

Theoretical and Computational Molecular Science

- K. OHTA, J. TAYAMA, S. SAITO and K. TOMINAGA**, “Vibrational Frequency Fluctuation of Ions in Aqueous Solutions Studied by Three-Pulse Infrared Photon Echo Method,” *Acc. Chem. Res.* **45**, 1982–1991 (2012).
- T. YAGASAKI and S. SAITO**, “Fluctuations and Relaxation Dynamics of Liquid Water Revealed by Linear and Nonlinear Spectroscopy,” *Annu. Rev. Phys. Chem.* **64**, 55–75 (2013).
- K. KIM and S. SAITO**, “Multiple Length and Time Scales of Dynamic Heterogeneities in Model Glass-Forming Liquids: A Systematic Analysis of Multi-Point and Multi-Time Correlations,” *J. Chem. Phys. (Special Topic: Glass Transition)* **138**, 12A506 (12 pages) (2013).
- M. HIGASHI, S. HIRAI, M. BANNO, K. OHTA, S. SAITO and K. TOMINAGA**, “Theoretical and Experimental Studies on Vibrational Energy Relaxation of the CO Stretching Mode of Acetone in Alcohol Solutions,” *J. Phys. Chem. B* **117**, 4723–4731 (2013).
- S. IMOTO, S. XANTHEAS and S. SAITO**, “Molecular Origin of the Difference in the HOH Bend of the IR Spectra between Liquid Water and Ice,” *J. Chem. Phys.* **138**, 054506 (8 pages) (2013).
- S. SAITO, I. OHMINE and B. BAGCHI**, “Frequency Dependence of Specific Heat in Supercooled Liquid Water and Emergence of Correlated Dynamics,” *J. Chem. Phys.* **138**, 094503 (7 pages) (2013).
- S. IMOTO, S. XANTHEAS and S. SAITO**, “Ultrafast Dynamics of Liquid Water: Frequency Fluctuations of the OH Stretch and the HOH Bend,” *J. Chem. Phys.* **139**, 044503 (7 pages) (2013).
- W. KURASHIGE, K. MUNAKATA, K. NOBUSADA and Y. NEGISHI**, “Synthesis of Stable $\text{Cu}_n\text{Au}_{25-n}$ Nanoclusters ($n = 1-9$) Using Selenolate Ligands,” *Chem. Commun.* **49**, 5447–5449 (2013).
- T. YASUIKE and K. NOBUSADA**, “Raman Enhancement by Plasmonic Excitation of Structurally-Characterized Metal Clusters: Au_8 , Ag_8 , and Cu_8 ,” *Phys. Chem. Chem. Phys.* **15**, 5424–5429 (2013).
- A. DAS, T. LI, K. NOBUSADA, Q. ZENG, N. L. ROSI and R. JIN**, “Total Structure and Optical Properties of a Phosphine/Thiolate-Protected Au_{24} Nanocluster,” *J. Am. Chem. Soc.* **134**, 20286–20289 (2012).
- W. KURASHIGE, M. YAMAGUCHI, K. NOBUSADA and Y. NEGISHI**, “Ligand-Induced Stability of Gold Nanoclusters: Thiolate versus Selenolate,” *J. Phys. Chem. Lett.* **3**, 2649–2652 (2012).
- M. NODA, T. YASUIKE, K. NOBUSADA and M. HAYASHI**, “Enhanced Raman Spectrum of Pyrazine with the Aid of Resonant Electron Dynamics in a Nearby Cluster,” *Chem. Phys. Lett.* **550**, 52–57 (2012).
- W. MIZUKAMI, Y. KURASHIGE and T. YANAI**, “More π Electrons Make a Difference: Emergence of Many Radicals on Graphene Nanoribbons Studied by Ab Initio DMRG Theory,” *J. Chem. Theory Comput.* **9**, 401–407 (2012).
- Y. KURASHIGE, G. K-L. CHAN and T. YANAI**, “Entangled Quantum Electronic Wavefunctions of the Mn_4Ca Cluster in Photosystem II,” *Nat. Chem.* **5**, 660–666 (2013).
- L. N. TRAN and T. YANAI**, “Correlated One-Body Potential from Second-Order Møller-Plesset Perturbation Theory: Alternative to Orbital-Optimized MP2 Method,” *J. Chem. Phys.* **138**, 224108 (12 pages) (2013).
- M. SAITOW, Y. KURASHIGE and T. YANAI**, “Highly Scalable Multireference Configuration Interaction Theory with Internal Contraction of Density Matrix Renormalization Group Wave Function,” *J. Chem. Phys.* **139**, 044118 (15 pages) (2013).
- R. FUKUDA and M. EHARA**, “Electronic Excitations of C_{60} Fullerene Calculated Using the Ab Initio Cluster Expansion Method,” *J. Chem. Phys.* **137**, 134304 (7 pages) (2012).
- R. FUKUDA, R. CHIDTHONG, R. CAMMI and M. EHARA**, “Optical Absorption and Fluorescence of PRODAN in Solution: Quantum Chemical Study Based on the SAC-CI method,” *Chem. Phys. Lett.* **552**, 53–57 (2012).
- N. V. KRYZHEVOI, M. TASHIRO, M. EHARA and L. S. CEDERBAUM**, “Interatomic Relaxation Effects in Double Core Ionization of Chain Molecules,” *J. Chem. Phys.* **137**, 154316 (10 pages) (2012).
- Y. MORISAWA, S. TACHIBANA, M. EHARA and Y. OZAKI**, “Elucidating Electronic Transitions from σ Orbitals of Liquid n - and Branched Alkanes by Far-ultraviolet Spectroscopy and Quantum Chemical Calculations,” *J. Phys. Chem. A* **116**, 11957–11964 (2012).
- S. NAMUANGRUK, R. FUKUDA, M. EHARA, J. MEEPRASERT, T. KHANASA, S. MORADA, T. KAEWIN, S. JUNGSTIWIWONG, T. SUDYOADSUK and V. PROMARAK**, “D-D- π -A Type Organic Dyes for Dye-Sensitized Solar Cells with a Potential of Direct Electron Injection and High Extinction Coefficient: Synthesis, Characterization, and Theoretical Investigation,” *J. Phys. Chem. C* **116**, 25653–25663 (2012).
- M. TASHIRO, M. NAKANO, M. EHARA, F. PENENT, L. ANDRIC, J. PALAUDOUX, K. ITO, Y. HIKOSAKA, N. KOUCHI and P. LABLANQUIE**, “Auger Decay of Molecular Double-Core Hole and Its Satellite States—Comparison of Experiment and Calculation,” *J. Chem. Phys.* **137**, 224306 (8 pages) (2012).
- R. N. DHITAL, C. KAMONSATIKUL, E. SOMSOOK, K. BOBUATONG, M. EHARA, S. KARANJIT and H. SAKURAI**, “Low Temperature Carbon–Chlorine Bond Activation by Bimetallic Gold/Palladium Alloy Nanoclusters: An Application to Ullmann Coupling,” *J. Am. Chem. Soc.* **134**, 20250–20253 (2012).
- R. FUKUDA and M. EHARA**, “Mechanism for Solvatochromic Shifts of Free Base Porphyrine Studied with Polarizable Continuum Models and Explicit Solute–Solvent Interactions,” *J. Chem. Theory Comput.* **9**, 470–480 (2013).
- S. YAMANAKA, K. KANDA, T. SAITO, Y. KITAGAWA, T. KAWAKAMI, M. EHARA, M. OKUMURA, H. NAKAMURA and K. YAMAGUCHI**, “Linear Response Function Approach for the Boundary Problem of QM/MM Methods,” *Int. J. Quantum Chem.* **113**, 336–341 (2013).
- S. KARANJIT, K. BOBUATONG, R. FUKUDA, M. EHARA and H. SAKURAI**, “Mechanism of Aerobic Oxidation of Methanol to Formic Acid on Au_8 : A DFT Study,” *Int. J. Quantum Chem.* **113**, 428–436 (2013).
- M. PROMKATKAEW, S. SURAMITR, T. KARPKIRD, M. EHARA and S. HANNONGBUA**, “Absorption and Emission Properties of Various Substituted Cinnamic Acids and Cinnamates, Based on TDDFT Investigation,” *Int. J. Quantum Chem.* **113**, 542–554 (2013).

- R. FUKUDA and M. EHARA**, "Theoretical Study on Electronic Excited States of Coronene and Its π -Extended Molecules Using SAC-CI Method," *Bull. Chem. Soc. Jpn.* **86**, 445–451 (2013).
- H. KUNYASU, A. SANAGAWA, D. NAKANE, T. IWASAKI, N. KAMBE, K. BOBUATONG, Y. LU and M. EHARA**, " σ -Bond Metathesis between M-X and RC(O)X' (M = Pt and Pd; X, X' = Cl, Br, and I): Facile Determination of the Relative ΔG s of the Oxidative Additions of RCO(X) to M(0) Complexes, Evidence by Density Functional Theory Calculation, and Synthetic Application," *Organometallics* **32**, 2026–2032 (2013).
- M. TASHIRO, N. V. KRZHEVOI, L. S. CEDERBAUM and M. EHARA**, "Polarization and Site Dependence of Interatomic Relaxation Effects in Double Core Hole States," *J. Phys. B* **46**, 164012 (6 pages) (2013).
- D. BOUSQUET, R. FUKUDA, P. MAITARAD, D. JACQUEMIN, I. CIOFINI, C. ADAMO and M. EHARA**, "Excited State Geometries of Heteroaromatic Compounds: A Comparative TD-DFT and SAC-CI Study," *J. Chem. Theory Comput.* **9**, 2368–2379 (2013).
- A. SANAGAWA, H. KUNYASU, T. IWASAKI, N. KAMBE, K. BOBUATONG and M. EHARA**, "Facile Halogen Exchange Method between Au(Cl)(L) and MeC(O)X (L = PPh₃ and IPr; X = Br and I) via σ -Bond Metathesis Supported by DFT Calculation," *Chem. Lett.* **42**, 831–832 (2013).
- R. FUKUDA and M. EHARA**, "Theoretical Study on the Electronic Excitations of Free-base Porphyrin-Ar₂ van der Waals Complexes," *J. Chem. Phys.* **139**, 074303 (10 pages) (2013).
- S. G. ITOH, T. MORISHITA and H. OKUMURA**, "Decomposition-Order Effects of Time-Integrator on Ensemble Averages for the Nosé-Hoover Thermostat," *J. Chem. Phys.* **139**, 064103 (10 pages) (2013).
- Y. MORI and H. OKUMURA**, "Pressure-Induced Helical Structure of a Peptide Studied by Simulated Tempering Molecular Dynamics Simulations," *J. Phys. Chem. Lett.* **4**, 2079–2083 (2013).
- H. OKUMURA and S. G. ITOH**, "Transformation of a Design Peptide between the α -Helix and β -Hairpin Structures by a Helix-Strand Replica-Exchange Molecular Dynamics Simulation," *Phys. Chem. Chem. Phys.* **15**, 13852–13861 (2013).
- S. G. ITOH and H. OKUMURA**, "Replica-Permutation Method with the Suwa-Todo Algorithm beyond the Replica-Exchange Method," *J. Chem. Theory Comput.* **9**, 570–581 (2013).
- T. MORISHITA, S. G. ITOH, H. OKUMURA and M. MIKAMI**, "On-the-Fly Reconstruction of Free-Energy Profiles Using Logarithmic Mean-Force Dynamics," *J. Comput. Chem.* **34**, 1375–1384 (2013).
- S. G. ITOH and H. OKUMURA**, "Coulomb Replica-Exchange Method: Handling Electrostatic Attractive and Repulsive Forces for Biomolecules," *J. Comput. Chem.* **34**, 622–639 (2013).
- T. SAKAGUCHI and H. OKUMURA**, "Cutoff Effect in the Nosé-Poincaré and Nosé-Hoover Thermostats," *J. Phys. Soc. Jpn.* **82**, 034001 (7 pages) (2013).
- C. RUNGNIM, T. RUNGROTMONGKOL, S. HANNONGBUA and H. OKUMURA**, "Replica Exchange Molecular Dynamics Simulation of Chitosan for Drug Delivery System Based on Carbon Nanotube," *J. Mol. Graphics Modell.* **39**, 183–192 (2013).
- H. NUMURA, T. KODA and H. OKUMURA**, "Probing a Non-Biaxial Behavior of Infinitely Thin Hard Platelets," *J. Phys. Soc. Jpn.* **81**, 114003 (6 pages) (2012).
- T. ISHIDA and H. SHIROTA**, "Dicationic versus Monocationic Ionic Liquids: Distinctive Ionic Dynamics and Dynamical Heterogeneity," *J. Phys. Chem. B* **117**, 1136–1150 (2013).
- S. NISHIZAWA, J. HASEGAWA and K. MATSUDA**, "Theoretical Investigation of the β Value of the Phenylene and Phenylene Ethynylene Units by Evaluating Exchange Interaction between Organic Radicals," *Chem. Phys. Lett.* **555**, 187–190 (2013).
- T. KAWATSU and J. HASEGAWA**, "Excitation Energy Transfer in GFP-X-CFP Model Peptides (X = amino acids): Direct vs. Through-Bridge Energy Transfers," *Int. J. Quantum Chem.* **113**, 563–568 (2013).
- T. KAWATSU and J. HASEGAWA**, "Sequentially Coupled Hole-Electron Transfer Pathways for Bridge-Mediated Triplet Excitation Energy Transfer," *J. Phys. Chem. C* **116**, 23252–23256 (2012).
- J. HASEGAWA, K. J. FUJIMOTO and T. KAWATSU**, "Configuration Interaction Picture for a Molecular Environment Using Localized Molecular Orbitals: The Excited States of Retinal Proteins," *J. Chem. Theory Comput.* **8**, 4452–4461 (2012).
- T. KAWATSU, K. MATSUDA and J. HASEGAWA**, "Singlet Excitation Energy Transfer Mediated by Local Exciton Bridges," *J. Phys. Chem. C* **116**, 13865–13876 (2012).
- J. HASEGAWA, K. FUJIMOTO and H. NAKATSUJI**, "Color Tuning in Human Cone Visual Pigments: The Role of the Protein Environment," *Prog. Theor. Chem. Phys.* **26**, 489–502 (2012).
- T. MORISHITA, S. G. ITOH, H. OKUMURA and M. MIKAMI**, "On-the-Fly Reconstruction of Free-Energy Profiles Using Logarithmic Mean-Force Dynamics," *J. Comput. Chem.* **34**, 1375–1384 (2013).

