Y.-L. LAI, T. OHIGASHI, N. KOSUGI, P. CHEN, D.-H. WEI, T.-F. GUO and Y.-J. HSU**, “Improve Hole Collection by Interfacial Chemical Redox Reaction at a Mesoscopic NiO/CH₃NH₃PbI₃ Heterojunction for Efficient Photovoltaic Cells,” *Adv. Mater. Interfaces* **3**, 1600135 (2016).
- T. OHIGASHI, A. ITO, K. SHINOHARA, S. TONE, M. KADO, Y. INAGAKI, Y.-F. WANG and N. KOSUGI**, “Observation of DNA and Protein Distributions in Mammalian Cell Nuclei Using STXM,” *AIP Conf. Proc.* **1696**, 020027 (2016).
- S. MITSUNOBU, M. ZHU, Y. TAKEICHI, T. OHIGASHI, H. SUGA, M. JINNO, H. MAKITA, M. SAKATA, K. ONO, K. MASE and Y. TAKAHASHI**, “Direct Direction of Fe(II) in Extracellular Polymeric Substances (EPS) at the Mineral–Microbe Interface in Bacterial Pyrite Leaching,” *Microbes Environ.* **31**, 63–69 (2016).
- K. IMAEDA and K. IMURA**, “Dye-Assisted Visualization of Plasmon Modes Excited in Single Gold Nanoplates,” *Chem. Phys. Lett.* **646**, 179–184 (2016).
- Y. NISHIYAMA, K. IMURA and H. OKAMOTO**, “Observation of Plasmon Wave Packet Motions via Femtosecond Time-Resolved Near-Field Imaging Techniques,” *Nano Lett.* **15**, 7657–7665 (2015).
- T. UCHIDA, Y. ICHIKAWA and K. IMURA**, “Optical Properties and Surface-Enhanced Raman Scattering Activity of Hexagonally Arranged Gold Nanoparticle Trimer,” *Chem. Phys. Lett.* **638**, 253–257 (2015).
- H. TANAKA, R. ARIMA, M. FUKUMORI, D. TANAKA, R. NEGISHI, Y. KOBAYASHI, S. KASAI, T. K. YAMADA and T. OGAWA**, “Method for Controlling Electrical Properties of Single-Layer Graphene Nanoribbons via Adsorbed Planar Molecular Nanoparticles,” *Sci. Rep.* **5**, 12341 (10 pages) (2015).
- T. K. YAMADA, T. ABE, N. M. K. NAZRIQ and T. IRISAWA**, “Electron-Bombarded <110>-Oriented Tungsten Tips for Stable Tunnelling Electron Emission,” *Rev. Sci. Instrum.* **87**, 033703 (7 pages) (2016).
- T. K. YAMADA, Y. SAKAGUCHI, L. GERHARD and W. WULFHEKEL**, “Temperature Control of the Growth of Iron Oxide Nanoislands on Fe(001),” *Jpn. J. Appl. Phys.* **55**, 08NB14 (5 pages) (2016).
- T. HIRAHARA, T. SHIRAI, T. HAJIRI, M. MATSUNAMI, K. TANAKA, S. KIMURA, S. HASEGAWA and K. KOBAYASHI**, “Role of Quantum and Surface-State Effects in the Bulk Fermi-Level Position of Ultrathin Bi Films,” *Phys. Rev. Lett.* **115**, 106803 (5 pages) (2015).
- A. V. MATETSKIY, I. A. KIBIREV, T. HIRAHARA, S. HASEGAWA, A. V. ZOTOV and A. A. SARANIN**, “Direct Observation of a Gap Opening in Topological Interface States of MnSe/Bi₂Se₃ Heterostructure,” *Appl. Phys. Lett.* **107**, 091604 (4 pages) (2015).

Materials Molecular Science

- O. SEKIZAWA, T. URUGA, Y. TAKAGI, K. NITTA, K. KATO, H. TANIDA, K. UESUGI, M. HOSHINO, E. IKENAGA, K. TAKESHITA, S. TAKAHASHI, M. SANO, H. AOYAGI, A. WATANABE, N. NARIYAMA, H. OHASHI, H. YUMOTO, T. KOYAMA, Y. SENBA, T. TAKEUCHI, Y. FURUKAWA, T. OHATA, T. MATSUSHITA, Y. ISHIZAWA, T. KUDO, H. KIMURA, H. YAMAZAKI, T. TANAKA, T. BIZEN, T. SEIKE, S. GOTO, H. OHNO, M. TAKATA, H. KITAMURA, T. ISHIKAWA, M. TADA, T. YOKOYAMA and Y. IWASAWA**, “SPRING-8 BL36XU: Catalytic Reaction Dynamics for Fuel Cells,” *J. Phys.: Conf. Ser.* **712**, 012142 (4 pages) (2016).
- S. YAMAZOE, S. TAKANO, W. KURASHIGE, T. YOKOYAMA, K. NITTA, Y. NEGISHI and T. TSUKUDA**, “Hierarchy of Bond Stiffnesses within Icosahedral-Based Gold Clusters Protected by Thiolates,” *Nat. Commun.* **7**, 10414 (7 pages) (2016).
- K. MOTOKURA, K. SAITOH, H. NODA, Y. UEMURA, W.-J. CHUN, A. MIYAJI, S. YAMAGUCHI and T. BABA**, “Co-Immobilization of a Palladium-Bisphosphine Complex and Strong Organic Base on a Silica Surface for Heterogeneous Synergistic Catalysis,” *ChemCatChem* **8**, 331–335 (2016).
- Y. UEMURA, D. KIDO, Y. WAKISAKA, H. UEHARA, T. OHBA, Y. NIWA, S. NOZAWA, T. SATO, K. ICHIYANAGI, R. FUKAYA, S. ADACHI, T. KATAYAMA, T. TOGASHI, S. OWADA, K. OGAWA, M. YABASHI, K. HATADA, S. TAKAKUSAGI, T. YOKOYAMA, B. OHTANI and K. ASAKURA**, “Dynamics of Photoelectrons and Structural Changes of Tungsten Trioxide Observed by Femtosecond Transient XAFS,” *Angew. Chem., Int. Ed.* **55**, 1364–1367 (2015).
- Y. WAKISAKA, Y. UEMURA, T. YOKOYAMA, H. ASAKURA, H. MORIMOTO, M. TABUCHI, D. OHSHIMA, T. KATO and S. IWATA**, “Anomalous Structural Behavior in the Metamagnetic Transition of FeRh Thin Films from a Local Viewpoint,” *Phys. Rev. B* **92**, 184408 (7 pages) (2015).
- Y. F. WANG, S. B. SINGH, M. V. LIMAYE, Y. C. SHAO, S. H. HSIEH, L. Y. CHEN, H. C. HSUEH, H. T. WANG, J. W. CHIOU, Y. C. YEH, C. W. CHEN, C. H. CHEN, S. C. RAY, J. WANG, W. F. PONG, Y. TAKAGI, T. OHIGASHI, T. YOKOYAMA and N. KOSUGI**, “Visualizing Chemical States and Defects Induced Magnetism of Graphene Oxide by Spatially Resolved-X-Ray Microscopy and Spectroscopy,” *Sci. Rep.* **5**, 15439 (12 pages) (2015).
- J. OKABAYASHI, S. MIYASAKA, K. HEMMI, K. TANAKA, S. TAJIMA, H. WADATI, A. TANAKA, Y. TAKAGI and T. YOKOYAMA**, “Investigating Orbital Magnetic Moments in Spinel-Type MnV₂O₄ Using X-Ray Magnetic Circular Dichroism,” *J. Phys. Soc. Jpn.* **84**, 104703 (5 pages) (2015).

