

**Theoretical and Computational Molecular Science**

- Y. MORI, K. OKAZAKI, T. MORI, K. KIM and N. MATSUBAYASHI**, "Learning Reaction Coordinates via Cross-Entropy Minimization: Application to Alanine Dipeptide," *J. Chem. Phys.* **153**, 054115 (8 pages) (2020).
- Y. NAM, M. KALATHINGAL, S. SAITO and J. Y. LEE**, "Tautomeric Effect of Histidine on  $\beta$ -Sheet Formation of Amyloid  $\beta$  1–40: 2D-IR Simulations," *Biophys. J.* **119**, 831–842 (2020).
- S.-I. KODA and S. SAITO**, "An Alternative Interpretation of the Slow KaiB-KaiC Binding of the Cyanobacterial Clock Proteins," *Sci. Rep.* **10**, 10439 (7 pages) (2020).
- T. MORI and S. SAITO**, "Dissecting the Dynamics during Enzyme Catalysis: A Case Study of Pin1 Peptidyl-Prolyl Isomerase," *J. Chem. Theory Comput.* **16**, 3396–3407 (2020).
- T. KATO, K. NOBUSADA and S. SAITO**, "Inverse Kohn-Sham Equations Derived from the Density Equation Theory," *J. Phys. Soc. Jpn.* **89**, 024301 (15 pages) (2020).
- S. SAITO, M. HIGASHI and G. R. FLEMING**, "Site-Dependent Fluctuations Optimize Electronic Energy Transfer in the Fenna-Matthews-Olson Protein," *J. Phys. Chem. B* **123**, 9762–9772 (2019).
- S. H. GAMOU, K. SHIMOSE, R. ENOKI, E. MINAMITANI, A. SHIOTARI, Y. KOTANI, K. TOYOKI, T. NAKAMURA, Y. SUGIMOTO, M. KOHDA, J. NITTA and S. MIWA**, "Detection of Spin-Transfer from Metal to Molecule by Magnetoresistance Measurement," *Nano Lett.* **20**, 75–80 (2020). DOI: 10.1021/acs.nanolett.9b03110
- K. SHIMIZU, W. LIU, W. LI, S. KASAMATSU, Y. ANDO, E. MINAMITANI and S. WATANABE**, "First-Principles Study of Li-Ion Distribution at  $\gamma$ -Li<sub>3</sub>PO<sub>4</sub>/Metal Interfaces," *Phys. Rev. Mater.* **4**, 015402 (10 pages) (2020). DOI: 10.1103/PhysRevMaterials.4.015402
- Z. NI, E. MINAMITANI, K. KAWAHARA, R. ARAFUNE, C.-L. LIN, N. TAKAGI and S. WATANABE**, "Mechanically Tunable Spontaneous Vertical Charge Redistribution in Few-Layer WTe<sub>2</sub>," *J. Phys. Chem. C* **124**, 2008–2012 (2020). DOI: 10.1021/acs.jpcc.9b10423
- X. YANG, Y. YUAN, Y. PENG, E. MINAMITANI, L. PENG, J.-J. XIAN, W.-H. ZHANG and Y.-S. FU**, "Observation of Short-Range Yu-Shiba-Rusinov States with Threefold Symmetry in Layered Superconductor 2H-NbSe<sub>2</sub>," *Nanoscale* **12**, 8174–8179 (2020). DOI: 10.1039/d0nr01383h
- K. IWATA, T. MIYAMACHI, E. MINAMITANI and F. KOMORI**, "Sensing Surface Lattice Strain with Kondo Resonance of Single Co Adatom," *Appl. Phys. Lett.* **116**, 051604 (4 pages) (2020). DOI: 10.1063/1.5142064
- P. MANO, E. MINAMITANI and S. WATANABE**, "Straintronic Effect for Superconductivity Enhancement in Li-Intercalated Bilayer MoS<sub>2</sub>," *Nanoscale Adv.* **3**, 3150–3155 (2020). DOI: 10.1039/D0NA00420K
- N. H. SHIMADA, E. MINAMITANI and S. WATANABE**, "Theoretical Prediction of Superconductivity in Monolayer h-BN Doped with Alkaline-Earth Metals (Ca, Sr, Ba)," *J. Phys.: Condens. Matter* **32**, 435002 (9 pages) (2020). DOI: 10.1088/1361-648X/aba674
- T. P. NGUYEN and A. ISHIZAKI**, Precise Determination of Excitation Energies in Condensed-Phase Molecular Systems Based on Exciton-Polariton Measurements," *Phys. Rev. Res.* **1**, 033019 (9 pages) (2019).
- A. ISHIZAKI**, "Prerequisites for Relevant Spectral Density and Convergence of Reduced Density Matrices at Low Temperatures," *J. Phys. Soc. Jpn.* **89**, 015001 (2 pages) (2020).