Photo-Molecular Science

- K. IMURA, K. UENO, H. MISAWA and H. OKAMOTO**, "Optical Field Imaging of Elongated Rectangular Nanovoids in Gold Thin Film," *J. Phys. Chem. C* **117**, 2449–2454 (2013).
- S. KIM, K. IMURA, M. LEE, T. NARUSHIMA, H. OKAMOTO and D. H. JEONG**, "Strong Optical Coupling between Mutually Orthogonal Plasmon Oscillations in a Silver Nanosphere-Nanowire Joined System," *Phys. Chem. Chem. Phys.* **15**, 4146–4153 (2013).
- T. SHIMADA, K. IMURA, H. OKAMOTO and M. KITAJIMA**, "Spatial Distribution of Enhanced Optical Fields in One-Dimensional Linear Arrays of Gold Nanoparticles Studied by Scanning Near-Field Optical Microscopy," *Phys. Chem. Chem. Phys.* **15**, 4265–4269 (2013).

LIST OF PUBLICATIONS

- T. NARUSHIMA and H. OKAMOTO**, "Circular Dichroism Nano-Imaging of Two-Dimensional Chiral Metal Nanostructures," *Phys. Chem. Chem. Phys.* **15**, 13805–13809 (2013).
- M. KITAJIMA, T. NARUSHIMA, T. KURASHINA, A. N. ITAKURA, S. TAKAMI, A. YAMADA, K. TERAISHI and A. MIYAMOTO**, "Stress Inversion from Initial Tensile to Compressive Side during Ultrathin Oxide Growth of the Si(100) Surface," *J. Phys.: Condens. Matter* **25**, 355007 (5 pages) (2013).
- H. AKAGI, T. KASAJIMA, T. KUMADA, R. ITAKURA, A. YOKOYAMA, H. HASEGAWA and Y. OHSHIMA**, "Isotope-Selective Ionization Utilizing Molecular Alignment and Non-Resonant Multiphoton Ionization," *Appl. Phys. B: Lasers Opt.* **109**, 75–80 (2012).
- S. MIYAKE and Y. OHSHIMA**, "Injection-Seeded Optical Parametric Amplifier for Generating Chirped Nanosecond Pulses," *Opt. Express* **21**, 5269–5274 (2013).
- M. NAKAJIMA, H. TOYOSHIMA, S. SATO, K. TANAKA, K. HOSHINA, H. KOHGUCHI, Y. SUMIYOSHI, Y. OHSHIMA and Y. ENDO**, "Electronic Spectroscopy of the HCCN Radical," *J. Chem. Phys.* **138**, 164309 (10 pages) (2013).
- M. HAYASHI and Y. OHSHIMA**, "Sub-Doppler Electronic Spectra of the Benzene-(He)_n Complexes," *Chem. Phys.* **419**, 131–137 (2013).
- H. KATSUKI, Y. KAYANUMA and K. OHMORI**, "Optically Engineered Quantum Interference of Delocalized Wavefunctions in a Bulk Solid: The Example of Solid *Para*-Hydrogen," *Phys. Rev. B* **88**, 014507 (6 pages) (2013).
- T. BREDTMANN, H. KATSUKI, J. MANZ, K. OHMORI and C. STEMMLE**, "Wavepacket Interferometry for Nuclear Densities and Flux Densities," *Mol. Phys.* **111**, 1691–1696 (2013). (invited paper)
- M. NAGASAKA, E. SERDAROGLU, R. FLESCHE, E. RÜHL and N. KOSUGI**, "Structures of Mixed Argon-Nitrogen Clusters," *J. Chem. Phys.* **137**, 214305 (7 pages) (2012).
- M. NAGASAKA, H. YUZAWA, T. HORIGOME, A. P. HITCHCOCK and N. KOSUGI**, "Electrochemical Reaction of Aqueous Iron Sulfate Solutions Studied by Fe L-Edge Soft X-Ray Absorption Spectroscopy," *J. Phys. Chem. C* **117**, 16343–16348 (2013).
- H. YAMANE and N. KOSUGI**, "Substituent-Induced Intermolecular Interaction in Organic Crystals Revealed by Precise Band-Dispersion Measurements," *Phys. Rev. Lett.* **111**, 086602 (5 pages) (2013).
- H. YAMANE and N. KOSUGI**, "Hybridized Electronic States in Potassium-Doped Picene Probed by Soft X-Ray Spectroscopies," *AIP Adv.* **2**, 042114 (6 pages) (2012).
- H. YAMANE, N. KOSUGI and T. HATSUI**, "Transmission-Grating Spectrometer for Highly Efficient and High-Resolution Soft X-Ray Emission Studies," *J. Electron Spectrosc. Relat. Phenom.* **188**, 155–160 (2013).
- T. YAJIMA, S. SAKAKIBARA, S. NARITSUKA, H. YAMANE, N. KOSUGI and T. MARUYAMA**, "Formation of Carbon Nanotube/n-type 6H-SiC Heterojunction by Surface Decomposition of SiC and Its Electric Properties," *Jpn. J. Appl. Phys.* **52**, 06GD01 (4 pages) (2013).
- J. PARK, S. W. JUNG, M.-C. JUNG, H. YAMANE, N. KOSUGI and H. W. YEOM**, "Self-Assembled Nanowires with Giant Rashba Split Bands," *Phys. Rev. Lett.* **110**, 036801 (5 pages) (2013).
- S. B. SINGH, L. T. YANG, Y. F. WANG, Y. C. SHAO, C. W. CHIANG, J. W. CHIOU, K. T. LIN, S. C. CHEN, B. Y. WANG, C. H. CHUANG, D. C. LING, W. F. PONG, M.-H. TSAI, H. M. TSAI, C. W. PAO, H. W. SHIU, C. H. CHEN, H.-J. LIN, J. F. LEE, H. YAMANE and N. KOSUGI**, "Correlation between P-Type Conductivity and Electronic Structure of Cr-Deficient CuCr_{1-x}O₂ (x = 0–0.1)," *Phys. Rev. B* **86**, 241103(R) (6 pages) (2012).
- V. KIMBERG, A. LINDBLAD, J. SÖDERSTRÖM, O. TRAVNIKOVA, C. NICOLAS, Y. P. SUN, F. GEL'MUKHANOV, N. KOSUGI and C. MIRON**, "Single-Molecule X-Ray Interferometry: Controlling Coupled Electron-Nuclear Quantum Dynamics and Imaging Molecular Potentials by Ultrahigh-Resolution Resonant Photoemission and Ab Initio Calculations," *Phys. Rev. X* **3**, 011017 (16 pages) (2013).
- A. LINDBLAD, V. KIMBERG, J. SÖDERSTRÖM, C. NICOLAS, O. TRAVNIKOVA, N. KOSUGI, F. GEL'MUKHANOV and C. MIRON**, "Vibrational Scattering Anisotropy in O₂-Dynamics beyond the Born-Oppenheimer Approximation," *New J. Phys.* **14**, 113018 (19 pages) (2012).
- B. DIERKER, E. SULJOTI, K. ATAK, K. M. LANGE, N. ENGEL, R. GOLNAK, M. DANTZ, K. HODECK, M. KHAN, N. KOSUGI and E. F. AZIZ**, "Probing Orbital Symmetry in Solution: Polarization-Dependent Resonant Inelastic Soft X-Ray Scattering on Liquid Micro-Jet," *New J. Phys.* **15**, 093025 (10 pages) (2013).
- K. ATAK, N. ENGEL, K. M. LANGE, R. GOLNAK, M. GOTZ, M. SOLDATOV, J.-E. RUBENSSON, N. KOSUGI and E. F. AZIZ**, "The Chemical Bond in Carbonyl and Sulfinyl Groups Studied by Soft X-Ray Spectroscopy and Ab Initio Calculations," *ChemPhysChem* **13**, 3106–3111 (2012).
- C. EVAIN, C. SZWAJ, S. BIELAWSKI, M. E. COUPRIE, M. HOSAKA, A. MOCHIHASHI and M. KATOH**, "Suppression of Self-Pulsing Instabilities in Free-Electron Lasers Using Delayed Optical Feedback," *Phys. Rev. S. T. Accel. Beams* **15**, 040701 (7 pages) (2012).
- M. HOSAKA, N. YAMAMOTO, Y. TAKASHIMA, C. SZWAJ, M. LE PARQUIRE, C. EVAIN, S. BIELAWSKI, M. ADACHI, T. TANIKAWA, S. KIMURA, M. KATOH, M. SHIMADA and T. TAKAHASHI**, "Saturation of the Laser-Induced Narrowband Coherent Synchrotron Radiation Process: Experimental Observation at a Storage Ring," *Phys. Rev. S. T. Accel. Beams* **16**, 020701 (8 pages) (2013).
- M. ADACHI, H. ZEN, T. KONOMI, J. YAMAZAKI, K. HAYASHI and M. KATOH**, "Design and Construction of UVSOR-III," *J. Phys.: Conf. Ser.* **425**, 042013 (5 pages) (2013).
- P. THOMA, A. SCHEURING, S. WUENSCH, K. IL'IN, A. SEMENOV, H-W HUEBERS, V. JUDIN, A-S. MUELLER, N. SMALE, M. ADACHI, S. TANAKA, S. KIMURA, M. KATOH, N. YAMAMOTO, M. HOSAKA, E. ROUSSEL, C. SZWAJ, S. BIELAWSKI and M. SIEGEL**, "High-Speed Y-Ba-Cu-O Direct Detection System for Monitoring Picosecond THz Pulses," *IEEE Trans. Terahertz Sci. Tech.* **3**, 81–86 (2013).
- Y. TAIRA, H. TOYOKAWA, R. KURODA, N. YAMAMOTO, M. ADACHI, S. TANAKA and M. KATOH**, "Photon-Induced Positron Annihilation Lifetime Spectroscopy Using Ultrashort Laser-Compton-Scattered Gamma-Ray Pulses," *Rev. Sci. Instrum.* **84**, 053305 (5 pages) (2013).