- K. YAMAMOTO, T. NAKAMURA and S. HIGASHIBAYASHI**, "Acid-Regulated Electron Transfer Disproportionation of a Non-Substituted Tetramethyl-biacridine Derivative," *Chem. Lett.* **44**, 1229–1231 (2015).
- P. PANDIT, T. NAKAMURA and S. HIGASHIBAYASHI**, "Synthesis and Acid-Responsive Electron Transfer Disproportionation of Non- and Tetramesityl-Substituted 1,1',9,9'-Bicarbazole," *Chem. Lett.* **44**, 1336–1338 (2015).
- T. NAKAMURA, K. FURUKAWA, T. TERAUCHI and Y. KOBAYASHI**, "Microscopic Evidence of a Metallic State in the One-Pot Organic Conductor, Ammonium Tetrathiapentalene Carboxylate," *Phys. Status Solidi RRL* **9**, 480–484 (2015).
- M. KIKUCHI, Y. SHINMURA, T. KAJI, T. KONO, Y. YOSHIDA and M. HIRAMOTO**, "Enhancing the Photocurrent in High-Photovoltage Organic Solar Cells by Doping," *Jpn. J. Appl. Phys.* **54**, 111601 (5 pages) (2015).
- C. OHASHI, Y. SHINMURA, M. KUBO and M. HIRAMOTO**, "ppm-Doping Effects in the Simplest n^+p -Homojunction Organic Photovoltaic Cells," *Org. Electron.* **27**, 151–154 (2015).
- Y. WATANABE, T. HARADA, H. KAWAI, T. KAJI, M. HIRAMOTO and K. NISHIYAMA**, "Emission Properties of [Eu(hfa)₃(phen)] and [Eu(hfa)₃(TPPO)₂] Dispersed in a Fibrous Network Comprising *p*-Chlorophenol + AOT Organogels," *J. Mol. Liq.* **217**, 51–56 (2016).
- F. BUSSOLOTTI, J. YANG, M. HIRAMOTO, T. KAJI, S. KERA and N. UENO**, "Direct Detection of Density of Gap States in C₆₀ Single Crystals by Photoemission Spectroscopy," *Rhys. Rev. B* **92**, 115102 (6 pages) (2015).
- S. KATSUBE, M. KINOSHITA, K. AMANO, T. SATO, Y. KATSUMOTO, T. UMECKY, T. TAKAMUKU, T. KAJI, M. HIRAMOTO, Y. TSURUNAGA and K. NISHIYAMA**, "Solvent Dependent Properties and Higher-Order Structures of Aryl Alcohols + AOT Molecular Gels," *Langmuir* **32**, 4352–4360 (2016).
- H. XU, S. TAO and D. JIANG**, "Proton Conductions in Crystalline and Porous Covalent Organic Frameworks," *Nat. Mater.* **15**, 722–727 (2016). DOI: 10.1038/NMAT4461
- C. GU, N. HUANG, Y. CHEN, H. ZHANG, S. ZHANG, F. LI, Y. MA and D. JIANG**, "Porous Organic Polymers with Tunable Work Functions and Selective Hole and Electron Conductions for Energy Conversions," *Angew. Chem., Int. Ed.* **55**, 3049–3053 (2016). DOI: 10.1002/anie.201510723
- J. GAO and D. JIANG**, "Covalent Organic Frameworks with Spatially Confined Guest Molecules in Nanochannels and Their Impacts on Crystalline Structures," *Chem. Commun.* **52**, 1498–1500 (2016). DOI: 10.1039/C5CC09225F
- C. GU, N. HUANG, Y. CHEN, L. QIN, H. XU, S. ZHANG, F. LI, Y. MA and D. JIANG**, " π -Conjugated Microporous Polymer Films: Designed Synthesis, Conducting Properties and Photoenergy Conversions," *Angew. Chem., Int. Ed.* **54**, 13594–13598 (2015). (Hot Paper) DOI: 10.1002/anie.201506570
- X. CHEN, M. ADDICOAT, E. JIN, H. XU, T. HAYASHI, F. XU, N. HUANG, S. IRLE and D. JIANG**, "Designed Synthesis of Double-Stage Two-Dimensional Covalent Organic Frameworks," *Sci. Rep.* **5**, 14650 (2015). DOI: 10.1038/srep.14650
- H. XU, J. GAO and D. JIANG**, "Stable, Crystalline, Porous, Covalent Organic Frameworks as a Platform for Chiral Organocatalysis," *Nat. Chem.* **7**, 905–912 (2015). DOI: 10.1038/NCHEM2352
- C. GU, N. HUANG, Y. WU, H. XU and D. JIANG**, "Design of AIE-Based Highly Photofunctional Porous Polymer Films with Controlled Thickness and Prominent Microporosity," *Angew. Chem., Int. Ed.* **54**, 11540–11544 (2015). DOI: 10.1002/anie.201504786
- S. DALAPATI, M. ADDICOAT, S. JIN, T. SAKURAI, J. GAO, H. XU, S. IRLE, S. SEKI and D. JIANG**, "Rational Design of Crystalline Supermicroporous Covalent Organic Frameworks with Triangular Topologies," *Nat. Commun.* **6**, 7786 (2015). DOI: 10.1038/ncomms8786
- N. HUANG, R. KRISHNA and D. JIANG**, "Tailor-Made Pore Surface Engineering in Covalent Organic Frameworks: Systematic Functionalization for Performance Screening," *J. Am. Chem. Soc.* **137**, 7079–7082 (2015). DOI: 10.1021/ja5b04300
- S. JIN, M. SUPUR, M. ADDICOAT, K. FURUKAWA, L. CHEN, T. NAKAMURA, S. FUKUZUMI, S. IRLE and D. JIANG**, "Creation of Superheterojunction Polymers via Direct Polycondensation: Segregated and Bicontinuous Donor–Acceptor π -Columnar Arrays in Covalent Organic Frameworks for Long-Lived Charge Separation," *J. Am. Chem. Soc.* **137**, 7817–7827 (2015). DOI: 10.1021/ja5b03553
- N. HUANG, X. DING, J. KIM, H. IHEE and D. JIANG**, "A Photoresponsive Smart Covalent Organic Framework," *Angew. Chem., Int. Ed.* **54**, 8704–8707 (2015). (VIP) DOI: 10.1002/anie.201503902
- N. HUANG, L. ZHAI, D. E. COUPRY, M. A. ADDICOAT, K. OKUSHITA, K. NISHIMURA, T. HEINE and D. JIANG**, "Multiple-Component Covalent Organic Frameworks," *Nat. Commun.* **7**, 12325 (12 pages) (2016).
- M. YAGI-UTSUMI, K. KATO and K. NISHIMURA**, "Membrane-Induced Dichotomous Conformation of Amyloid β with the Disordered N-Terminal Segment Followed by the Stable C-Terminal β Structure," *PLoS One* **11**, 0146405 (10 pages) (2016).
- T. IJIMA, T. YAMASE and K. NISHIMURA**, "Molecular and Electron–Spin Structures of a Ring-Shaped Mixed-Valence Polyoxovanadate (IV, V) Studied by ¹¹B and ²³Na Solid-State NMR Spectroscopy and DFT Calculations," *Solid State Nucl. Magn. Reson.* **76–77**, 15–23 (2016).
- Y. NONOGUCHI, M. NAKANO, T. MURAYAMA, H. HAGINO, S. HAMA, K. MIYAZAKI, R. MATSUBARA, M. NAKAMURA and T. KAWAI**, "Simple Salt-Coordinated *n*-Type Nanocarbon Materials Stable in Air," *Adv. Funct. Mater.* **26**, 3021–3028 (2016).
- H. KOJIMA, R. ABE, M. ITO, Y. TOMATSU, F. FUJIWARA, R. MATSUBARA, N. YOSHIMOTO and M. NAKAMURA**, "Giant Seebeck Effect in Pure Fullerene Thin Films," *Appl. Phys. Express* **8**, 121301 (4 pages) (2015).
- R. MATSUBARA, Y. SAKAI, T. NOMURA, M. SAKAI, K. KUDO, Y. MAJIMA, D. KNIPP and M. NAKAMURA**, "Quantitative Investigation of the Effect of Gate-Dielectric Surface Treatments on Limiting Factors of Mobility in Organic Thin-Film Transistors," *J. Appl. Phys.* **118**, 175502 (9 pages) (2015).