- T. P. NGUYEN, Q. T. PHAM and A. ISHIZAKI**, "Controlling the Nonadiabatic Electron-Transfer Reaction Rate through Molecular-Vibration Polaritons in the Ultrastrong Coupling Regime," *Sci. Rep.* **10**, 7318 (11 pages) (2020).
- Y. FUJIHASHI, R. SHIMIZU and A. ISHIZAKI**, "Generation of Pseudo-Sunlight via Quantum Entangled Photons and the Interaction with Molecules," *Phys. Rev. Res.* **2**, 023256 (7 pages) (2020).
- A. ISHIZAKI**, "Probing Excited-State Dynamics with Quantum Entangled Photons: Correspondence to Coherent Multidimensional Spectroscopy," *J. Chem. Phys.* **153**, 051102 (7 pages) (2020). [Editor's Pick]
- H. TSUNOYAMA, A. OHNUMA, K. TAKAHASHI, A. VELLOTH, M. EHARA, N. ICHIKUNI, M. TABUCHI and A. NAKAJIMA**, "Enhanced Oxygen Reduction Activity of Platinum Subnanocluster Catalysts through Charge Redistribution," *Chem. Commun.* **55**, 12603–12606 (2019).
- Y.-X. ZHAO, M.-Y. LI, P. ZHAO, M. EHARA and X. ZHAO**, "New Insight into U@C<sub>80</sub>: Missing U@D<sub>3</sub>(31921)-C<sub>80</sub> and Nuanced Enantiomers of U@C<sub>1</sub>(28324)-C<sub>80</sub>," *Inorg. Chem.* **58**, 14159–14166 (2019).
- Y. MAEDA, H. MURAKOSHI, H. TAMBO, P. ZHAO, K. KURODA, M. YAMADA, X. ZHAO, S. NAGASE and M. EHARA**, "Thermodynamic Control of Quantum Defects on Single-Walled Carbon Nanotubes," *Chem. Commun.* **55**, 13757–13760 (2019).
- T. YANG, C. KONG, S. YANG, Z. YANG, S. YANG and M. EHARA**, "Reaction Mechanism, Norbornene and Ligand Effects, and Origins of Meta-Selectivity of Pd/Norbornene-Catalyzed C–H Activation," *Chem. Sci.* **11**, 113–125 (2020).
- P. ZHAO, B. BOEKFA, T. NISHITOBA, N. TSUNOJI, T. SANO, T. YOKOI, M. OGURA and M. EHARA**, "Theoretical Study on <sup>31</sup>P NMR Chemical Shifts of Phosphorus-Modified CHA Zeolites," *Microporous Mesoporous Mater.* **294**, 109908 (12 pages) (2020).
- M.-Y. LI, Y.-X. ZHAO, Y.-B. HAN, K. YUAN, S. NAGASE, M. EHARA and X. ZHAO**, "Theoretical Investigation of the Key Roles in Fullerene-Formation Mechanisms: Enantiomer and Enthalpy," *ACS Appl. Nano Mater.* **3**, 547–554 (2020).
- S. HU, P. ZHAO, W. SHEN, M. EHARA, Y. XIE, T. AKASAKA and X. LU**, "Crystallographic Characterization of Er<sub>2</sub>C<sub>2</sub>@C<sub>80-88</sub>: Cluster Stretching with Cage Elongation," *Inorg. Chem.* **59**, 1940–1946 (2020).
- H. YOSHIDA, M. EHARA, U. DEVA PRIYAKUMAR, T. KAWAI and T. NAKASHIMA**, "Enantioseparation and Chiral Induction in Ag<sub>29</sub> Nanoclusters with Intrinsic Chirality," *Chem. Sci.* **11**, 2394–2400 (2020).
- S. SARTYOUNGKUL, M. EHARA and H. SAKURAI**, "Time-Dependent Density Functional Theory Investigation of Excited State Intramolecular Proton Transfer in Tris(2-hydroxyphenyl)triazasumanene," *J. Phys. Chem. A* **124**, 1227–1234 (2020).
- T. SADHUKHAN, A. JUNKAEW, P. ZHAO, H. MIURA, T. SHISHIDO and M. EHARA**, "Importance of the Pd and Surrounding Site in Hydrosilylation of Internal Alkynes by Palladium-Gold Alloy Catalyst," *Organometallics* **39**, 528–537 (2020).

## LIST OF PUBLICATIONS

- M.-Y. LI, Z.-B. GAO, Y.-B. HAN, Y.-X. ZHAO, K. YUAN, S. NAGASE, M. EHARA and X. ZHAO**, “Potential Molecular Semiconductor Devices: Cyclo- $C_n$  ( $n = 10$  and  $14$ ) with Higher Stabilities and Aromaticities than Acknowledged Cyclo- $C_{18}$ ,” *Phys. Chem. Chem. Phys.* **22**, 4823–4831 (2020).
- M. PROMKATKAEW, S. SURAMITR, T. KARPKIRD, M. EHARA and S. HANNONGBUA**, “DFT/TD-DFT Investigation on the Photoinduced Electron Transfer of Diruthenium and Viologen Complexes,” *J. Lumin.* **222**, 117121 (9 pages) (2020).