- B. H. MIN, J. B. HONG, J. H. YUN, T. IIZUKA, S. KIMURA, Y. BANG and Y. S. KWON**, "Optical Properties of the Iron-Based Superconductor LiFeAs Single Crystal," *New J. Phys.* **15**, 073029 (13 pages) (2013).
- K. IMURA, T. HAJIRI, M. MATSUNAMI, S. KIMURA, M. KANEKO, T. ITO, Y. NISHI, N. K. SATO and H. S. SUZUKI**, "Angle Resolved Photoemission Spectroscopy on Mixed-Valent $\text{Sm}_{1-x}\text{Y}_x\text{S}_2$," *J. Korean Phys. Soc.* **62**, 2028–2032 (2013).
- Y. UFUKTEPE, A. H. FARHA, S. KIMURA, T. HAJIRI, F. KARADAG, M. A. AL MAMUN, A. A. ELMUSTAFA, G. MYNENI and H. E. ELSAYED-ALI**, "Structural, Electronic, and Mechanical Properties of Niobium Nitride Prepared by Thermal Diffusion in Nitrogen," *Mater. Chem. Phys.* **141**, 393–400 (2013).
- M. MATSUNAMI, T. HAJIRI, H. MIYAZAKI, M. KOSAKA and S. KIMURA**, "Strongly Hybridized Electronic Structure of YbAl_2 : An Angle-Resolved Photoemission Study," *Phys. Rev. B* **87**, 165141 (5 pages) (2013).
- T. WATANABE, K. OKIMURA, T. HAJIRI, S. KIMURA and J. SAKAI**, "Phase Selective Growth and Characterization of Vanadium Dioxide Films on Silicon Substrates," *J. Appl. Phys.* **113**, 163503 (6 pages) (2013).
- J. YAMAGUCHI, A. SEKIYAMA, M. Y. KIMURA, H. SUGIYAMA, Y. TOMIDA, G. FUNABASHI, S. KOMORI, T. BALASHOV, W. WULFHEKEL, T. ITO, S. KIMURA, A. HIGASHIYA, K. TAMASAKU, M. YABASHI, T. ISHIKAWA, S. YEO, S.-I. LEE, F. IGA, T. TAKABATAKE and S. SUGA**, "Different Evolution of Intrinsic Gap in Strongly Correlated SmB_6 in Contrast to YbB_{12} ," *New J. Phys.* **15**, 043042 (12 pages) (2013).
- V. GURITANU, P. WISSGOTT, T. WEIG, H. WINKLER, J. SICHELSCHEMIDT, M. SCHEFFLER, A. PROKOFIEV, S. KIMURA, T. IIZUKA, A. M. STRYDOM, M. DRESSEL, F. STEGLICH, K. HELD and S. PASCHEN**, "Anisotropic Optical Conductivity of the Putative Kondo Insulator CeRu_4Sn_6 ," *Phys. Rev. B* **87**, 115129 (5 pages) (2013).
- M. HOSAKA, N. YAMAMOTO, Y. TAKASHIMA, C. SZWAJ, M. LE PARQUIER, C. EVAIN, S. BIELAWSKI, M. ADACHI, H. ZEN, T. TANIKAWA, S. KIMURA, M. KATOH, M. SHIMADA and T. TAKAHASHI**, "Saturation of the Laser-Induced Narrowband Coherent Synchrotron Radiation Process: Experimental Observation at a Storage Ring," *Phys. Rev. S. T. Accel. Beams* **16**, 020701 (8 pages) (2013).
- P. THOMA, A. SCHEURING, S. WÜNSCH, K. IL'IN, A. SEMENOV, H.-W. HÜBERS, V. JUDIN, A.-S. MÜLLER, N. SMALE, M. ADACHI, S. TANAKA, S. KIMURA, M. KATOH, N. YAMAMOTO, M. HOSAKA, E. ROUSSEL, C. SZWAJ, S. BIELAWSKI and M. SIEGEL**, "High-Speed Y-Ba-Cu-O Direct Detection System for Monitoring Picosecond THz Pulses," *IEEE Trans. Terahertz Sci. Tech.* **3**, 81–86 (2013).
- J. SICHELSCHEMIDT, A. HERZOG, H. S. JEEVAN, C. GEIBEL, F. STEGLICH, T. IIZUKA and S. KIMURA**, "Far-Infrared Optical Conductivity of CeCu_2Si_2 ," *J. Phys.: Condens. Matter* **25**, 065602 (4 pages) (2013).
- S. KIMURA and H. OKAMURA**, "Infrared and Terahertz Spectroscopy of Strongly Correlated Electron Systems under Extreme Conditions," *J. Phys. Soc. Jpn.* **82**, 021004 (28 pages) (2013).
- T. HAJIRI, R. NIWA, T. ITO, M. MATSUNAMI, Y. J. SONG, S. KIMURA and Y. S. KWON**, "Polarization-Dependent Three-Dimensional Angle-Resolved Photoemission Study on LiFeAs," *J. Phys.: Conf. Ser.* **391**, 012125 (4 pages) (2012).
- H. MIYAZAKI, H. MOMIYAMA, T. HAJIRI, T. ITO, K. IMURA, M. MATSUNAMI and S. KIMURA**, "Fabrication of Single Crystalline EuO Thin Films with SrO Buffer Layer on SrTiO_3 Substrate," *J. Phys.: Conf. Ser.* **391**, 012047 (4 pages) (2012).
- S. KIMURA, T. IIZUKA, Y. MURO, J. KAJINO and T. TAKABATAKE**, "Anisotropic Gap Formation in $\text{CeM}_2\text{Al}_{10}$ ($M = \text{Ru, Os}$)," *J. Phys.: Conf. Ser.* **391**, 012030 (4 pages) (2012).
- V. GURITANU, S. SEIRO, J. SICHELSCHEMIDT, N. CAROCA-CANALES, T. IIZUKA, S. KIMURA, C. GEIBEL and F. STEGLICH**, "Optical Study of Archetypal Valence-Fluctuating Eu-Systems," *Phys. Rev. Lett.* **109**, 247207 (5 pages) (2012).
- T. HIRAHARA, N. FUKUI, T. SHIRASAWA, M. YAMADA, M. AITANI, H. MIYAZAKI, M. MATSUNAMI, S. KIMURA, T. TAKAHASHI, S. HASEGAWA and K. KOBAYASHI**, "Atomic and Electronic Structure of Ultrathin Bi(111) Films Grown on Bi_2Te_3 (111) Substrates: Evidence for a Strain-Induced Topological Phase Transition," *Phys. Rev. Lett.* **109**, 227401 (5 pages) (2012).
- F. CHEN, Q. GE, M. XU, Y. ZHANG, X. SHEN, W. JI, M. MATSUNAMI, S. KIMURA, J. HU and D. FENG**, "The Orbital Characters of Low-Energy Electronic Structure in Iron-Chalcogenide Superconductor $\text{K}_x\text{Fe}_{2-y}\text{Se}_2$," *Chin. Sci. Bull.* **57**, 3829 (7 pages) (2012).
- H. IWAYAMA, M. NAGASONO, J. R. HARRIES and E. SHIGEMASA**, "Demonstration of Up-Conversion Fluorescence from Ar Clusters in Intense Free-Electron-Laser Fields," *Opt. Express* **20**, 23174–23179 (2012).
- H. IWAYAMA, N. SISOURAT, P. LABLANQUIE, F. PENENT, J. PALAUDOUX, L. ANDRIC, J. H. D. ELAND, K. BUČAR, M. ŽITNIK, Y. VELKOV, Y. HIKOSAKA, M. NAKANO and E. SHIGEMASA**, "A Local Chemical Environment Effect in Site-Specific Auger Spectra of Ethyl Trifluoroacetate," *J. Chem. Phys.* **138**, 024306 (6 pages) (2013).
- S.-M. HUTTULA, P. LABLANQUIE, L. ANDRIC, J. PALAUDOUX, M. HUTTULA, S. SHEINERMAN, E. SHIGEMASA, Y. HIKOSAKA, K. ITO and F. PENENT**, "Decay of a 2p Inner-Shell Hole in an Ar^+ Ion," *Phys. Rev. Lett.* **110**, 113002 (5 pages) (2013).
- M. NAKANO, F. PENENT, M. TASHIRO, T. P. GROZDANOV, M. ŽITNIK, S. CARNIATO, P. SELLES, L. ANDRIC, P. LABLANQUIE, J. PALAUDOUX, E. SHIGEMASA, H. IWAYAMA, Y. HIKOSAKA, K. SOEJIMA, I. H. SUZUKI, N. KOUCHI and K. ITO**, "Single Photon K^{-2} and $\text{K}^{-1}\text{K}^{-1}$ Double Core Ionization in C_2H_{2n} ($n = 1-3$), CO, and N_2 as a Potential New Tool for Chemical Analysis," *Phys. Rev. Lett.* **110**, 163001 (5 pages) (2013).
- M. N. PIANCASTELLI, R. GUILLEMIN, M. SIMON, H. IWAYAMA and E. SHIGEMASA**, "Ultrafast Dynamics in C 1s Core-Excited CF_4 Revealed by Two-Dimensional Resonant Auger Spectroscopy," *J. Chem. Phys.* **138**, 234305 (5 pages) (2013).
- K. TAMASAKU, M. NAGASONO, H. IWAYAMA, E. SHIGEMASA, Y. INUBUSHI, T. TANAKA, K. TONO, T. TOGASHI, T. SATO, T. KATAYAMA, T. KAMESHIMA, T. HATSUI, M. YABASHI and T. ISHIKAWA**, "Double Core-Hole Creation by Sequential Attosecond Photoionization," *Phys. Rev. Lett.* **111**, 043001 (5 pages) (2013).
- M. YABASHI, H. TANAKA, T. TANAKA, H. TOMIZAWA, T. TOGASHI, M. NAGASONO, T. ISHIKAWA, J. R. HARRIES, Y. HIKOSAKA, A. HISHIKAWA, K. NAGAYA, N. SAITO, E. SHIGEMASA and K. UEDA**, "Compact XFEL and AMO Sciences: SACL A and SCSS," *J. Phys. B* **46**, 164001 (19 pages) (2013).