Life and Coordination-Complex Molecular Science

- N. MURAKI and S. AONO, "Structural Basis for Heme Recognition by HmuT Responsible for Heme Transport to the Heme Transporter in *Corynebacterium glutamicum*," *Chem. Lett.* **45**, 24–26 (2015).
- N. MURAKI, C. KITATSUJI, M. OGURA, T. UCHIDA, K. ISHIMORI and S. AONO, "Structural Characterization of Heme Environmental Mutants of CgHmuT that Shuttles Heme Molecules to Heme Transporters," *Int. J. Mol. Sci.* **17**, 829 (10 pages) (2016).
- M. YAGI-UTSUMI, T. SATOH and K. KATO, "Structural Basis of Redox-Dependent Substrate Binding of Protein Disulfide Isomerase," *Sci. Rep.* **5**, 13909 (2015).
- H. YAGI, Y. ZHANG, M. YAGI-UTSUMI, T. YAMAGUCHI, S. IIDA, Y. YAMAGUCHI and K. KATO, "Backbone ^1H , ^{13}C , and ^{15}N Resonance Assignments of the Fc Fragment of Human Immunoglobulin G Glycoprotein," *Biomol. NMR Assign.* **9**(2), 257–260 (2015).
- K. INAGAKI, T. SATOH, M. YAGI-UTSUMI, A.-C. LE GULLUCHE, T. ANZAI, Y. UEKUSA, Y. KAMIYA and K. KATO, "Redox-Coupled Structural Changes of the Catalytic α' Domain of Protein Disulfide Isomerase," *FEBS Lett.* **589**, 2690–2694 (2015).
- Y. ISODA, H. YAGI, T. SATOH, M. SHIBATA-KOYAMA, K. MASUDA, M. SATOH, K. KATO and S. IIDA, "Importance of the Side Chain at Position 296 of Antibody Fc in Interactions with Fc γ RIIIa and Other Fc γ Receptors," *PLoS One* **10**, e0140120 (2015).
- K. ISHII, H. ENDA, M. NODA, M. KAJINO, A. KIM, E. KURIMOTO, K. SATO, A. NAKANO, Y. KOBAYASHI, H. YAGI, S. UCHIYAMA and K. KATO, "pH-Dependent Assembly and Segregation of the Coiled-Coil Segments of Yeast Putative Cargo Receptors Emp46p and Emp47p," *PLoS One* **10**, e0140287 (2015).
- R. THAMMAPORN, M. YAGI-UTSUMI, T. YAMAGUCHI, P. BOONSRI, P. SAPARPAKORN, K. CHOOWONGKOMON, S. TECHASAKUL, K. KATO and S. HANNONGBUA, "NMR Characterization of HIV-1 Reverse Transcriptase Binding to Various Non-Nucleoside Reverse Transcriptase Inhibitors with Different Activities," *Sci. Rep.* **5**, 15806 (2015).
- S. NINAGAWA, T. OKADA, Y. SUMITOMO, S. HORIMOTO, T. SUGIMOTO, T. ISHIKAWA, S. TAKEDA, T. YAMAMOTO, T. SUZUKI, Y. KAMIYA, K. KATO and K. MORI, "Forcible Destruction of Severely Misfolded Mammalian Glycoproteins by the Non-Glycoprotein ERAD Pathway," *J. Cell Biol.* **211**, 775–784 (2015).
- T. ZHU, T. YAMAGUCHI, T. SATOH and K. KATO, "A Hybrid Strategy for The Preparation of ^{13}C -Labeled High-Mannose-Type Oligosaccharides with Terminal Glucosylation for NMR Study," *Chem. Lett.* **44**, 1744–1746 (2015).
- Y. KANEMATSU, Y. KAMIYA, K. MATSUO, K. GEKKO, K. KATO and M. TACHIKAWA, "Isotope Effect on the Circular Dichroism Spectrum of Methyl α -D-Glucopyranoside in Aqueous Solution," *Sci. Rep.* **5**, 17900 (2015).
- K. ISHII, M. NODA, H. YAGI, R. THAMMAPORN, S. SEETAHA, T. SATOH, K. KATO and S. UCHIYAMA, "Disassembly of the Self-Assembled, Double-Ring Structure of Proteasome $\alpha 7$ Homo-Tetradecamer by $\alpha 6$," *Sci. Rep.* **5**, 18167 (2015).
- M. YAGI-UTSUMI, K. KATO and K. NISHIMURA, "Membrane-Induced Dichotomous Conformation of Amyloid β with the Disordered N-Terminal Segment Followed by the Stable C-Terminal β Structure," *PLoS One* **11**, e0146405 (2016).
- S. SEETAHA, M. YAGI-UTSUMI, T. YAMAGUCHI, K. ISHII, S. HANNONGBUA, K. CHOOWONGKOMON and K. KATO, "Application of Site-Specific Spin Labeling for NMR Detecting Inhibitor-Induced Conformational Change of HIV-1 Reverse Transcriptase," *ChemMedChem* **11**, 363–366 (2016).
- T. SATOH, T. TOSHIMORI, G. YAN, T. YAMAGUCHI and K. KATO, "Structural Basis for Two-Step Glucose Trimming by Glucosidase II Involved in ER Glycoprotein Quality Control," *Sci. Rep.* **6**, 20575 (2016).
- R. THAMMAPORN, K. ISHII, M. YAGI-UTSUMI, S. UCHIYAMA, S. HANNONGBUA and K. KATO, "Mass Spectrometric Characterization of HIV-1 Reverse Transcriptase Interactions with Non-Nucleoside Reverse Transcriptase Inhibitors," *Biol. Pharm. Bull.* **39**, 450–454 (2016).
- R. INOUE, T. TAKATA, N. FUJII, K. ISHII, S. UCHIYAMA, N. SATO, Y. OBA, K. WOOD, K. KATO, N. FUJII and M. SUGIYAMA, "New Insight into the Dynamical System of αB -Crystallin Oligomers," *Sci. Rep.* **6**, 29208 (2016).
- H. ITO, H. KAJI, A. TOGAYACHI, P. AZADI, M. ISHIHARA, R. GEYER, C. GALUSKA, H. GEYER, K. KAKEHI, M. KINOSHITA, N. G. KARLSSON, C. JIN, K. KATO, H. YAGI, S. KONDO, N. KAWASAKI, N. HASHII, D. KOLARICH, K. STAVENHAGEN, N. H. PACKER, M. THAYSEN-ANDERSEN, M. NAKANO, N. TANIGUCHI, A. KURIMOTO, Y. WADA, M. TAJIRI, P. YANG, W. CAO, H. LI, P. M. RUDD and H. NARIMATSU, "Comparison of Analytical Methods for Profiling N- and O-Linked Glycans from Cultured Cell Lines: HUPO Human Disease Glycomics/Proteome Initiative Multi-Institutional Study," *Glycoconjugate J.* **33**, 405–415 (2016).
- H. ISOJIMA, R. IINO, Y. NIITANI, H. NOJI and M. TOMISHIGE, "Direct Observation of Intermediate States during the Stepping Motion of Kinesin-1," *Nat. Chem. Biol.* **12**, 290–297 (2016).
- Y. MATSUMOTO, S. SAKAKIHARA, A. GRUSHNIKOV, K. KIKUCHI, H. NOJI, A. YAMAGUCHI, R. IINO, Y. YAGI and K. NISHINO, "A Microfluidic Channel Method for Rapid Drug-Susceptibility Testing of *Pseudomonas aeruginosa*," *PLoS One* **11**, e0148797 (2016).
- L. SHENG and K. KURIHARA, "Generation of Catalytic Amphiphiles in a Self-Reproducing Giant Vesicle," *Chem. Lett.* **45**, 598–600 (2016).
- L. SHENG and K. KURIHARA, "Transformation of Oil Droplets into Giant Vesicles," *Chem. Commun.* **52**, 7786–7789 (2016).