- Q. M. PHUNG, Y. KOMORI, T. YANAI, T. SOMMERFELD and M. EHARA**, “Combination of a Voronoi-Type Complex Absorbing Potential with the XMS-CASPT2 Method and Pilot Applications,” *J. Chem. Theory Comput.* **16**, 2606–2616 (2020).
- B. ZHU, M. EHARA and S. SAKAKI**, “Propene Oxidation Catalysis and Electronic Structure of  $M_{55}$  Particle ( $M = \text{Pd}$  or  $\text{Rh}$ ): Differences and Similarities between  $\text{Pd}_{55}$  and  $\text{Rh}_{55}$ ,” *Phys. Chem. Chem. Phys.* **22**, 11783–11796 (2020).
- H. YOSHIDA, J. KUMAR, M. EHARA, Y. OKAJIMA, F. ASANOMA, T. KAWAI and T. NAKASHIMA**, “Impact of Enantiomeric Ligand Composition on the Photophysical Properties of Chiral  $\text{Ag}_{29}$  Nanoclusters,” *Bull. Chem. Soc. Jpn.* **93**, 834–840 (2020).
- T. SHIRAOGAWA and M. EHARA**, “Theoretical Design of Photofunctional Molecular Aggregates for Optical Properties: An Inverse Design Approach,” *J. Phys. Chem. C* **124**, 13329–13337 (2020).
- M.-Y. LI, Y.-X. ZHAO, Y.-B. HAN, K. YUAN, K.-N. ZHANG, Y.-Q. CHEN, M. EHARA, S. NAGASE and X. ZHAO**, “Covalent Interactions Depended on the Distances between Metals and Fullerenes for Thermodynamically Stable  $M@C_{78}$  ( $M = \text{La}, \text{Ce}, \text{and Sm}$ )”, *Inorg. Chem. Front.* **7**, 2538–2547 (2020).
- H. OKUMURA and S. G. ITOH**, “Molecular Dynamics Simulations of Amyloid- $\beta$ (16-22) Peptide Aggregation at Air-Water Interfaces,” *J. Chem. Phys.* **151**, 095101 (12 pages) (2020).
- M. YAMAUCHI and H. OKUMURA**, “Replica Sub-Permutation Method for Molecular Dynamics and Monte Carlo Simulations,” *J. Comput. Chem.* **40**, 2694–2711 (2019).
- N. MURAKI, K. ISHII, S. UCHIYAMA, S. G. ITOH, H. OKUMURA and S. AONO**, “Structural Characterization of HypX Responsible for CO Biosynthesis in the Maturation of NiFe-Hydrogenase,” *Commun. Biol.* **2**, 385 (12 pages) (2019).
- T. FUJITA, Y. NOGUCHI and T. HOSHI**, “Revisiting the Charge-Transfer States at Pentacene/ $C_{60}$  Interfaces with the GW/Bethe-Salpeter Equation Approach,” *Materials* **13**, 2728 (15 pages) (2020).
- M. I. MAHMOOD, H. NOGUCHI and K. OKAZAKI**, “Curvature Induction and Sensing of the F-BAR Protein Pacsin1 on Lipid Membranes via Molecular Dynamics Simulations,” *Sci. Rep.* **9**, 14557 (11 pages) (2019).
- J. WARNAU, D. WÖHLERT, K. OKAZAKI, Ö. YILDIZ, A. P. GAMIZ-HERNANDEZ, V. R. I. KAILA, W. KÜHLBRANDT and G. HUMMER**, “Ion Binding and Selectivity of the  $\text{Na}^+/\text{H}^+$  Antiporter  $\text{MjNhaP1}$  from Experiment and Simulation,” *J. Phys. Chem. B* **124**, 336–344 (2020).
- K. OKAZAKI, A. NAKAMURA and R. IINO**, “Chemical-State-Dependent Free Energy Profile from Single-Molecule Trajectories of Biomolecular Motors: Application to Processive Chitinase,” *J. Phys. Chem. B* **124**, 6475–6487 (2020).
- Y. MORI, K. OKAZAKI, T. MORI, K. KIM and N. MATUBAYASI**, “Learning Reaction Coordinates via Cross-Entropy Minimization: Application to Alanine Dipeptide,” *J. Chem. Phys.* **153**, 054115 (8 pages) (2020).
- T. ISHIDA**, “Theoretical Investigation of Dissolution and Decomposition Mechanisms of a Cellulose Fiber in Ionic Liquids,” *J. Phys. Chem. B* **124**, 3090–3102 (2020).
- S. SUMITA and Y. YANASE**, “Superconductivity Induced by Fluctuations of Momentum-Based Multipoles,” *Phys. Rev. Res.* **2**, 033225 (19 pages) (2020).