LIST OF PUBLICATIONS

- Y. SATO and T. TAIRA**, “Temperature Dependencies of Stimulated Emission Cross Section for Nd-Doped Solid-State Laser Materials,” *Opt. Mater. Express* **2**, 1076–1087 (2012).
- H. ISHIZUKI and T. TAIRA**, “Half-Joule Output Optical-Parametric Oscillation by Using 10-mm-Thick Periodically Poled Mg-Doped Congruent LiNbO₃,” *Opt. Express* **20**, 20002–20010 (2012).
- Y. DENG, A. SCHWARZ, H. FATTAHI, M. UEFFING, X. GU, M. OSSIANDER, T. METZGER, V. PERVAK, H. ISHIZUKI, T. TAIRA, T. KOBAYASHI, G. MARCUS, F. KRAUSZ, R. KIENBERGER and N. KARPOWICZ**, “Carrier-Envelope-Phase-Stable, 1.2 mJ, 1.5 Cycle Laser Pulses at 2.1 μm ,” *Opt. Lett.* **37**, 4973–4975 (2012).
- K. FURUI, J. HAYASHI, T. OKADA, N. NAKATSUKA, T. TAIRA, T. HORI and F. AKAMATSU**, “Study on Laser Induced Ignition for Methane-Air Mixtures with Pico-Second Pulse Duration Laser,” *Trans. Jpn. Soc. Mech. Eng. B* **78**, 2004–2014 (2012). (in Japanese)
- M. HEMMER, A. THAI, M. BAUDISCH, H. ISHIZUKI, T. TAIRA and J. BIEGERT**, “18- μJ Energy, 160-kHz Repetition Rate, 250-MW Peak Power Mid-IR OPCPA,” *Chin. Opt. Lett.* **11**, 013202 (3 pages) (2013).
- V. KEMLIN, D. JEGOUSO, J. DEBRAY, P. SEGONDS, B. BOULANGER, B. MENAERT, H. ISHIZUKI and T. TAIRA**, “Widely Tunable Optical Parametric Oscillator in a 5 mm-thick 5%MgO:PPLN Partial Cylinder,” *Opt. Lett.* **38**, 860–862 (2013).
- M. TSUNEKANE, N. PAVEL and T. TAIRA**, “Simultaneously 3-Point Ignitable, Nd:YAG/Cr:YAG Ceramic Micro-Lasers,” *Rev. Laser Eng.* **41**, 119–124 (2013). (in Japanese)
- M. TSUNEKANE and T. TAIRA**, “High Peak Power, Passively Q-Switched Yb:YAG/Cr:YAG Micro-Lasers,” *IEEE J. Quantum Electron.* **49**, 454–461 (2013).
- Y. SATO, J. AKIYAMA and T. TAIRA**, “Orientation Control of Micro-Domains in Anisotropic Laser Ceramics,” *Opt. Mater. Express* **3**, 829–841 (2013).
- R. BHANDARI and T. TAIRA**, “Palm-Top Size Megawatt Peak Power Ultraviolet Microlaser,” *Opt. Eng.* **52**, 076102 (6 pages) (2013).
- P. ZUO, T. FUJI, T. HORIO, S. ADACHI and T. SUZUKI**, “Simultaneous Generation of Ultrashort Pulses at 158 and 198 nm in a Single Filamentation Cell by Cascaded Four-Wave Mixing in Ar,” *Appl. Phys. B: Lasers Opt.* **108**, 815–819 (2012).
- Y. NOMURA, H. SHIRAI, K. ISHII, N. TSURUMACHI, A. A. VORONIN, A. M. ZHELTIKOV and T. FUJI**, “Phase-Stable Sub-Cycle Mid-Infrared Conical Emission from Filamentation in Gases,” *Opt. Express* **20**, 24741–24747 (2012).
- T. FUJI and Y. NOMURA**, “Generation of Phase-Stable Sub-Cycle Mid-Infrared Pulses from Filamentation in Nitrogen,” *Appl. Sci.* **3**, 122–138 (2013).
- Y. NOMURA, Y. T. WANG, T. KOZAI, H. SHIRAI, A. YABUSHITA, C. W. LUO, S. NAKANISHI and T. FUJI**, “Single-Shot Detection of Mid-Infrared Spectra by Chirped-Pulse Upconversion with Four-Wave Difference Frequency Generation in Gases,” *Opt. Express* **21**, 18249–18254 (2013).
- M. TSUBOUCHI, M. NAGAI and Y. OHSHIMA**, “Terahertz Tomography of a Photo-Induced Carrier Based on Pump-Probe Spectroscopy Using Counterpropagation Geometry,” *Opt. Lett.* **37**, 3528–3530 (2012).
- M. TSUBOUCHI and T. KUMADA**, “Development of High-Efficiency Etalons with an Optical Shutter for Terahertz Laser Pulses,” *Opt. Express* **20**, 28500–28506 (2012).
- Y. IMAMURA and T. HATSUI**, “Theoretical Study on Valence Excitations of Multiply Ionized States for Envelope Measurement of X-Ray Free-Electron-Laser Pulses,” *Phys. Rev. A* **87**, 043413 (5 pages) (2013).
- T. R. M. BARENDS, L. FOUCAR, R. L. SHOEMAN, S. BARI, S. W. EPP, R. HARTMANN, G. HAUSER, M. HUTH, C. KIESER, L. LOMB, K. MOTOMURA, K. NAGAYA, C. SCHMIDT, R. STRECKER, D. ANIELSKI, R. BOLL, B. ERK, H. FUKUZAWA, E. HARTMANN, T. HATSUI, P. HOLL, Y. INUBUSHI, T. ISHIKAWA, S. KASSEMAYER, C. KAISER, F. KOECK, N. KUNISHIMA, M. KURKA, D. ROLLES, B. RUDEK, A. RUDENKO, T. SATO, C.-D. SCHROETER, H. SOLTAU, L. STRUEDER, T. TANAKA, T. TOGASHI, K. TONO, J. ULLRICH, S. YASE, S. WADA, M. YAO, M. YABASHI, K. UEDA and I. SCHLICHTING**, “Anomalous Signal from S Atoms in Protein Crystallographic Data from an X-Ray Free-Electron Laser,” *Acta Crystallogr., Sect. D: Biol. Crystallogr.* **69**, 838–842 (2013).
- T. TANAKA, S. GOTO, T. HARA, T. HATSUI, H. OHASHI, K. TOGAWA, M. YABASHI and H. TANAKA**, “Undulator Commissioning by Characterization of Radiation in X-Ray Free Electron Lasers,” *Phys. Rev. S. T. Accel. Beams* **15**, 110701 (10 pages) (2012).
- K. OKAMOTO, T. KOZAWA, K. OIKAWA, T. HATSUI, M. NAGASONO, T. KAMESHIMA, T. TOGASHI, K. TONO, M. YABASHI, H. KIMURA, Y. SENBA, H. OHASHI, R. FUJIYOSHI and T. SUMIYOSHI**, “Effect of Ultrahigh-Density Ionization of Resist Films on Sensitivity Using Extreme-Ultraviolet Free-Electron Laser,” *Appl. Phys. Express* **5**, 096701 (3 pages) (2012).
- Y. INUBUSHI, K. TONO, T. TOGASHI, T. SATO, T. HATSUI, T. KAMESHIMA, K. TOGAWA, T. HARA, T. TANAKA, H. TANAKA, T. ISHIKAWA and M. YABASHI**, “Determination of the Pulse Duration of an X-Ray Free Electron Laser Using Highly Resolved Single-Shot Spectra,” *Phys. Rev. Lett.* **109**, 144801 (4 pages) (2012).
- T. ISHIKAWA, H. AOYAGI, T. ASAKA, Y. ASANO, N. AZUMI, T. BIZEN, H. EGO, K. FUKAMI, T. FUKUI, Y. FURUKAWA, S. GOTO, H. HANAOKI, T. HARA, T. HASEGAWA, T. HATSUI, A. HIGASHIYA, T. HIRONO, N. HOSODA, M. ISHII, T. INAGAKI, Y. INUBUSHI, T. ITOGA, Y. JOTI, M. KAGO, T. KAMESHIMA, H. KIMURA, Y. KIRIHARA, A. KIYOMICHI, T. KOBAYASHI, C. KONDO, T. KUDO, H. MAESAKA, X. M. MARÉCHAL, T. MASUDA, S. MATSUBARA, T. MATSUMOTO, T. MATSUSHITA, S. MATSUI, M. NAGASONO, N. NARIYAMA, H. OHASHI, T. OHATA, T. OHSHIMA, S. ONO, Y. OTAKE, C. SAJI, T. SAKURAI, T. SATO, K. SAWADA, T. SEIKE, K. SHIRASAWA, T. SUGIMOTO, S. SUZUKI, S. TAKAHASHI, H. TAKEBE, K. TAKESHITA, K. TAMASAKU, H. TANAKA, R. TANAKA, T. TANAKA, T. TOGASHI, K. TOGAWA, A. TOKUHISA, H. TOMIZAWA, K. TONO, S. WU, M. YABASHI, M. YAMAGA, A. YAMASHITA, K. YANAGIDA, C. ZHANG, T. SHINTAKE, H. KITAMURA and N. KUMAGAI**, “A Compact X-Ray Free-Electron Laser Emitting in the Sub-Ångström Region,” *Nat. Photonics* **6**, 540–544 (2012).
- Y. IMAMURA and T. HATSUI**, “Interplay of Strong Chemical Bonds and the Repulsive Coulomb Force in the Metastable States of Triply Ionized Homonuclear Molecules: A Theoretical Study of N₂³⁺ and O₂³⁺,” *Phys. Rev. A* **85**, 012524 (6 pages) (2012).

T. KUDO, K. TONO, M. YABASHI, T. TOGASHI, T. SATO, Y. INUBUSHI, M. OMODANI, Y. KIRIHARA, T. MATSUSHITA, K. KOBAYASHI, M. YAMAGA, S. UCHIYAMA and T. HATSUI, "A Photodiode Amplifier System for Pulse-by-Pulse Intensity Measurement of an X-Ray Free Electron Laser," *Rev. Sci. Instrum.* **83**, 043108 (6 pages) (2012).

Materials Molecular Science

O. SEKIZAWA, T. URUGA, M. TADA, K. NITTA, K. KATO, H. TANIDA, 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, T. YOKOYAMA and Y. IWASAWA, "New XAFS Beamline for Structural and Electronic Dynamics of Nanoparticle Catalysts in Fuel Cells under Operating Conditions," *J. Phys.: Conf. Ser.* **430**, 012020 (6 pages) (2013).

K. EGUCHI, Y. TAKAGI, T. NAKAGAWA and T. YOKOYAMA, "Passivating Effect of Si(111)-($\sqrt{3}\times\sqrt{3}$)Ag and Si₃N₄/Si(111)-(8×8) Buffer Layers," *J. Phys.: Conf. Ser.* **430**, 012129 (6 pages) (2013).

T. YOKOYAMA and K. EGUCHI, "Anisotropic Thermal Expansion and Cooperative Invar/Anti-Invar Effects in Mn Alloys," *Phys. Rev. Lett.* **110**, 075901 (5 pages) (2013).

T. NAKAGAWA, Y. TAKAGI, T. YOKOYAMA, T. METHFESSEL, S. DIEHL and H.-J. ELMERS, "Giant Magnetic Anisotropy Energy and Coercivity in Fe Island and Atomic Wire on W(110)," *Phys. Rev. B* **86**, 144418 (5 pages) (2012).

T. YOKOYAMA, "Path Integral Effective Classical Potential Method Applied to Anharmonicity and Quantum Effects in Thermal Expansion of Invar Alloy," *e-J. Surf. Sci. Nanotech.* **10**, 486–492 (2012).

T. SAIDA, O. SEKIZAWA, N. ISHIGURO, K. UESUGI, M. HOSHINA, T. URUGA, S. OHKOSHI, T. YOKOYAMA and M. TADA, "4D Visualization of Structures/Chemical States of Pt/C Cathode Catalyst Layers in Polymer Electrolyte Fuel Cells by 3D-Laminography-XAFS," *Angew. Chem., Int. Ed.* **51**, 10311–10314 (2012).

M. TADA, S. ZHANG, S. MALWADKAR, N. ISHIGURO, J. SOGA, Y. NAGAI, K. TEZUKA, H. IMOTO, S. O.-Y.-MATSUO, S. OHKOSHI and Y. IWASAWA, "The Active Phase of Nickel/Ordered Ce₂Zr₂O_x Catalysts with a Discontinuous ($x = 7-8$) in Methane Steam Reforming," *Angew. Chem., Int. Ed.* **51**, 9361–9365 (2012). [HOT PAPER]

T. SAIDA, O. SEKIZAWA, N. ISHIGURO, K. UESUGI, M. HOSHINA, T. URUGA, S. OHKOSHI, T. YOKOYAMA and M. TADA, "4D Visualization of a Cathode Catalyst Layer in a Polymer Electrolyte Fuel Cell by 3D-Laminography-XAFS," *Angew. Chem., Int. Ed.* **51**, 10311–10314 (2012).

S. ZHANG, S. MURATSUGU, N. ISHIGURO, S. OHKOSHI and M. TADA, "Perovskite NaCeTi₂O₆-Supported Ni Catalysts for CH₄ Steam Reforming," *ChemCatChem* **4**, 1783–1790 (2012). [Back Cover of Issue 11].

S. MURATSUGU, Z. WENG, H. NAKAI, K. ISOBE, T. SASAKI and M. TADA, "Surface-Assisted Transfer Hydrogenation Catalysis on a γ -Al₂O₃-Supported Ir Dimer," *Phys. Chem. Chem. Phys.* **14**, 16023–16031 (2012).

S. MURATSUGU and M. TADA, "Molecularly Imprinted Ru Complex Catalyst Systems Integrated on Oxide Surfaces," *Acc. Chem. Res.* **46**, 300–311 (2013).

S. NAGAMATSU, T. ARAI, M. YAMAMOTO, T. OHKURA, H. OYANAGI, T. ISHIZAKA, H. KAWANAMI, T. URUGA, M. TADA and Y. IWASAWA, "Potential-Dependent Restructuring and Hysteresis in the Structural and Electronic Transformations of Pt/C, Au(Core)-Pt(Shell)/C, and Pd(Core)-Pt(Shell)/C Cathode Catalysts in Polymer Electrolyte Fuel Cells Characterized by *in situ* X-Ray Absorption Fine Structure," *J. Phys. Chem. C* **117**, 13094–13107 (2013).