- H. TSUKAMOTO, Y. KUBO, D. L. FARRENS, M. KOYANAGI, A. TERAOKA and Y. FURUTANI**, "Retinal Attachment Instability Is Diversified among Mammalian Melanopsins," *J. Biol. Chem.* **290**, 27176–27187 (2015).
- Y. FURUTANI, H. SHIMIZU, Y. ASAI, S. OIKI and H. KANDORI**, "Specific Interactions between Alkali Metal Cations and the KcsA Channel Studied Using ATR-FTIR Spectroscopy," *Biophys. Physicobiol.* **12**, 37–45 (2015).
- Y. INOKUCHI, T. EBATA, T. IKEDA, T. HAINO, T. KIMURA, H. GUO and Y. FURUTANI**, "New Insights into Metal Ion-Crown Ether Complexes Revealed by SEIRA Spectroscopy," *New J. Chem.* **39**, 8673–8680 (2015).
- M. SRISA-ART and Y. FURUTANI**, "Simple and Rapid Fabrication of PDMS Microfluidic Devices Compatible with FTIR Microspectroscopy," *Bull. Chem. Soc. Jpn.* **89**, 195–202 (2016).
- Y. M. A. YAMADA, A. OHNO, T. SATO and Y. UOZUMI**, "Instantaneous Click Chemistry by a Copper-Containing Polymeric Membrane-Installed Microflow Catalytic Reactor," *Chem. –Eur. J.* **21**, 17269–17273 (2015).
- G. SHEN, H. ZHOU, P. DU, S. LIU, K. ZOU and Y. UOZUMI**, "Brønsted Acid-Catalyzed Selective C–C Bond Cleavage of 1,3-Diketones: A Facile Synthesis of 4(3H)-Quinazolinones in Aqueous Ethyl Lactate," *RSC Adv.* **5**, 85646–85651 (2015).
- G. HAMASAKA, F. SAKURAI and Y. UOZUMI**, "A Vesicular Self-Assembled Amphiphilic Palladium NNC-Pincer Complex-Catalyzed Allylic Arylation of Allyl Acetates with Sodium Tetraarylborates in Water," *Tetrahedron* **71**, 6437–6441 (2015).
- G. HAMASAKA, Y. TSUJI and Y. UOZUMI**, "Organoborane-Catalyzed Hydrogenation of Unactivated Aldehydes with a Hantzsch Ester as a Synthetic NAD(P)H Analogue," *Synlett* **26**, 2037–2041 (2015).
- Y.-H. KIN, J. HAN, B. Y. JUNG, H. BAEK, Y. M. A. YAMADA, Y. UOZUMI and Y.-S. LEE**, "Production of Valuable Esters from Oleic Acid with a Porous Polymeric Acid Catalyst without Water Removal," *Synlett* **27**, 29–32 (2016).
- J.-C. HIERSO and Y. UOZUMI**, "Cluster Preface: Heterogeneous Catalysis," *Synlett* **27**, 1177–1178 (2016).
- A. OHTAKA, T. KOTERA, A. SAKON, K. UEDA, G. HAMASAKA, Y. UOZUMI, O. SHIMOMURA and R. NOMURA**, "Fluoride-Free Hiyama Coupling Reaction Catalyzed by Linear Polystyrene-Stabilized PdO Nanoparticles in Water: Specific Reactivity of PdO Nanoparticles over Pd Nanoparticles," *Synlett* **27**, 1202–1206 (2016).
- S. YAN, S. PAN, T. OSAKO and Y. UOZUMI**, "Recyclable Polystyrene-Supported Copper Catalysts for the Aerobic Oxidative Homocoupling of Terminal Alkynes," *Synlett* **27**, 1232–1236 (2016).
- H. BAEK, M. MINAKAWA, Y. M. A. YAMADA, J. W. HAN and Y. UOZUMI**, "In-Water and Neat Batch and Continuous-Flow Direct Esterification and Transesterification by a Porous Polymeric Acid Catalyst," *Sci. Rep.* **6**, 25925 (2016).
- A. OHTAKA, M. KOZONO, K. TAKAHASHI, G. HAMASAKA, Y. UOZUMI, T. SHINAGAWA, O. SHIMOMURA and R. NOMURA**, "Linear Polystyrene-Stabilized Pt Nanoparticles Catalyzed Indole Synthesis in Water via Aerobic Alcohol Oxidation," *Chem. Lett.* **45**, 758–760 (2016).