- K. IMAMURA, T. YAMAZAKI, D. YOKOGAWA, M. HIGASHI and H. SATO**, “Nuclear Magnetic Shielding of Molecule in Solution Based on Reference Interaction Site Model Self-Consistent Field with Spatial Electron Density Distribution,” *J. Chem. Phys.* **152**, 194102 (11 pages) (2020).
- H. NAKANO, M. HIGASHI and H. SATO**, “Uniform Potential Difference Scheme to Evaluate Effective Electronic Couplings for Superexchange Electron Transfer in Donor–Bridge–Acceptor Systems,” *J. Chem. Phys.* **152**, 224103 (13 pages) (2020).

## Photo-Molecular Science

- M. MIZOGUCHI, Y. ZHANG, M. KUNIMI, A. TANAKA, S. TAKEDA, N. TAKEI, V. BHARTI, K. KOYASU, T. KISHIMOTO, D. JAKSCH, A. GLÄTZLE, M. KIFFNER, G. MASELLA, G. PUPILLO, M. WEIDEMÜLLER and K. OHMORI**, “Ultrafast Creation of Overlapping Rydberg Electrons in an Atomic BEC and Mott-Insulator Lattice,” *Phys. Rev. Lett.* **124**, 253201 (7 pages) (2020).
- H. KATSUKI, Y. OHTSUKI, T. AJIKI, H. GOTO and K. OHMORI**, “Engineering Quantum Wave-Packet Dispersion with a Strong Non-Resonant Femtosecond Laser Pulse,” *arXiv* 1910.08241 (2019).
- H. SAKAI (Hamamatsu Photonics K.K.), K. OHMORI (NINS), T. ANDO (Hamamatsu Photonics K.K.), N. TAKEI (NINS), H. TOYODA, Y. OHTAKE, T. HYODO and Y. TAKIGUCHI (Hamamatsu Photonics K.K.)**, Patent Publication (15<sup>th</sup> Nov. 2018), “Quantum Simulator and Quantum Simulation Method.”
- H. SAKAI (Hamamatsu Photonics K.K.), K. OHMORI (NINS), T. ANDO (Hamamatsu Photonics K.K.), N. TAKEI (NINS), H. TOYODA, Y. OHTAKE, T. HYODO and Y. TAKIGUCHI (Hamamatsu Photonics K.K.)**, US Patent (3<sup>rd</sup> Nov. 2020), “Quantum Simulator and Quantum Simulation Method.”

- F. MATSUI, S. MAKITA, H. MATSUDA, T. YANO, E. NAKAMURA, K. TANAKA, S. SUGA and S. KERA**, "Photoelectron Momentum Microscope at BL6U of UVSOR-III Synchrotron," *Jpn. J. Appl. Phys.* **59**, 067001 (9 pages) (2020). DOI: 10.35848/1347-4065/ab9184
- F. MATSUI, S. MAKITA, H. MATSUDA, T. UEBA, T. HORIGOME, H. YAMANE, K. TANAKA, S. KERA and N. KOSUGI**, "Bulk and Surface Band Dispersion Mapping of the Au(111) Surface by Acceptance-Cone Tunable PES System," *e-J. Surf. Sci. Nanotechnol.* **18**, 18–23 (2020). DOI: 10.1380/ejssnt.2020.18
- G. D'AVINO, S. DUHM, R. DELLA VALLE, G. HEIMEL, M. OEHZELT, S. KERA, N. UENO, D. BELJONNE and I. SALZMANN**, "Electrostatic Interactions Shape Molecular Organization and Electronic Structure of Organic Semiconductor Blends," *Chem. Mater.* **32**, 1261–1271 (2020). DOI: 10.1021/acs.chemmater.9b04763
- J. YANG, S.-X. REN, T. YAMAGUCHI, M. MEISSNER, L. CHENG, L. ZHOU, S. IDETA, K. TANAKA and S. KERA**, "Valence Band Dispersion Measured in the Surface Normal Direction of  $\text{CH}_3\text{NH}_3\text{PbI}_3$  Single Crystals," *Appl. Phys. Express* **13**, 011009 (4 pages) (2020). DOI: 10.7567/1882-0786/ab6134
- H. YAMANE, F. MATSUI, T. UEBA, T. HORIGOME, S. MAKITA, K. TANAKA, S. KERA and N. KOSUGI**, "Acceptance-Cone-Tunable Electron Spectrometer for Highly-Efficient Constant Energy Mapping," *Rev. Sci. Instrum.* **90**, 093102 (7 pages) (2019). DOI: 10.1063/1.5109453
- Y. NAKAYAMA, S. KERA and N. UENO**, "Photoelectron Spectroscopy on Single Crystals of Organic Semiconductors: Experimental Electronic Band Structure for Optoelectronic Properties," *J. Mater. Chem. C* **8**, 9090–9132 (2020). DOI: 10.1039/D0TC00891E [Invited review]
- Y. HIKOSAKA, T. KANEYASU, M. FUJIMOTO, H. IWAYAMA and M. KATOH**, "Coherent Control in the Extreme Ultraviolet and Attosecond Regime by Synchrotron Radiation," *Nat. Commun.* **10**, 4988 (5 pages) (2019).