L. WANG, S. YAMAMOTO, S. MALWADKAR, S. NAGAMATSU, T. SASAKI, K. HAYASHIZAKI, M. TADA and Y. IWASAWA, "Direct Synthesis of Phenol from Benzene and O₂, Regulated by NH₃ on Pt/β and Pt-Re/ZSM-5 Catalysts," *ChemCatChem* **5**, 2203–2206 (2013).

M. WAKI, S. MURATSUGU and M. TADA, "Rate Enhancement for Hexose Sugar Oxidation on an Ethynylpyridine-Functionalized Pt/Al₂O₃ Catalyst with Induced Chirality," *Chem. Commun.* **49**, 7283–7285 (2013). [Inside Back Cover].

S. MURATSUGU, M. H. LIM, T. ITOH, W. THUMRONGPATANARKS, M. KONDO, S. MASAOKA, T. S. A. HOR and M. TADA, "Dispersed Ru Nanoclusters Transformed from a Grafted Trinuclear Ru Complex on SiO₂ for Selective Alcohol Oxidation," *Dalton Trans.* **42**, 12611–12619 (2013). [Inside Front Cover].

O. SEKIZAWA, T. URUGA, M. TADA, K. NITTA, K. KATO, H. TANIDA, 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, T. YOKOYAMA and Y. IWASAWA, "New XAFS Beamline for Structural and Electronic Dynamics of Nanoparticle Catalysts in Fuel Cells under Operating Conditions," *J. Phys.: Conf. Ser.* **430**, 012020 (6 pages) (2013).

T. TSUJI, T. URUGA, K. NITTA, K. KAWAMURA, M. MIZUMAKI, M. SUZUKI, O. SEKIZAWA, N. ISHIGURO, M. TADA, H. OHASHI, H. YAMAZAKI, H. YUMOTO, T. KOYAMA, Y. SENBA, T. TAKEUCHI, Y. TERADA, N. NARIYAMA, K. TAKESHITA, A. FUJIWARA, S. GOTO, M. YAMAMOTO, M. TAKATA and T. ISHIKAWA, "Development of Fast Scanning Microscopic XAFS Measurement System," *J. Phys.: Conf. Ser.* **430**, 012019 (6 pages) (2013).

M. SUZUKI, N. KAWAMURA, M. MIZUMAKI, Y. TERADA, T. URUGA, A. FUJIWARA, H. YAMAZAKI, H. YUMOTO, T. KOYAMA, Y. SENBA, T. TAKEUCHI, H. OHASHI, N. NARIYAMA, K. TAKESHITA, H. KIMURA, T. MATSUSHITA, Y. FURUKAWA, T. OHATA, Y. KONDO, J. ARIAKE, J. RICHTER, P. FONS, O. SEKIZAWA, N. ISHIGURO, M. TADA, S. GOTO, M. YAMAMOTO, M. TAKATA and T. ISHIKAWA, "A Hard X-Ray Nanospectroscopy Station at SPring-8 BL39XU," *J. Phys.: Conf. Ser.* **430**, 012017 (4 pages) (2013).

LIST OF PUBLICATIONS

- T. NAITO, T. KARASUDANI, K. OHARA, T. TAKANO, Y. TAKAHASHI, T. INABE, K. FURUKAWA and T. NAKAMURA**, "Simultaneous Control of Carriers and Localized Spins with Light in Organic Materials," *Adv. Mater.* **24**, 6153–6157 (2012).
- D. SAKAMAKI, A. ITO, K. FURUKAWA, T. KATO, M. SHIRO and K. TANAKA**, "A Polymacrocyclic Oligoarylamine with a Pseudobeltane Motif: Towards a Cylindrical Multispin System," *Angew. Chem., Int. Ed.* **51**, 12776–12781 (2012).
- S. JIN, X. DING, X. FENG, M. SUPUR, K. FURUKAWA, S. TAKAHASHI, M. ADDICOAT, M. E. EL-KHOULY, T. NAKAMURA, S. IRLE, S. FUKUZUMI, A. NAGAI and D. JIANG**, "Charge Dynamics in A Donor–Acceptor Covalent Organic Framework with Periodically Ordered Bicontinuous Heterojunctions," *Angew. Chem., Int. Ed.* **52**, 2017–2021 (2013).
- Y. FUNASAKO, T. INAGAKI, T. MOCHIDA, T. SAKURAI, H. OHTA, K. FURUKAWA and T. NAKAMURA**, "Organometallic Ionic Liquids from Alkyloctamethylferrocenium Cations: Thermal Properties, Crystal Structures, and Magnetic Properties," *Dalton Trans.* **42**, 8317–8327 (2013).
- Y. MORINAKA, S. SATO, A. WAKAMIYA, H. NIKAWA, N. MIZOROGI, F. TANABE, M. MURATA, K. KOMATSU, K. FURUKAWA, T. KATO, S. NAGASE, T. AKASAKA and Y. MURATA**, "X-Ray Observation of a Helium Atom and Placing a Nitrogen Atom Inside He@C₆₀ and He@C₇₀," *Nat. Commun.* **4**, 1554 (5 pages) (2013).
- M. KUBO, Y. SHINMURA, N. ISHIYAMA, T. KAJI and M. HIRAMOTO**, "Invertible Organic Photovoltaic Cells with Heavily-Doped Organic/Metal Ohmic Contacts," *Appl. Phys. Express* **5**, 092302 (3 pages) (2012).
- N. ISHIYAMA, M. KUBO, T. KAJI and M. HIRAMOTO**, "Tandem Photovoltaic Cells Formed in Single Fullerene Films by Impurity Doping," *Appl. Phys. Lett.* **101**, 233303 (3 pages) (2012).
- Y. SHINMURA, M. KUBO, T. KAJI and M. HIRAMOTO**, "Improved Photovoltaic Characteristics by MoO₃-Doping to Thick Hole Transporting Films," *Jpn. J. Appl. Phys.* **52**, 04CR12 (4 pages) (2013).
- K. YOKOYAMA, T. KAJI and M. HIRAMOTO**, "Double Co-Deposited Layered Organic Photovoltaic Cells with Sensitivity through the Visible to Near-Infrared," *Jpn. J. Appl. Phys.* **52**, 04CR06 (4 pages) (2013).
- N. ISHIYAMA, T. YOSHIOKA, T. KAJI and M. HIRAMOTO**, "Tuning of Barrier Parameters of *n*-Type Schottky Junction in Photovoltaic Co-Deposited Films by Doping," *Appl. Phys. Express* **6**, 012301 (3 pages) (2013).
- N. ISHIYAMA, M. KUBO, T. KAJI and M. HIRAMOTO**, "Tandem Organic Solar Cells Formed in Co-Deposited Films by Doping," *Org. Electron.* **14**, 1793–1796 (2013).
- X. LIU, Y. XU, Z. GUO, A. NAGAI and D. JIANG**, "Super Absorbent Conjugated Microporous Polymers: A Synergistic Structural Effect on Exceptional Uptake of Amines," *Chem. Commun.* **49**, 3233–3235 (2013).
- A. NAGAI, X. CHEN, X. FENG, X. DING, Z. GUO and D. JIANG**, "A Squaraine-Linked Covalent Organic Framework," *Angew. Chem., Int. Ed.* **52**, 3770–3774 (2013). (Hot Paper)
- S. JIN, X. DING, X. FENG, M. SUPUR, K. FURUKAWA, S. TAKAHASHI, M. ADDICOAT, M. E. EL-KHOULY, T. NAKAMURA, S. IRLE, S. FUKUZUMI, A. NAGAI and D. JIANG**, "Charge Dynamics in a Donor–Acceptor Covalent Organic Framework with Periodically Ordered Bicontinuous Heterojunctions," *Angew. Chem., Int. Ed.* **52**, 2017–2021 (2013). (Inside Cover)
- X. CHEN, M. ADDICOAT, S. IRLE, A. NAGAI and D. JIANG**, "Control Crystallinity and Porosity of Covalent Organic Frameworks through Managing Interlayer Interactions Based on Self-Complementary π -Electronic Force," *J. Am. Chem. Soc.* **135**, 546–549 (2013).
- Y. XU, A. NAGAI and D. JIANG**, "Core-Shell Conjugated Microporous Polymers: A New Strategy for Exploring Color-Tunable and -Controllable Light Emissions," *Chem. Commun.* **49**, 1591–1593 (2013). (Inside Cover)
- X. FENG, Y. DONG and D. JIANG**, "Star-Shaped Two-Dimensional Covalent Organic Frameworks," *CrystEngComm* **15**, 1508–1511 (2013). (Themed Issue for COFs)
- X. DING, X. FENG, A. SAEKI, S. SEKI, A. NAGAI and D. JIANG**, "Conducting Metallophthalocyanine 2D Covalent Organic Frameworks: The Role of Central Metals in Controlling π -Electronic Functions," *Chem. Commun.* **48**, 8952–8954 (2012).
- M. TANIO and K. NISHIMURA**, "Intramolecular Allosteric Interaction in the Phospholipase C- δ 1 Pleckstrin Homology Domain," *Biochim. Biophys. Acta, Proteins Proteomics* **1834**, 1034–1043 (2013).
- M. TANIO and K. NISHIMURA**, "Analysis of the Phospholipase C- δ 1 Pleckstrin Homology Domain Using Native Polyacrylamide Gel Electrophoresis," *Anal. Biochem.* **431**, 106–114 (2012).
- K. YAZAWA, F. SUZUKI, Y. NISHIYAMA, T. OHATA, A. AOKI, K. NISHIMURA, H. KAJI and T. ASAKURA**, "Determination of Accurate ¹H Positions of Alanine Tripeptide with Anti-Parallel and Parallel β -Sheet Structures by High Resolution ¹H Solid State NMR and GIPAW Chemical Shift Calculation," *Chem. Commun.* **48**, 11199–11201 (2012).
- A. TSUTSUMI, N. JAVKHLANTUGS, A. KIRA, M. UMEYAMA, I. KAWAMURA, K. NISHIMURA, K. UEDA and A. NAITO**, "Structure and Orientation of Bovine Lactoferrampin in the Mimetic Bacterial Membrane as Revealed by Solid-State NMR and Molecular Dynamics Simulation," *Biophys. J.* **103**, 1–9 (2012).
- E. HASEGAWA, E. TOSAKA, A. YONEOKA, Y. TAMURA, S. TAKIZAWA, M. TOMURA and Y. YAMASHITA**, "Photoinduced Electron Transfer Reaction of α -Bromomethyl Substituted Benzocyclic β -Keto Esters with Amines: Selective Reaction Pathways Depending on Nature of Amine Radical Cations," *Res. Chem. Intermed.* **39**, 247–267 (2013).
- K. SUGANUMA, K. HORIUCHI, H. MATSUDA, H. N. CHENG, A. AOKI and T. ASAKURA**, "NMR Analysis and Chemical Shift Calculations of Poly(lactic acid) Dimer Model Compounds with Different Tacticities," *Polym. J.* **44**, 838–844 (2012).
- K. YAZAWA, F. SUZUKI, Y. NISHIYAMA, T. OHATA, A. AOKI, K. NISHIMURA, H. KAJI, T. SHIMIZU and T. ASAKURA**, "Determination of Accurate ¹H Positions of an Alanine Tripeptide with Anti-Parallel and Parallel β -Sheet Structures by High Resolution ¹H Solid State NMR and GIPAW Chemical Shift Calculation," *Chem. Commun.* **48**, 11199–11201 (2012).