- T. OSAKO, Y. M. A. YAMADA and Y. UOZUMI**, "Application of Heterogeneous Polymer-Supported Catalysts to Continuous Flow Systems," *J. Synth. Org. Chem., Jpn.* **74**, 621–630 (2016).
- N. MOMIYAMA, T. NARUMI and M. TERADA**, "Design of a Brønsted Acid with Two Different Acidic Sites: Synthesis and Application of Aryl Phosphinic Acid–Phosphoric Acid as a Brønsted Acid Catalyst," *Chem. Commun.* **51**, 16976–16979 (2015).
- N. MOMIYAMA, K. FUNAYAMA, H. NODA, M. YAMANAKA, N. AKASAKA, S. ISHIDA, T. IWAMOTO and M. TERADA**, "Hydrogen Bonds-Enabled Design of a C₁-Symmetric Chiral Brønsted Acid Catalyst," *ACS Catal.* **6**, 949–956 (2016).
- N. MOMIYAMA, H. OKAMOTO, J. KIKUCHI, T. KORENAGA and M. TERADA**, "Perfluorinated Aryls in the Design of Chiral Brønsted Acid Catalysts: Catalysis of Enantioselective [4+2] Cycloadditions and Ene-Reactions of Imines with Alkenes by Chiral Mono-Phosphoric Acids with Perfluoroaryls," *ACS Catal.* **6**, 1198–1204 (2016).
- J. KIKUCHI, N. MOMIYAMA and M. TERADA**, "Chiral Phosphoric Acid-Catalyzed Diastereo- and Enantioselective Mannich-Type Reaction between Enamides and Thiazolones," *Org. Lett.* **18**, 2521–2513 (2016).
- M. OKAMURA, M. KONDO, R. KUGA, Y. KURASHIGE, T. YANAI, S. HAYAMI, V. K. K. PRANEETH, M. YOSHIDA, K. YONEDA, S. KAWATA and S. MASAOKA**, "A Pentanuclear Iron Catalyst Designed for Water Oxidation," *Nature* **530**, 465–468 (2016).
- K. KITAMOTO, M. OGAWA, G. AJAYAKUMAR, S. MASAOKA, H.-B. KRAATZ and K. SAKAI**, "Molecular Photo-Charge-Separators Enabling Single-Pigment-Driven Multi-Electron Transfer and Storage Leading to H₂ Evolution from Water," *Inorg. Chem. Front.* **3**, 671–680 (2016).
- N. NARITA, T. ENOMOTO, S. MASAOKA and N. KUSAKABE**, "Titanium May Produce Abiotic Oxygen Atmospheres on Habitable Exoplanets," *Sci. Rep.* **5**, 13977 (2015).
- G. NAKAMURA, M. KONDO, M. CRISALLI, S. K. LEE, A. SHBATA, P. C. FORD and S. MASAOKA**, "Syntheses and Properties of Phosphine-Substituted Ruthenium(II) Polypyridine Complexes with Nitrogen Oxides," *Dalton Trans.* **44**, 17189–17200 (2015).
- T. ITOH, M. KONDO, H. SAKAMOTO, K. WAKABAYASHI, M. KANAIKE, K. ITAMI and S. MASAOKA**, "Porous Frameworks Constructed by Non-Covalent Linking of Substitution-Inert Metal Complexes," *Dalton Trans.* **44**, 15334–15342 (2015).
- A. FUKATSU, M. KONDO, Y. OKABE and S. MASAOKA**, "Electrochemical Analysis of Iron Porphyrin-Catalyzed CO₂ Reduction under Photoirradiation," *J. Photochem. Photobiol., A* **313**, 143–148 (2015).
- T. KOSHIYAMA, N. KANDA, K. IWATA, M. HONJO, S. ASADA, T. HATAE, Y. TSUJI, M. YOSHIDA, M. OKAMURA, R. KUGA, S. MASAOKA and M. OHBA**, "Regulation of Cerium(IV)-Driven O₂ Evolution Reaction Using Composites of Liposome and Lipophilic Ruthenium Complexes," *Dalton Trans.* **44**, 15126–15129 (2015).