- T. KANEYASU, Y. HIKOSAKA, M. FUJIMOTO, H. IWAYAMA and M. KATOH**, "Controlling the Orbital Alignment in Atoms Using Cross-Circularly Polarized Extreme Ultraviolet Wave Packet," *Phys. Rev. Lett.* **123**, 233401 (5 pages) (2019).
- L. GUO, H. YAMAGUCHI, M. YAMAMOTO, F. MATSUI, G. WANG, F. LIU, P. YANG, E. R. BATISTA, N. A. MOODY, Y. TAKASHIMA and M. KATOH**, "Graphene as Reusable Substrate for Bialkali Photocathodes," *Appl. Phys. Lett.* **116**, 251903 (5 pages) (2020).
- K. FUJIMORI, M. KITAURA, Y. TAIRA, M. FUJIMOTO, H. ZEN, S. WATANABE, K. KAMADA, Y. OKANO, M. KATOH, M. HOSAKA, J. YAMAZAKI, T. HIRADE, Y. KOBAYASHI and A. OHNISHI**, "Visualizing Cation Vacancies in  $\text{Ce:Gd}_3\text{Al}_2\text{Ga}_3\text{O}_{12}$  Scintillators by Gamma-Ray-Induced Positron Annihilation Lifetime Spectroscopy," *Appl. Phys. Express* **13**, 085505 (4 pages) (2020).
- K. ALI, H. OHGAKI, H. ZEN, T. KII, T. HAYAKAWA, T. SHIZUMA, H. TOYOKAWA, Y. TAIRA, V. IANCU, G. TURTURICA, C. ALEXANDRU UR, M. FUJIMOTO and M. KATOH**, "Selective Isotope CT Imaging Based on Nuclear Resonance Fluorescence Transmission Method," *IEEE Trans. Nucl. Sci.* **67**(8), 1976–1984 (2020).
- T. KANEYASU, Y. HIKOSAKA, M. FUJIMOTO, H. IWAYAMA and M. KATOH**, "Polarization Control in a Crossed Undulator without a Monochromator," *New J. Phys.* **22**, 083062 (8 pages) (2020).
- K. FUJIMORI, M. KITAURA, Y. TAIRA, M. FUJIMOTO, H. ZEN, S. WATANABE, K. KAMADA, Y. OKANO, M. KATOH, M. HOSAKA, J. YAMAZAKI, T. HIRADE, Y. KOBAYASHI and A. OHNISHI**, "Visualizing Cation Vacancies in  $\text{Ce:Gd}_3\text{Al}_2\text{Ga}_3\text{O}_{12}$  Scintillators by Gamma-Ray-Induced Positron Annihilation Lifetime Spectroscopy," *Appl. Phys. Express* **13**, 085505 (4 pages) (2020).
- D. PINEK, T. ITO, K. FURUTA, Y. KIM, M. IKEMOTO, S. IDETA, K. TANAKA, M. NAKATAKE, P.L. FEVRE, F. BERTRAN and T. OUISSE**, "Near Fermi Level Electronic Structure of  $\text{Ti}_3\text{SiC}_2$  Revealed by Angle-Resolved Photoemission Spectroscopy," *Phys. Rev. B* **102**, 075111 (11 pages) (2020).
- H. ANZAI, K. MORIKAWA, H. SHIONO, H. SATO, S. IDETA, K. TANAKA, T. ZHUANG, K. T. MATSUMOTO and K. HIRAKO**, "Temperature Dependence of the Kondo Resonance in the Photoemission Spectra of the Heavy-Fermion Compounds  $\text{Yb}_X\text{Cu}_4$  ( $X = \text{Mg, Cd, and Sn}$ )," *Phys. Rev. B* **101**, 235160 (7 pages) (2020).
- F. MATSUI, S. MAKITA, H. MATSUDA, T. YANO, E. NAKAMURA, K. TANAKA, S. SUGA and S. KERA**, "Photoelectron Momentum Microscope at BL6U of UVSOR-III Synchrotron," *Jpn. J. Appl. Phys.* **59**, 067001 (9 pages) (2020).
- J. YANG, S.-X. REN, T. YAMAGUCHI, M. MEISSNER, L. CHENG, L. ZHOU, S. IDETA, K. TANAKA and S. KERA**, "Valence Band Dispersion Measured in the Surface Normal Direction of  $\text{CH}_3\text{NH}_3\text{PbI}_3$  Single Crystals," *Appl. Phys. Express* **13**, 011009 (4 pages) (2020).
- S. IDETA, N. MURAI, M. NAKAJIMA, R. KAJIMOTO and K. TANAKA**, "Experimental Investigation of the Suppressed Superconducting Gap and Double-Resonance Mode in  $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ ," *Phys. Rev. B* **100**, 235135 (7 pages) (2019).