- D. AYTEMIZ, W. SAKIYAMA, Y. SUZUKI, N. NAKAIZUMI, R. TANAKA, Y. OGAWA, Y. TAKAGI, Y. NAKAZAWA and T. ASAKURA, "Small-Diameter Knitted Silk Vascular Grafts (3mm Diameter) with a Double-Raschel Knitted Silk Tube Coated with Silk Fibroin Sponge," *Adv. Healthcare Mater.* **2**, 361–368 (2013).
- N. KUBOYAMA, H. KIBA, K. ARAI, R. UCHIDA, Y. TANIMOTO, U. K. BHAWAL, Y. ABIKO, S. MIYAMOTO, D. KNIGHT, T. ASAKURA and N. NISHIYAMA, "Silk Fibroin-Based Scaffolds for Bone Regeneration," *J. Biomed. Mater. Res. Part B: Appl. Biomater.* **101**, 295–302 (2013).
- T. ASAKURA, Y. SUZUKI, Y. NAKAZAWA, K. YAZAWA, G. P. HOLLAND and J. L. YARGER, "Silk Structure Studied with Nuclear Magnetic Resonance," *Prog. Nucl. Magn. Reson. Spectrosc.* **69**, 23–68 (2013).
- Y. SUZUKI, Y. NAKAZAWA, D. AYTEMIZ, T. KOMATSU, K. MIYAZAKI, S. YAMASAKI and T. ASAKURA, "Development of Silk/Polyurethane Small-diameter Vascular Graft by Electrospinning," *Seikei-Kakou* **25**, 181–187 (2013). (in Japanese)
- T. ASAKURA, "From Determination of Silk Structure to Application of Silk to Vascular Graft," *SEN'I GAKKAISHI* **69**, 145–148 (2013). (in Japanese)
- S. MIYAMOTO, R. KOYANAGI, Y. NAKAZAWA, A. NAGANO, Y. ABIKO, M. INADA, C. MIYAURA and T. ASAKURA, "Bombyx Mori Silk Fibroin Scaffolds for Bone Regeneration Studied by Bone Differentiation Experiment," *J. Biosci. Bioeng.* **115**, 575–578 (2013).

Life and Coordination-Complex Molecular Science

- T. ISHIDA and S. AONO, "A Model Theoretical Study on Ligand Exchange Reactions of CoaA," *Phys. Chem. Chem. Phys.* **15**, 6139–6148 (2013).
- H. SAWAI, M. YAMANAKA, H. SUGIMOTO, Y. SHIRO and S. AONO, "Structural Basis for the Transcriptional Regulation of Heme Homeostasis in *Lactococcus lactis*," *J. Biol. Chem.* **287**, 30755–30768 (2012).
- M. S. CHANDAK, T. NAKAMURA, K. MAKABE, T. TAKENAKA, A. MUKAIYAMA, T. K. CHAUDHURI, K. KATO and K. KUWAJIMA, "The H/D-Exchange Kinetics of the *Escherichia coli* Co-Chaperonin GroES Studied by 2D NMR and DMSO-Quenched Exchange Methods," *J. Mol. Biol.* **425**, 2541–2560 (2013).
- M. S. CHANDAK, T. NAKAMURA, T. TAKENAKA, T. K. CHAUDHURI, M. YAGI-UTSUMI, J. CHEN, K. KATO and K. KUWAJIMA, "The Use of Spin Desalting Columns in DMSO-Quenched H/D-Exchange NMR Experiments," *Protein Sci.* **22**, 486–491 (2013).
- K. MAKABE, T. NAKAMURA and K. KUWAJIMA, "Structural Insights into the Stability Perturbations Induced by N-Terminal Variation in Human and Goat α -Lactalbumin," *Protein Eng., Des. Sel.* **26**, 165–170 (2013).
- A. MUKAIYAMA, T. NAKAMURA, K. MAKABE, K. MAKI, Y. GOTO and K. KUWAJIMA, "Native-State Heterogeneity of β_2 -Microglobulin as Revealed by Kinetic Folding and Real-Time NMR Experiments," *J. Mol. Biol.* **425**, 257–272 (2013).
- A. MUKAIYAMA, T. NAKAMURA, K. MAKABE, K. MAKI, Y. GOTO and K. KUWAJIMA, "The Molten Globule of β_2 -Microglobulin Accumulated at pH 4 and Its Role in Protein Folding," *J. Mol. Biol.* **425**, 273–291 (2013).
- T. NAKAMURA, T. AIZAWA, R. KARIYA, S. OKADA, M. DEMURA, K. KAWANO, K. MAKABE and K. KUWAJIMA, "Molecular Mechanisms of the Cytotoxicity of Human α -Lactalbumin Made Lethal to Tumor Cells (HAMLET) and Other Protein-Oleic Acid Complexes," *J. Biol. Chem.* **288**, 14408–14416 (2013).
- H. SEKIGUCHI, A. NAKAGAWA, K. MORIYA, K. MAKABE, K. ICHIYANAGI, S. NOZAWA, T. SATO, S. ADACHI, K. KUWAJIMA, M. YOHDA and Y.C. SASAKI, "ATP Dependent Rotational Motion of Group II Chaperonin Observed by X-Ray Single Molecule Tracking," *PLoS One* **8**, e64176 (2013).
- M. YAGI-UTSUMI, T. KUNIHARA, T. NAKAMURA, Y. UEKUSA, K. MAKABE, K. KUWAJIMA and K. KATO, "NMR Characterization of the Interaction of GroEL with Amyloid β as a Model Ligand," *FEBS Lett.* **587**, 1605–1609 (2013).
- Y. UEKUSA, S. MIMURA, H. SASAKAWA, E. KURIMOTO, E. SAKATA, S. OLIVIER, H. YAGI, F. TOKUNAGA, K. IWAI and K. KATO, "Backbone and Side Chain ^1H , ^{13}C , and ^{15}N Assignments of the Ubiquitin-Like Domain of Human HOIL-1L, an Essential Component of Linear Ubiquitin Chain Assembly Complex," *Biomol. NMR Assignments* **6**, 177–180 (2012).
- S. KONDO, H. YAGI, Y. KAMIYA, A. ITO, M. KUHARA, A. KUDOH, N. TAKAHASHI and K. KATO, "N-Glycosylation Profiles of Chicken Immunoglobulin Y Glycoproteins Expressed by Different Production Vehicles," *J. Glycomics Lipidomics* **S5**, 002 (2012).
- M. YAGI-UTSUMI, S. YOSHIKAWA, Y. YAMAGUCHI, Y. NISHI, E. KURIMOTO, Y. ISHIDA, T. HOMMA, J. HOSEKI, Y. NISHIKAWA, T. KOIDE, K. NAGATA and K. KATO, "NMR and Mutational Identification of the Collagen-Binding Site of the Chaperone Hsp47," *PLoS One* **7**, e45930 (2012).
- D. FUJITA, K. SUZUKI, S. SATO, M. YAGI-UTSUMI, Y. YAMAGUCHI, N. MIZUNO, T. KUMASAKA, M. TAKATA, M. NODA, S. UCHIYAMA, K. KATO and M. FUJITA, "Protein Encapsulation within Synthetic Molecular Hosts," *Nat. Commun.* **3**, 1093 (2012).
- T. FUJII, M. URUSHIHARA, H. KASHIDA, H. ITO, X. LIANG, M. YAGI-UTSUMI, K. KATO and H. ASANUMA, "Reversed Assembling of Dyes in an RNA Duplex Compared with Those in DNA," *Chem. –Euro. J.* **18**, 13304–13313 (2012).
- T. YAMAGUCHI, T. UNO, Y. UEKUSA, M. YAGI-UTSUMI and K. KATO, "Ganglioside-Embedding Small Bicelles for Probing Membrane-Landing Processes of Intrinsically Disordered Proteins," *Chem. Commun.* **49**, 1235–1237 (2013).
- Y. KAMIYA, K. YANAGI, T. KITAJIMA, T. YAMAGUCHI, Y. CHIBA and K. KATO, "Application of Metabolic ^{13}C Labeling in Conjunction with High-Field Nuclear Magnetic Resonance Spectroscopy for Comparative Conformational Analysis of High Mannose-Type Oligosaccharides," *Biomolecules* **3**, 108–123 (2013).
- M. YAGI-UTSUMI, Y. YAMAGUCHI, P. BOONSRI, T. IGUCHI, K. OKEMOTO, S. NATORI and K. KATO, "Stable Isotope-Assisted NMR Characterization of Interaction between Lipid A and Sarcotoxin IA, a Cecropin-Type Antibacterial Peptide," *Biochem. Biophys. Res. Commun.* **431**, 136–140 (2013).

LIST OF PUBLICATIONS

- G. MONDAL, H. YAGI, K. KATO and B. P. CHATTERJEE**, “Multidimensional HPLC Analysis of N-Linked Glycans of Serum Alpha-1-Acid Glycoprotein in Chronic Hepatitis B and Hepatitis B-Induced Liver Cirrhosis Patients,” *Trends Carbohydr. Res.* **5**, 11–19 (2013).
- M. SUGIYAMA, H. SAHASHI, E. KURIMOTO, S. TAKATA, H. YAGI, K. KANAI, E. SAKATA, Y. MINAMI, K. TANAKA and K. KATO**, “Spatial Arrangement and Functional Role of α Subunits of Proteasome Activator PA28 in Hetero-Oligomeric Form,” *Biochem. Biophys. Res. Commun.* **432**, 141–145 (2013).
- S. KITAZAWA, T. KAMEDA, M. YAGI-UTSUMI, K. SUGASE, N. J. BAXTER, K. KATO, M. P. WILLIAMSON and R. KITAHARA**, “Solution Structure of the Q41N Variant of Ubiquitin as a Model for the Alternatively Folded N₂ State of Ubiquitin,” *Biochemistry* **52**, 1874–1885 (2013).
- K. KUMOI, T. SATOH, K. MURATA, T. HIROMOTO, T. MIZUSHIMA, Y. KAMIYA, M. NODA, S. UCHIYAMA, H. YAGI and K. KATO**, “An Archaeal Homolog of Proteasome Assembly Factor Functions as a Proteasome Activator,” *PLoS One* **8**, e60294 (2013).
- T. FUJIMORI, Y. KAMIYA, K. NAGATA, K. KATO and N. HOSOKAWA**, “Endoplasmic Reticulum Lectin XTP3-B Inhibits Endoplasmic Reticulum-Associated Degradation of a Misfolded α 1-Antitrypsin Variant,” *FEBS J.* **8**, 1563–1575 (2013).
- M. S. CHANDAK, T. NAKAMURA, T. TAKENAKA, T. K. CHAUDHURI, M. YAGI-UTSUMI, J. CHEN, K. KATO and K. KUWAJIMA**, “The Use of Spin Desalting Columns in DMSO-Quenched H/D-Exchange NMR Experiments,” *Protein Sci.* **22**, 486–491 (2013).
- T. YAMAGUCHI, Y. KAMIYA, Y.-M. CHOO, S. YAMAMOTO and K. KATO**, “Terminal Spin Labeling of a High-Mannose-Type Oligosaccharide for Quantitative NMR Analysis of Its Dynamic Conformation,” *Chem. Lett.* **42**, 544–546 (2013).
- M. YAGI-UTSUMI, T. KUNIHARA, T. NAKAMURA, Y. UEKUSA, K. MAKABE, K. KUWAJIMA and K. KATO**, “NMR Characterization of the Interaction of GroEL with Amyloid β as a Model Ligand,” *FEBS Lett.* **587**, 1605–1609 (2013).
- S.-J. YOON, N. UTKINA, M. SADILEK, H. YAGI, K. KATO and S. HAKOMORI**, “Self-Recognition of High-Mannose Type Glycans Mediating Adhesion of Embryonal Fibroblasts,” *Glycoconjugate J.* **30**, 485–496 (2013).
- N. NISHIDA, M. YAGI-UTSUMI, F. MOTOJIMA, M. YOSHIDA, I. SHIMADA and K. KATO**, “Nuclear Magnetic Resonance Approaches for Characterizing Interactions between the Bacterial Chaperonin GroEL and Unstructured Proteins,” *J. Biosci. Bioeng.* **116**, 160–164 (2013).
- E. KURIMOTO, K. KUROKI, Y. YAMAGUCHI, M. YAGI-UTSUMI, T. IGAKI, T. IGUCHI, K. MAENAKA and K. KATO**, “Structural and Functional Mosaic Nature of MHC Class I Molecules in Their Peptide-Free Form,” *Mol. Immunol.* **55**, 393–399 (2013).
- M. S. CHANDAK, T. NAKAMURA, K. MAKABE, T. TAKENAKA, A. MUKAIYAMA, T. K. CHAUDHURI, K. KATO and K. KUWAJIMA**, “The H/D-Exchange Kinetics of the *Escherichia coli* Co-Chaperonin GroES Studied by 2D NMR and DMSO-Quenched Exchange Methods,” *J. Mol. Biol.* **425**, 2541–2560 (2013).
- T. KURAHASHI and H. FUJII**, “Comparative Spectroscopic Studies of Iron(III) and Manganese(III) Salen Complexes Having a Weakly-Coordinating Triflate Axial Ligand,” *Bull. Chem. Soc. Jpn.* **85**, 940–947 (2012). (BCSJ Award Article)
- Z. CONG, S. YANAGISAWA, T. KURAHASHI, T. OGURA, S. NAKASHIMA and H. FUJII**, “Synthesis, Characterization, and Reactivity of Hypochlorito-Iron(III) Porphyrin Complexes,” *J. Am. Chem. Soc.* **134**, 20617–20620 (2012).
- T. KURAHASHI and H. FUJII**, “Unique Ligand Radical Character of an Activated Cobalt Salen Catalyst that is Generated by Aerobic Oxidation of a Cobalt(II) Salen Complex,” *Inorg. Chem.* **52**, 3908–3919 (2013).
- H. ITO, M. SUMII, A. KAWANABE, Y. FAN, Y. FURUTANI, L. S. BROWN and H. KANDORI**, “Comparative FTIR Study of a New Fungal Rhodopsin,” *J. Phys. Chem. B* **116**, 11881–11889 (2012).
- Y. FURUTANI, K. FUJIWARA, T. KIMURA, T. KIKUKAWA, M. DEMURA and H. KANDORI**, “Dynamics of Dangling Bonds of Water Molecules in *pharaonis* Halorhodopsin during Chloride Ion Transportation,” *J. Phys. Chem. Lett.* **3**, 2964–2969 (2012).
- Y. FURUTANI, H. SHIMIZU, Y. ASAI, T. FUKUDA, S. OIKI and H. KANDORI**, “ATR-FTIR Spectroscopy Revealed the Different Vibrational Modes of the Selectivity Filter Interacting with K⁺ and Na⁺ in the Open and Collapsed Conformations of the KcsA Potassium Channel,” *J. Phys. Chem. Lett.* **3**, 3806–3810 (2012).
- Y. FURUTANI, T. OKITSU, L. REISSIG, M. MIZUNO, M. HOMMA, A. WADA, Y. MIZUTANI and Y. SUDO**, “Large Spectral Change Due to Amide Modes of a β -Sheet upon the Formation of an Early Photointermediate of Middle Rhodopsin,” *J. Phys. Chem. B* **117**, 3449–3458 (2013).
- H. GUO, T. KIMURA and Y. FURUTANI**, “Distortion of the Amide-I and -II Bands of an α -Helical Membrane Protein, *pharaonis* Halorhodopsin, Depends on Thickness of Gold Films Utilized for Surface-Enhanced Infrared Absorption Spectroscopy,” *Chem. Phys.* **419**, 8–16 (2013).
- Y. FURUTANI, T. KIMURA and K. OKAMOTO**, “Development of a Rapid Buffer-Exchange System for Time-Resolved ATR-FTIR Spectroscopy with the Step-Scan Mode,” *Biophysics* **9**, 123–129 (2013).
- Y. M. A. YAMADA, S. M. SARKAR and Y. UOZUMI**, “Amphiphilic Self-Assembled Polymeric Copper Catalyst to Parts per Million Levels: Click Chemistry,” *J. Am. Chem. Soc.* **134**, 9285–9290 (2012).
- Y. M. A. YAMADA, H. OHTA, Y. YUYAMA and Y. UOZUMI**, “Polymeric Bimetallic Catalyst-Promoted In-Water Dehydrative Alkylation of Ammonia and Amines with Alcohols,” *Synthesis* **45**, 2093–2100 (2012).
- R. HUDSON, G. HAMASAKA, T. OSAKO, Y. M. A. YAMADA, C.-J. LI, Y. UOZUMI and A. MOORES**, “Highly Efficient Iron(0) Nanoparticle-Catalyzed Hydrogenation in Water in Flow,” *Green Chem.* **15**, 2141–2148 (2012).
- A. OHTAKA, E. SAKAGUCHI, T. YAMAGUCHI, G. HAMASAKA, Y. UOZUMI, O. SHIMOMURA and R. NOMURA**, “A Recyclable ‘Boomerang’ Linear Polystyrene-Stabilized Pd Nanoparticles for the Suzuki Coupling Reaction of Aryl Chlorides in Water,” *ChemCatChem* **5**, 2167–2169 (2012).