LIST OF PUBLICATIONS

T. KURAHASHI, “Reverse Catalase Reaction: Dioxxygen Activation via Two-Electron Transfer from Hydroxide to Dioxxygen Mediated By a Manganese(III) Salen Complex,” *Inorg. Chem.* **54**, 8356–8366 (2015).

R. NARAYANAN, A. VELLOTH, T. KURAHASHI, H. FUJII and M. HADA, “The Origin of Relative Stability of Di- μ -oxo M-M Chiral Salen Complexes [M-M = Ti(IV)-Ti(IV), V(IV)-V(IV), Cr(IV)-Cr(IV), and Mn(IV)-Mn(IV)]: A Quantum-Chemical Analysis,” *Bull. Chem. Soc. Jpn.* **89**, 447–454 (2016).

O. SHOJI, T. FUJISHIRO, K. NISHIO, Y. KANO, H. KIMOTO, S. CHIEN, H. ONODA, A. MURAMATSU, S. TANAKA, A. HORI, H. SUGIMOTO, Y. SHIRO and Y. WATANABE, “A Substrate-Binding-State Mimic of H₂O₂-Dependent Cytochrome P450 Produced by One-point Mutagenesis and Peroxygenation of Non-native Substrates,” *Catal. Sci. Tech.* **6**, 5806–5811 (2016).

S. D. MUNDAY, O. SHOJI, Y. WATANABE, L. L. WONG and S. G. BELL, “Improved Oxidation of Aromatic and Aliphatic Hydrocarbons Using Rate Enhancing Variants of P450Bm3 in Combination with Decoy Molecules,” *Chem. Commun.* **52**, 1036–1039 (2016).

H. ONODA, O. SHOJI and Y. WATANABE, “Acetate Anion-Triggered Peroxygenation of Non-Native Substrates by Wild-Type Cytochrome P450s,” *Dalton Trans.* **44**, 15316–15323 (2015).

M. SAKAGUCHI, T. KIMURA, T. NISHIDA, T. TOSHA, H. SUGIMOTO, Y. YAMAGUCHI, S. YANAGISAWA, G. UENO, H. MURAKAMI, H. AGO, M. YAMAMOTO, T. OGURA, Y. SHIRO and M. KUBO, “A Nearly On-Axis Spectroscopic System for Simultaneously Measuring UV-Visible Absorption and X-Ray Diffraction in the SPring-8 Structural Genomics Beamline,” *J. Synchrotron Radiat.* **23**, 334–338 (2016).