- G. VINCINI, S. TAJIMA, S. MIYASAKA and K. TANAKA**, "Multilayer Effects in  $\text{Bi}_2\text{Sr}_2\text{Ca}_2\text{Cu}_3\text{O}_{10+z}$  Superconductors," *Supercond. Sci. Technol.* **32**, 113001 (12 pages) (2019).
- M. HORIO, K. KOSHIISHI, S. NAKATA, K. HAGIWARA, Y. OTA, K. OKAZAKI, S. SHIN, S. IDETA, K. TANAKA, A. TAKAHASHI, T. OHGI, T. ADACHI, Y. KOIKE and A. FUJIMORI**, " $d$ -Wave Superconducting Gap Observed in Protect-Annealed Electron-Doped Cuprate Superconductors  $\text{Pr}_{1.3-x}\text{La}_{0.7}\text{Ce}_x\text{CuO}_4$ ," *Phys. Rev. B* **100**, 054517 (5 pages) (2019).
- Y. OHTSUBO, Y. YAMASHITA, J. KISHI, S. IDETA, K. TANAKA, H. YAMANE, J. E. RAULT, P. LE. FEVRE, F. BERTRAN and S. KIMURA**, "Temperature-Driven Modification of Surface Electronic Structure on Bismuth, a Topological Border Material," *J. Phys. D: Appl. Phys.* **52**, 254002 (6 pages) (2019).
- T. MATSUSHITA, T. MURO, T. YOKOYA, K. TERASHIMA, Y. KATO, H. MATSUI, N. MAEJIMA, Y. HASHIMOTO and F. MATSUI**, "Theory for High-Angular-Resolution Photoelectron Holograms Considering the Inelastic Mean Free Path and the Formation Mechanism of Quasi-Kikuchi Band," *Phys. Status Solidi B* **257**, 2000117 (5 pages) (2020).
- L. GUO, H. YAMAGUCHI, M. YAMAMOTO, F. MATSUI, G. WANG, F. LIU, P. YANG, E. R. BATISTA, N. A. MOODY, Y. TAKASHIMA and M. KATOH**, "Graphene as Reusable Substrate for Bialkali Photocathodes," *Appl. Phys. Lett.* **116**, 251903 (5 pages) (2020).
- F. MATSUI, S. MAKITA, H. MATSUDA, T. YANO, E. NAKAMURA, K. TANAKA, S. SUGA and S. KERA**, "Photoelectron Momentum Microscope at BL6U of UVSOR-III Synchrotron," *Jpn. J. Appl. Phys.* **59**, 067001 (9 pages) (2020).

## LIST OF PUBLICATIONS

- H. MATSUDA and F. MATSUI**, "Principle and Basic Design of Omnidirectional Photoelectron Acceptance Lens," *Jpn. J. Appl. Phys.* **59**, 046503 (11 pages) (2020).
- I. I. OGORODNIKOV, M. V. KUZNETSOV, F. MATSUI, D. Y. USACHOV and L. V. YASHINA**, "Enhanced Surface Sensitivity of X-Ray Photoelectron Holography through the Example of Bi<sub>2</sub>Te<sub>3</sub>(111) Surface," *Appl. Surf. Sci.* **505**, 144531 (6 pages) (2020).
- T. MATSUSHITA, T. MURO, F. MATSUI, N. HAPPO and K. HAYASHI**, "Data Processing for Atomic Resolution Holography," *Jpn. J. Appl. Phys.* **59**, 020502 (10 pages) (2020).
- F. MATSUI, S. MAKITA, H. MATSUDA, T. UEBA, T. HORIGOME, H. YAMANE, K. TANAKA, S. KERA and N. KOSUGI**, "Bulk and Surface Band Dispersion Mapping of the Au(111) Surface by Acceptance-Cone Tunable PES System," *e-J. Surf. Sci. Nanotechnol.* **18**, 18–23 (2020).
- F. MATSUI, S. MAKITA, H. MATSUDA, T. OHIGASHI, H. YAMANE and N. KOSUGI**, "Identification of Twinning-Induced Edges on the Cleaved Graphite Crystal Surface," *J. Phys. Soc. Jpn.* **88**, 114704 (3 pages) (2019).
- F. MATSUI, K. YASUDA, N. MAEJIMA, H. MATSUDA, T. MATSUSHITA and H. DAIMON**, "Chemical and Magnetic Properties of Polycrystalline Iron Surface Revealed by Auger Electron Holography, Spectroscopy, and Microscopy," *Jpn. J. Appl. Phys.* **58**, 110602 (8 pages) (2019).
- H. YAMANE, F. MATSUI, T. UEBA, T. HORIGOME, S. MAKITA, K. TANAKA, S. KERA and N. KOSUGI**, "Acceptance-Cone-Tunable Electron Spectrometer for Highly-Efficient Constant Energy Mapping," *Rev. Sci. Instrum.* **90**, 093102 (7 pages) (2019).