- T. ITOH, M. KONDO, M. KANAIKE and S. MASAOKA**, "Arene-Perfluoroarene Interactions for Crystal Engineering of Metal Complexes: Controlled Self-Assembly of Paddle-Wheel Dimers," *CrystEngComm* **15**, 6122–6126 (2013).
- S. MURATSUGU, M. H. LIM, T. ITOH, W. THUMRONGPATANARAKS, M. KONDO, S. MASAOKA, T. S. A. HOR and M. TADA**, "Dispersed Ru Nanoclusters Transformed from a Grafted Trinuclear Ru Complex on SiO₂ for Selective Alcohol Oxidation," *Dalton Trans.* **42**, 12611–12619 (2013).
- M. KOBAYASHI, S. MASAOKA and K. SAKAI**, "Photoinduced Hydrogen Evolution from Water Based on a Z-Scheme Photosynthesis by a Simple Platinum(II) Terpyridine Derivative," *Angew. Chem., Int. Ed.* **51**, 7431–7434 (2012).
- S. TAKIZAWA, E. RÉMOND, F. A. ARTEAGA, Y. YOSHIDA, V. SRIDHARAN, J. BAYARDON, S. JUGÉ and H. SASAI**, "P-Chirogenic Organocatalysts: Application to the Aza-Morita-Baylis-Hillman (Aza-MBH) Reaction of Ketimines," *Chem. Commun.* **49**, 8392–8394 (2013).
- V. SRIDHARAN, L. FAN, S. TAKIZAWA, T. SUZUKI and H. SASAI**, "Pd(II)-SDP-Catalyzed Enantioselective 5-Exo-Dig Cyclization of γ -Alkynoic Acids: Application to the Synthesis of Functionalized Dihydrofuran-2(3H)-ones Containing a Chiral Quaternary Carbon Center," *Org. Biomol. Chem.* **11**, 5936–5943 (2013).
- S. TAKIZAWA, F. A. ARTEAGA, Y. YOSHIDA, M. SUZUKI and H. SASAI**, "Organocatalyzed Formal [2+2] Cycloaddition of Ketimines with Allenates: Facile Access to Azetidines with a Chiral Tetrasubstituted Carbon Stereogenic Center," *Org. Lett.* **15**, 4142–4145 (2013).
- S. TAKIZAWA, T. M.-N. NGUYEN, A. GROSSMANN, M. SUZUKI, D. ENDERS and H. SASAI**, "Facile Synthesis of α -Methylidene- γ -Butyrolactones: Intramolecular Rauhut-Currier Reaction Promoted by Chiral Acid-Base Organocatalysts," *Tetrahedron* **69**, 1202–1209 (2013).
- S. TAKIZAWA, F. A. ARTEAGA, Y. YOSHIDA, J. KODERA, Y. NAGATA and H. SASAI**, "Vanadium-Catalyzed Enantioselective Friedel-Crafts-Type Reactions," *Dalton Trans.* **42**, 11787–11790 (2013).
- R. K. M. GABR, T. HATAKEYAMA, K. TAKENAKA, S. TAKIZAWA, Y. OKADA, M. NAKAMURA and H. SASAI**, "DFT Study on 5-Endo-Trig-Type Cyclization of 3-Alkenoic Acids Using Pd-SPRIX Catalyst: Importance of the Rigid Spiro Framework for Both Selectivity and Reactivity," *Chem. –Eur. J.* **19**, 9518–9525 (2013).
- T. KUSAKABE, T. TAKAHASHI, R. SHEN, A. IKEDA, Y. D. DHAGE, Y. KANNO, Y. INOUE, H. SASAI, T. MOCHIDA and K. KATO**, "Carbonylation of Propargyl Carbamates with Palladium(II) Bisoxazoline Catalysts: Efficient Synthesis of 5-Methyl-3(2H)-furanones," *Angew. Chem., Int. Ed.* **52**, 7845–7849 (2013).
- E. RÉMOND, J. BAYARDON, S. TAKIZAWA, Y. ROUSSELIN, H. SASAI and S. JUGÉ**, "o-(Hydroxyalkyl) P-Chirogenic Phosphines as Functional Chiral Lewis Bases," *Org. Lett.* **15**, 1870–1873 (2013).
- T. SUZUKI, Y. ISHIZAKA, K. GHOZATI, D.-Y. ZHOU, K. ASANO and H. SASAI**, "Enantioselective Multicatalytic Synthesis of α -Benzyl- β -hydroxyindan-1-ones," *Synthesis* **45**, 2134–2136 (2013).
- Y. YOSHIDA, S. TAKIZAWA and H. SASAI**, "Design and Synthesis of Spiro Bis(1,2,3-triazolium) Salts As Chiral Ionic Liquids," *Tetrahedron: Asymmetry* **23**, 843–851 (2012).
- G. DISTEFANO, H. SUZUKI, M. TSUJIMOTO, S. ISODA, S. BRACCO, A. COMOTTI, P. SOZZANI, T. UEMURA and S. KITAGAWA**, "Highly Ordered Alignment of a Vinyl Polymer by Host–Guest Cross-Polymerization," *Nat. Chem.* **5**, 335–341 (2013).
- T. UEMURA, G. WASHINO, N. YANAI and S. KITAGAWA**, "Controlled Encapsulation of Photo-Responsive Macromolecules in Porous Coordination Polymer," *Chem. Lett.* **42**, 222–223 (2013).
- N. YANAI, T. UEMURA and S. KITAGAWA**, "Behavior of Binary Guests in a Porous Coordination Polymer," *Chem. Mater.* **24**, 4744–4749 (2012).
- Y. IKEZOE, G. WASHINO, T. UEMURA, S. KITAGAWA and H. MATSUI**, "Autonomous Motors of a Metal-Organic Framework Powered by Reorganization of Self-Assembled Peptides at Interfaces," *Nat. Mater.* **11**, 1081–1085 (2012).
- H. IRIEDA, T. MORITA, K. MAKI, M. HOMMA, H. AIBA and Y. SUDO**, "Photo-Induced Regulation of the Chromatic Adaptive Gene Expression by Anabaena Sensory Rhodopsin," *J. Biol. Chem.* **287**, 32485–32493 (2012).
- L. REISSIG, T. IWATA, T. KIKUKAWA, M. DEMURA, N. KAMO, H. KANDORI and Y. SUDO**, "The Influence of Halide Binding on the Hydrogen Bonding Network in the Active Site of *Salinibacter* Sensory Rhodopsin I," *Biochemistry* **51**, 8802–8813 (2012).
- Y. FURUTANI, T. OKITSU, L. REISSIG, M. MIZUNO, M. HOMMA, A. WADA, Y. MIZUTANI and Y. SUDO**, "Large Spectral Change due to Amide Modes of a β -Sheet upon the Formation of an Early Photointermediate of Middle Rhodopsin," *J. Phys. Chem. B* **117**, 3449–3458 (2013).
- A. MORI, J. YAGASAKI, M. HOMMA, L. REISSIG and Y. SUDO**, "Investigation of the Chromophore Binding Cavity in the 11-*cis* Acceptable Microbial Rhodopsin MR," *Chem. Phys.* **419**, 23–29 (2013).
- Y. SUDO, A. OKAZAKI, H. ONO, J. YAGASAKI, S. SUGO, M. KAMIYA, L. REISSIG, K. INOUE, K. IHARA, H. KANDORI, S. TAKAGI and S. HAYASHI**, "A Blue-Shifted Light-Driven Proton Pump for Neural Silencing," *J. Biol. Chem.* **288**, 20624–20632 (2013).
- T. TSUKAMOTO, K. INOUE, H. KANDORI and Y. SUDO**, "Thermal and Spectroscopic Characterization of a Proton Pumping Rhodopsin from an Extreme Thermophile," *J. Biol. Chem.* **288**, 21581–21592 (2013).