Research Center of Integrative Molecular Systems

I. ANZAI, K. TOICHI, E. TOKUDA, A. MUKAIYAMA, S. AKIYAMA and Y. FURUKAWA, “Screening of Drugs Inhibiting *In vitro* Oligomerization of Cu/Zn-Superoxide Dismutase with a Mutation Causing Amyotrophic Lateral Sclerosis,” *Front. Mol. Biosci.* **3**, 40 (2016). doi: 10.3389/fmolb.2016.00040

E. NANGO, S. AKIYAMA, S. MAKI-YONEKURA, Y. ASHIKAWA, Y. KUSAKABE, E. KRAYUKHINA, T. MARUNO, S. UCHIYAMA, N. NUEMKET, K. YONEKURA, M. SHIMIZU, N. ATSUMI, N. YASUI, T. HIKIMA, M. YAMAMOTO, Y. KOBAYASHI and A. YAMASHITA, “Taste Substance Binding Elicits Conformational Change of Taste Receptor T1r Heterodimer Extracellular Domains,” *Sci. Rep.* **6**, 25745 (2016). doi: 10.1038/srep25745

Y. FURUKAWA, Y. SUZUKI, M. FUKUOKA, K. NAGASAWA, K. NAKAGOME, H. SHIMIZU, A. MUKAIYAMA and S. AKIYAMA, “A Molecular Mechanism Realizing Sequence-Specific Recognition of Nucleic Acids by TDP-43,” *Sci. Rep.* **6**, 20576 (2016). doi: 10.1038/srep20576

Y. FURUKAWA, I. ANZAI, S. AKIYAMA, M. IMAI, F. J. C. CRUZ, T. SAIO, K. NAGASAWA, T. NOMURA and K. ISHIMORI, “Conformational Disorder of the Most Immature Cu,Zn-Superoxide Dismutase Leading to Amyotrophic Lateral Sclerosis,” *J. Biol. Chem.* **291**, 4144–4155 (2016).

***Y.-R. LIN, *N. KOGA, R. TATSUMI-KOGA, G. LIU, A. F. CLOUSER, G. T. MONTELLIONE and D. BAKER** (*Y.-R. Lin and N. Koga contributed equally), “Control over Overall Shape and Size in De Novo Designed Proteins,” *Proc. Natl. Acad. Sci. U.S.A.* **112**, E5478–E5485 (2015).

K. G. NAKAMURA, Y. SHIKANO and Y. KAYANUMA, “Influence of Pulse Width and Detuning on Coherent Phonon Generation,” *Phys. Rev. B* **92**, 144304 (7 pages) (2015).

A. HOSOYA, K. MARUYAMA and Y. SHIKANO, “Operational Derivation of Boltzmann Distribution with Maxwell’s Demon Model,” *Sci. Rep.* **5**, 17011 (9 pages) (2015).

S. GOTO, R. W. TUCKER and T. J. WALTON, “Classical Dynamics of Free Electromagnetic Laser Pulses,” *Nucl. Instrum. Methods Phys. Res., Sect. B* **369**, 40–44 (2016).

S. GOTO, R. W. TUCKER and T. J. WALTON, “The Dynamics of Compact Laser Pulses,” *J. Phys. A: Math. Theor.* **49**, 265203 (11 pages) (2016).

T. HORIKIRI, M. YAMAGUCHI, K. KAMIDE, Y. MATSUO, T. BYRNES, N. ISHIDA, A. LÖFFLER, S. HÖFLING, Y. SHIKANO, T. OGAWA, A. FORCHEL and Y. YAMAMOTO, “High-Energy Side-Peak Emission of Exciton-Polariton Condensates in High Density Regime,” *Sci. Rep.* **6**, 25655 (11 pages) (2016).

K. G. NAKAMURA, K. OHYA, H. TAKAHASHI, T. TSURUTA, H. SASAKI, S. UOZUMI, K. NORIMATSU, M. KITAJIMA, Y. SHIKANO and Y. KAYANUMA, “Spectrally Resolved Detection in Transient-Reflectivity Measurements of Coherent Optical Phonons in Diamond,” *Phys. Rev. B* **94**, 024303 (7 pages) (2016).

Y.-X. ZHANG, S. WU, Z.-B. CHEN and Y. SHIKANO, “Ground-State Cooling of a Dispersively Coupled Optomechanical System in the Unresolved Sideband Regime via a Dissipatively Coupled Oscillator,” *Phys. Rev. A* **94**, 023823 (11 pages) (2016).