- D. Y. USACHOV, A. V. TARASOV, F. MATSUI, M. MUNTWILER, K. A. BOKAI, V. O. SHEVELEV, O. Y. VILKOV, M. V. KUZNETSOV, L. V. YASHINA, C. LAUBSCHAT, A. COSSARO, L. FLOREANO, A. VERDINI and D. V. VYALIKH**, "Decoding the Structure of Interfaces and Impurities in 2D Materials by Photoelectron Holography," *2D Mater.* **6**, 045046 (13 pages) (2019).
- F. MATSUI and H. MATSUDA**, "Electrostatic Lens, and Parallel Beam Generation Device and Parallel Beam Convergence Device which use Electrostatic Lens and Collimator," US 10614992, 2020.04.07 patented.
- M. NAGASAKA and H. IWAYAMA**, "Photoelectron Based Soft X-Ray Detector for Removing High Order X Rays," *Rev. Sci. Instrum.* **91**, 083103 (7 pages) (2020).
- M. NAGASAKA**, "Soft X-Ray Absorption Spectroscopy in the Low-Energy Region Explored Using an Argon Gas Window," *J. Synchrotron Radiat.* **27**, 959–962 (2020).
- M. NAGASAKA, H. YUZAWA and N. KOSUGI**, "Microheterogeneity in Aqueous Acetonitrile Solution Probed by Soft X-Ray Absorption Spectroscopy," *J. Phys. Chem. B* **124**, 1259–1265 (2020).
- M. NAGASAKA, H. YUZAWA, N. TAKADA, M. AOYAMA, E. RÜHL and N. KOSUGI**, "Laminar Flow in Microfluidics Investigated by Spatially-Resolved Soft X-Ray Absorption and Infrared Spectroscopy," *J. Chem. Phys.* **151**, 114201 (7 pages) (2019).
- T. MANSIKKALA, M. PATANEN, A. KARKONEN, R. KORPINEN, A. PRANOVICH, T. OHIGASHI, S. SWARAJ, J. SEITOSONEN, J. RUOKOLAINEN, M. HUTTULA, P. SARANPAA and R. PIISPANEN**, "Lignans in Knotwood of Norway Spruce: Localisation with Soft X-Ray Microscopy and Scanning Transmission Electron Microscopy with Energy Dispersive X-Ray Spectroscopy," *Molecules* **25**, 2997 (22 pages) (2020).
- Y. LU, Y. F. WANG, Y. C. HUANG, J. L. CHEN, C. L. CHEN, Y. C. LIN, Y. G. LIN, W. F. PONG, T. OHIGASHI, N. KOSUGI, C. H. KUO, W. C. CHOU and C. L. DONG**, "Effect of Fe<sub>2</sub>Co<sub>3</sub> Coating on ZnO Nanowires in Photoelectrochemical Water Splitting: A Synchrotron X-Ray Spectroscopic and Spectromicroscopic Investigation," *Sol. Energy Mater. Sol. Cells* **209**, 110469 (7 pages) (2020).
- M. NAGASAKA and H. IWAYAMA**, "Photoelectron Based Soft X-Ray Detector for Removing High Order X Rays," *Rev. Sci. Instrum.* **91**, 083103 (7 pages) (2020).
- A. FERTE, J. PALAUDOUX, F. PENENT, H. IWAYAMA, E. SHIGEMASA, Y. HIKOSAKA, K. SOEJIMA, K. ITO, P. LABLANQUIE, R. TAIEB and S. CARNIATO**, "Advanced Computation Method for Double Core Hole Spectra: Insight into the Nature of Intense Shake-up Satellites," *J. Phys. Chem. Lett.* **11**, 4359 (11 pages) (2020).
- Y. HIKOSAKA, H. IWAYAMA and T. KANEYASU**, "Zeeman Quantum Beats of Helium Rydberg States Excited by Synchrotron Radiation," *J. Synchrotron Radiat.* **27**, 675 (6 pages) (2020).
- S. KOSUGI, N. SUZUKI, KUMAGAI, H. IWAYAMA, E. SHIGEMASA, F. KOIKE and Y. AZUMA**, "Dominance of Angular Momentum Exchange in the PCI Recapture of Photoelectrons Revealed by High Resolution Auger Electron Measurements of Kr," *J. Phys. B* **52**, 245002 (6 pages) (2019).
- T. KANEYASU, Y. HIKOSAKA, M. FUJIMOTO, H. IWAYAMA and M. KATO**, "Controlling the Orbital Alignment in Atoms Using Cross-Circularly Polarized Extreme Ultraviolet Wave Packet," *Phys. Rev. Lett.* **123**, 233401 (5 pages) (2019).
- Y. HIKOSAKA, T. KANEYASU, M. FUJIMOTO, H. IWAYAMA and M. KATO**, "Coherent Control in the Extreme Ultraviolet and Attosecond Regime by Synchrotron Radiation," *Nat. Commun.* **10**, 4988 (5 pages) (2019).