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- A. MUKAIYAMA, T. NAKAMURA, K. MAKABE, K., MAKI, Y. GOTO and K. KUWAJIMA, "Native-State Heterogeneity of β 2-Microglobulin as Revealed by Kinetic Folding and Real-Time NMR Experiments," *J. Mol. Biol.* **425**, 257–272 (2013).
- A. MUKAIYAMA, T. NAKAMURA, K. MAKABE, K., MAKI, Y. GOTO and K. KUWAJIMA, "The Molten Globule of β 2-Microglobulin Accumulated at pH 4 and Its Role in Protein Folding," *J. Mol. Biol.* **425**, 273–291 (2013).
- M. S. CHANDAK, T. NAKAMURA, K. MAKABE, T. TAKENAKA, A. MUKAIYAMA, T. K. CCAUDHURI, K. KATO and K. KUWAJIMA, "The H/D-Exchange Kinetics of the *Escherichia coli* Co-Chaperonin GroES Studied by 2D NMR and DMSO-Quenched Exchange Methods," *J. Mol. Biol.* **425**, 2541–2560 (2013).
- L. BANCHI, G. COSTAGLIOLA, A. ISHIZAKI and P. GIORDA, "An Analytical Continuation Approach for Evaluating Emission Lineshapes of Molecular Aggregates and the Adequacy of Multichromophoric Förster Theory," *J. Chem. Phys.* **138**, 184107 (14 pages) (2013).
- Y. SHIKANO, "The Counterfactual Process in Weak Values," *Phys. Scr.* **T151**, 014015 (3 pages) (2012).
- Y. SHIKANO, T. WADA and J. HORIKAWA, "The Discrete-Time Quantum Walk as a Stochastic Process in Quantum Mechanics," *Phys. Scr.* **T151**, 014016 (5 pages) (2012).
- H. KOBAYASHI, G. PUENTES and Y. SHIKANO, "Extracting Joint Weak Values from Two-Dimensional Spatial Displacements," *Phys. Rev. A* **86**, 053805 (4 pages) (2012).
- T. HORIKIRI, Y. MATSUO, Y. SHIKANO, A. LOFFLER, S. HOFLING, A. FORCHEL and Y. YAMAMOTO, "Temperature Dependence of Highly Excited Exciton Polaritons in Semiconductor Microcavities," *J. Phys. Soc. Jpn.* **82**, 084709 (10 pages) (2013).
- Y. SUSA, Y. SHIKANO and A. HOSOYA, "Reply to "Comment on "Optimal Probe Wave Function of Weak-Value Amplification,""" *Phys. Rev. A* **87**, 046102 (2 pages) (2013).
- M. GONULOL, A. EKREM, Y. SHIKANO and O. E. MUSTECAPELIOGLU, "Survival Probability in a Quantum Walk on a One-Dimensional Lattice with Partially Absorbing Traps," *J. Comput. Theor. Nanosci.* **10**, 1596–1600 (2013).
- A. U. C. HARDAL, P. XUE, Y. SHIKANO, O. E. MUSTECAPELIOGLU and B. C. SANDERS, "Discrete-Time Quantum Walk with Nitrogen-Vacancy Centers in Diamond Coupled to a Superconducting Flux Qubit," *Phys. Rev. A* **88**, 022303 (11 pages) (2013).
- H. M. YAMAMOTO, M. NAKANO, M. SUDA, Y. IWASA, M. KAWASAKI and R. KATO, "A Strained Organic Field-Effect Transistor with a Gate-Tunable Superconducting Channel," *Nat. Commun.* **4**, 2379 (7 pages) (2013).
- H. M. YAMAMOTO, J. UENO and R. KATO, "Critical Behavior of a Filling-Controlled Mott-Transition Observed at an Organic Field-Effect-Transistor Interface," *Eur. Phys. J. Special Topics* **222**, 1057–1063 (2013).
- N. TAKUBO, N. TAJIMA, H. M. YAMAMOTO, H. CUI and R. KATO, "Lattice Distortion Stabilizes the Photoinduced Metallic Phase in the Charge-Ordered Organic Salts (BEDT-TTF)₃X₂ (X = ReO₄, ClO₄)," *Phys. Rev. Lett.* **110**, 227401 (2013).
- Y. KOSAKA, H. M. YAMAMOTO, A. TAJIMA, A. NAKAO, H. CUI and R. KATO, "Supramolecular Ni(dmit)₂ Salts with Halopyridinium Cations—Development of Multifunctional Molecular Conductors with the Use of Competing Supramolecular Interactions," *CrystEngComm* **15**, 3200–3211 (2013).
- N. TAKUBO, N. TAJIMA, H. M. YAMAMOTO and R. KATO, "Observation of Photo-Induced Insulator-to-Metal Transition in Charge-Ordered α -(BEDT-TTF)₂I₃ Thin Crystal by Simultaneous Transport and Optical Measurement," *J. Lumin.* **137**, 237–240 (2013).
- D. WATANABE, M. YAMASHITA, S. TONEGAWA, Y. OSHIMA, H. M. YAMAMOTO, R. KATO, I. SHEIKIN, K. BEHNIA, T. TERASHIMA, S. UJI, T. SHIBAUCHI and Y. MATSUDA, "Novel Pauli-Paramagnetic Quantum Phase in a Mott Insulator," *Nat. Commun.* **3**, 1090 (6 pages) (2012).
- T. KISS, A. CHAINANI, H. M. YAMAMOTO, T. MIYAZAKI, T. AKIMOTO, T. SHIMOJIMA, K. ISHIZUKA, S. WATANABE, C.-T. CHEN, A. FUKAYA, R. KATO and S. SHIN, "Quasiparticles and Fermi Liquid Behaviour in an Organic Metal," *Nat. Commun.* **3**, 1089 (6 pages) (2012).
- T. MURAHASHI, S. KIMURA, K. TAKASE, S. OGOSHI and K. YAMAMOTO, "Bridging π -Coordination of Pyrrole and Indole over a Pd^I–Pd^I Bond," *Chem. Commun.* **49**, 4310–4312 (2013).
- T. MURAHASHI, K. TAKASE, K. USUL, S. KIMURA, M. FUJIMOTO, T. UEMURA, S. OGOSHI and K. YAMAMOTO, "Trinuclear Palladium Addition to Unsaturated Carbo-cycles," *Dalton Trans.* **42**, 10626–10632 (2013).
- F. ANGER, R. SCHOLZ, E. ADAMSKI, K. BROCH, A. GERLACH, Y. SAKAMOTO, T. SUZUKI and F. SCHREIBER, "Optical Properties of Fully and Partially Fluorinated Rubrene in Films and Solution," *Appl. Phys. Lett.* **102**, 013308 (5 pages) (2013).
- E. KAYAHARA, T. IWAMOTO, T. SUZUKI and S. YAMAGO, "Selective Synthesis of [6]-, [8]-, and [10]Cycloparaphenylenes," *Chem. Lett.* **42**, 621–623 (2013).
- H. KON and T. NAGATA, "New Ternary Ligands Consisting of a N₄ Bridging Ligand and Two Terpyridines, and Their Co(II) and Ni(II) Dinuclear Complexes. Structure, Redox Properties, and Reaction with Acid," *Dalton Trans.* **42**, 5697–5705 (2013).
- H. YAMAZAKI, T. UENO, K. AISO, M. HIRAHARA, T. AOKI, T. NAGATA, S. IGARASHI and M. YAGI, "Synthesis, Characterization and Heterogeneous Catalysis for Water Oxidation of a Di-Manganese Complex with 4'-(4-pyridyl)-2,2':6',2''-Terpyridine," *Polyhedron* **52**, 455–460 (2013).
- H. YAMAZAKI, S. IGARASHI, T. NAGATA and M. YAGI, "Substituent Effects on Core Structures and Heterogeneous Catalytic Activities of Mn^{III}(μ -O)₂Mn^{IV} Dimers with 2,2':6',2''-Terpyridine Derivative Ligands for Water Oxidation," *Inorg. Chem.* **51**, 1530–1539 (2012).

- O. SOPHIPHUN, J. WITTAYAKUN, R. N. DHITAL, S. HAESUWANNAKIJ, A. MURUGADOSS and H. SAKURAI**, "Gold/Palladium Bimetallic Alloy Nanoclusters Stabilized by Chitosan as Highly Efficient and Selective Catalyst for Homocoupling of Arylboronic Acid," *Aust. J. Chem.* **65**, 1238–1243 (2012).
- P. KAEWMATI, E. SOMSOOK, R. N. DHITAL and H. SAKURAI**, "Aerobic Oxygenation of Phenylboronic Acid Promoted by Thiol under Gold-Free Conditions: A Warning against Gold Nanoparticle Catalysis," *Tetrahedron Lett.* **53**, 6104–6106 (2012).
- H. KITAHARA and H. SAKURAI**, "Addition versus Oxygenative Cleavage: Two Contradictory Reactivities in the Reaction of *N*-Benzyl 4-Pentenylamine Catalyzed by Colloidal Nanogold under Aerobic Conditions," *Chem. Lett.* **41**, 1328–1330 (2012).
- B. M. SCHMIDT, S. SEKI, B. TOPOLINSKI, K. OHKUBO, S. FUKUZUMI, H. SAKURAI and D. LENTZ**, "Electronic Properties of Trifluoromethylated Corannulenes," *Angew. Chem., Int. Ed.* **51**, 11385–11388 (2012).
- R. N. DHITAL, C. KAMONSATIKUL, E. SOMSOOK, K. BOBUATONG, M. EHARA and H. SAKURAI**, "Low-Temperature Carbon–Chlorine Bond Activation by Bimetallic Gold/Palladium Alloy Nanoclusters: An Application to Ullmann Coupling," *J. Am. Chem. Soc.* **134**, 20250–20253 (2012).
- A. MURUGADOSS, K. OKUMURA and H. SAKURAI**, "Bimetallic AuPd Nanocluster Catalysts with Controlled Atomic Gold Distribution for Oxidative Dehydrogenation of Tetralin," *J. Phys. Chem. C* **116**, 26776–26783 (2012).
- J. MACK, Y. MORITA, S. HIGASHIBAYASHI, H. SAKURAI and N. KOBAYASHI**, "Magnetic Circular Dichroism Spectroscopy and Electronic Structures of C_3 Symmetry Buckybowls," *Chem. Phys. Lett.* **556**, 188–194 (2013).
- S. KARANJIT, K. BOBUATONG, R. FUKUDA, M. EHARA and H. SAKURAI**, "Mechanism of the Aerobic Oxidation of Methanol to Formic Acid on Au₈: A DFT Study," *Int. J. Quantum Chem.* **113**, 428–436 (2013).
- R. N. DHITAL, C. KAMONSATIKUL, E. SOMSOOK, Y. SATO and H. SAKURAI**, "Aryl Iodides as Strong Inhibitor for Gold and Gold-Based Bimetallic *quasi*-Homogeneous Catalysis," *Chem. Commun.* **49**, 2542–2544 (2013).
- B. M. SCHMIDT, B. TOPOLINSKI, S. HIGASHIBAYASHI, T. KOJIMA, M. KAWANO, D. LENTZ and H. SAKURAI**, "The Synthesis of Hexafluorosumanene and its Congeners," *Chem. –Eur. J.* **19**, 3282–3286 (2013).
- B. B. SHRESTHA, S. KARANJIT, G. PANDA, S. HIGASHIBAYASHI and H. SAKURAI**, "Synthesis of Substituted Sumanenes by Aromatic Electrophilic Substitution Reactions," *Chem. Lett.* **42**, 386–388 (2013).
- K. MAEYAMA, T. TSUKAMOTO, M. SUZUKI, S. HIGASHIBAYASHI and H. SAKURAI**, "Nanosized Palladium-Catalyzed Suzuki–Miyaura Coupling Polymerization: Synthesis of Soluble Aromatic Poly(ether ketone)s," *Polymer J.* **45**, 401–405 (2013).
- S. HIGASHIBAYASHI, S. ONOGI, H. K. SRIVASTAVA, G. N. SASTRY, Y.-T. WU and H. SAKURAI**, "Stereo-electronic Effect of Curved Aromatic Structure Favouring the Unexpected *Endo* Conformation of Benzylic Substituted Sumanene," *Angew. Chem., Int. Ed.* **52**, 7314–7316 (2013).
- S. KUNISHIGE, M. KAWABATA, M. BABA, T. YAMANAKA, Y. MORITA, S. HIGASHIBAYASHI and H. SAKURAI**, "Jet Spectroscopy of Buckybowl: Electronic and Vibrational Structures in the S_0 and S_1 States of Triphenylene and Sumanene," *J. Chem. Phys.* **139**, 044313 (8 pages) (2013).