- G. KOBAYASHI, Y. HINUMA, S. MATSUOKA, A. WATANABE, I. MUHAMMAD, M. HIRAYAMA, M. YONEMURA, T. KAMIYAMA, I. TANAKA and R. KANNO, "Pure H⁻ Conduction in Oxyhydrides," *Science* **351**, 1314–1317 (2016).
- G. KOBAYASHI, Y. IRII, F. MATSUMOTO, A. ITO, Y. OHSAWA, S. YAMAMOTO, Y. CUI, J.-Y. SON and Y. SATO, "Improving Cycling Performance of Li[Li_{0.2}Ni_{0.18}Co_{0.03}Mn_{0.58}]O₂ through Combination of Al₂O₃-Based Surface Modification and Stepwise Pre-Cycling," *J. Power Sources* **303**, 250–256 (2016).
- M. IQBAL, K. SUZUKI, G. KOBAYASHI, G. ZHAO, M. HIRAYAMA and R. KANNO, "Lithium Ion Conduction in Doped LaLiO₂ System," *Solid State Ionics* **285**, 33–37 (2016).
- K SOMA, S. KOININGS, G. KOBAYASHI and S. TAKEDA, "B12-O-05 Towards Dynamics Electron Holographic Analysis of Solid State Electrochemical Devices at Operating Condition," *Microscopy* **64**, i21 (2015).
- S. TSUSHIMA, W. HUNG, P. DEEVANHXAY, G. KOBAYASHI, R. KANNO and S. HIRAI, "In Situ X-Ray Visualization of Lithiation Process in Porous Graphite Electrode in an Operating Li-Ion Cell," *ChemElectroChem* **2**, 1535–1540 (2015).
- Y. KAWASUGI, K. SEKI, Y. EDAGAWA, Y. SATO, J. PU, T. TAKENOBU, S. YUNOKI, H. M. YAMAMOTO and R. KATO, "Electron–Hole Doping Asymmetry of Fermi Surface Reconstructed in a Simple Mott Insulator," *Nat. Commun.* **7**, 12356 (2016).
- S. YASUZUKA, S. UJI, T. KONOIKE, T. TERASHIMA, D. GRAF, E. S. CHOI, J. S. BROOKS, H. M. YAMAMOTO and R. KATO, "Shubnikov–de Haas Effect and Angular-Dependent Magnetoresistance in Layered Organic Conductor β⁺-(ET)(TCNQ)," *J. Phys. Soc. Jpn.* **85**, 084701 (7 pages) (2016).
- H. YAMAKAWA, T. MIYAMOTO, T. MORIMOTO, H. YADA, Y. KINOSHITA, M. SOTOME, N. KIDA, K. YAMAMOTO, K. IWANO, Y. MATSUMOTO, S. WATANABE, Y. SHIMOI, M. SUDA, H. M. YAMAMOTO, H. MORI and H. OKAMOTO, "Novel Electronic Ferroelectricity in an Organic Charge-Order Insulator Investigated with Terahertz-Pump Optical-Probe Spectroscopy," *Sci. Rep.* **6**, 20571 (2016).
- E. KAYAHARA, R. QU, M. KOJIMA, T. IWAMOTO, T. SUZUKI and S. YAMAGO, "Ligand-Controlled Synthesis of [3]- and [4]Cyclo-9,9-dimethyl-2,7-fluorenes through Triangle- and Square-Shaped Platinum Intermediates," *Chem. –Eur. J.* **21**, 18939–18943 (2015).
- Y. KURODA, Y. SAKAMOTO, T. SUZUKI, E. KAYAHARA and S. YAMAGO, "Tetracyclo(2,7-carbazole)s: Diatropicity and Paratropicity of Inner Regions of Nanohoops," *J. Org. Chem.* **81**, 3356–3363 (2016).
- S. HIGASHIBAYASHI, P. PANDIT, R. HARUKI, S. ADACHI and R. KUMAI, "Redox-Dependent Transformation of Hydrazinobuckybowl Between Curved and Planar Geometries," *Angew. Chem., Int. Ed.* **55**, 10830–10834 (2016).
- T. TSUKAMOTO, K. MAEYAMA, S. HIGASHIBAYASHI and H. SAKURAI, "Thermal Stability, Solubility, and Fluorescence Property of Poly(arylene vinylene ketone)s Bearing 1,1'-Binaphthylene Units," *React. Funct. Polym.* **100**, 123–129 (2016).
- K. YAMAMOTO and S. HIGASHIBAYASHI, "Synthesis of Three-Dimensional Butterfly Slit-Cyclobisazaanthracenes and Hydrazinobisanthenes via One-Step Cyclodimerization and Their Properties," *Chem. –Eur. J.* **22**, 663–671 (2016).
- T. TSUKAMOTO, K. MAEYAMA, S. HIGASHIBAYASHI and H. SAKURAI, "Synthesis and Characterization of Poly(arylene vinylene ketone)s Bearing 1,1'-Binaphthylene Units through Mizoroki-Heck Coupling Polymerization," *Chem. Lett.* **44**, 1780–1782 (2015).
- K. KANAHARA, MD M. R. BADAL, S. HATANO, M. ABE, S. HIGASHIBAYASHI, N. TAKASHINA and H. SAKURAI, "Intra- and Intermolecular Reactivity of Triplet Sumanenetrione," *Bull. Chem. Soc. Jpn.* **88**, 1612–1617 (2015).
- K. MAEYAMA, T. TSUKAMOTO, H. KUMAGAI, S. HIGASHIBAYASHI and H. SAKURAI, "Synthesis of Organosoluble and Fluorescent Aromatic Polyketones Bearing 1,1'-Binaphthyl Units through Suzuki-Miyaura Coupling Polymerization," *Polym. Bull.* **72**, 2903–2916 (2015).
- P. PANDIT, T. NAKAMURA and S. HIGASHIBAYASHI, "Synthesis and Acid-Responsive Electron Transfer Disproportionation of Non- and Tetramesityl-Substituted 1,1',9,9'-Bicarbazole," *Chem. Lett.* **44**, 1336–1338 (2015).
- K. YAMAMOTO, T. NAKAMURA and S. HIGASHIBAYASHI, "Acid-Regulated Electron Transfer Disproportionation of a Non-Substituted Tetramethyl-biacridine Derivative," *Chem. Lett.* **44**, 1229–1231 (2015).
- K. YAMAMOTO, S. KIMURA and T. MURAHASHI, "σ-π Continuum in Indole–Pd(II) Complexes," *Angew. Chem., Int. Ed.* **55**, 5322–5326 (2016).
- K. MASAI, K. SHIRATO, K. YAMAMOTO, Y. KURASHIGE and T. MURAHASHI, "A Mechanistic Insight into Metal-Cluster π-Envelopment: A Dual Binding Mode Involving Bent and Planar Ligand-Conformers," *Chem. Commun.* **52**, 6247–6430 (2016).