- M. IMAI, Y. YOKOTA, I. TANABE, K. INAGAKI, Y. MORIKAWA and K. FUKUI**, "Correlation between Mobility and Hydrogen Bonding Network of Water at Electrified-Graphite Electrode Using Molecular Dynamics Simulation," *Phys. Chem. Chem. Phys.* **22**, 1767–1773 (2020).
- D. OKAUE, I. TANABE, S. ONO, K. SAKAMOTO, T. SATO, A. IMANISHI, Y. MORIKAWA, J. TAKEYA and K. FUKUI**, "Ionic-Liquid-Originated Carrier Trapping Dynamics at the Interface in Electric Double-Layer Organic FET Revealed by Operando Interfacial Analyses," *J. Phys. Chem. C* **124**, 2543–2552 (2020).
- Y. MORINO, Y. YOKOTA, H. HARA, K. BANDO, S. ONO, A. IMANISHI, Y. OKADA, H. MATSUI, T. UEMURA, J. TAKEYA and K. FUKUI**, "Rapid Improvements in Charge Carrier Mobility at Ionic Liquid/Pentacene Single Crystal Interfaces by Self-Cleaning," *Phys. Chem. Chem. Phys.* **22**, 6131–6135 (2020).

- P. E. EVANS, T. KOMESU, L. ZHANG, D.-F. SHAO, A. J. YOST, S. KUMAR, E. F. SCHWIER, K. SHIMADA, E. TSYMBAL, X. HONG and P. A. DOWBEN, "Detection of Decoupled Surface and Bulk States in Epitaxial Orthorhombic SrIrO<sub>3</sub> Thin Films," *AIP Adv.* **10**, 045027 (5 pages) (2020).
- D. GENG, K. YU, S. YUE, J. CAO, W. LI, D. MA, C. CUI, M. ARITA, S. KUMAR, E. F. SCHWIER, K. SHIMADA, P. CHENG, L. CHEN, K. WU, Y. YAO and B. FENG, "Experimental Evidence of Monolayer AlB<sub>2</sub> with Symmetry-Protected Dirac Cones," *Phys. Rev. B* **101**, 161407(R) (5 pages) (2020).
- A. SINGH, S. KUMAR, M. SINGHA, P. SINGHA, R. SINGH, V. K. GANGWAR, A. LAKHANI, S. PATIL, E. F. SCHWIER, T. MATSUMURA, K. SHIMADA, A. K. GHOSH and S. CHATTERJEE, "Anomalous Hall Effect in Cu Doped Topological Insulator Bi<sub>2</sub>Te<sub>3</sub>," *J. Phys.: Condens. Matter* **32**, 305602 (11 pages) (2020).
- A. G. RYBKIN, A. A. RYBKINA, A. V. TARASOV, D. A. PUDIKOV, I. I. KLIMOVSKIKH, O. YU. VILKOV, A. E. PETUKHOV, D. Y. USACHOV, D. A. ESTYUNIN, V. Y. VOROSHININ, A. VARYKHALOV, G. DI SANTO, L. PETACCIA, E. F. SCHWIER, K. SHIMADA, A. KIMURA and A. M. SHIKIN, "A New Approach for Synthesis of Epitaxial Nano-Thin Pt<sub>5</sub>Gd Alloy via Intercalation Underneath a Graphene," *Appl. Surf. Sci.* **526**, 146687 (8 pages) (2020).
- Y. ZHANG, K. DENG, X. ZHANG, M. WANG, Y. WANG, C. LIU, J.-W. MEI, S. KUMAR, E. F. SCHWIER, K. SHIMADA, C. CHEN and B. SHEN, "In-Plane Antiferromagnetic Moments and Magnetic Polaron in the Axion Topological Insulator Candidate EuIn<sub>2</sub>As<sub>2</sub>," *Phys. Rev. B* **101**, 205126 (7 pages) (2020).
- M. ZHENG, E. F. SCHWIER, H. IWASAWA and K. SHIMADA, "High-Resolution Angle-Resolved Photoemission Study of Oxygen Adsorbed Fe/MgO(001)," *Chin. Phys. B* **29**, 067901 (9 pages) (2020).
- X. WU, J. LI, X.-M. MA, Y. ZHAN, Y. LIU, C.-S. ZHOU, J. SHAO, Q. WANG, Y.-J. HAO, Y. FENG, E. F. SCHWIER, S. KUMAR, H. SUN, P. LIU, K. SHIMADA, K. MIYAMOTO, T. OKUDA, K. WANG, M. XIE, C. CHEN, Q. LIU, C. LIU and Y. ZHAO, "Distinct Topological Surface States on the Two Terminations of MnBi<sub>4</sub>Te<sub>7</sub>," *Phys. Rev. X* **10**, 031013 (10 pages) (2020).
- M. NURMAMAT, K. OKAMOTO, S. ZHU, T. V. MENSCHIKOVA, I. P. RUSINOV, V. O. KOROSTELEV, K. MIYAMOTO, T. OKUDA, T. MIYASHITA, X. WANG, Y. ISHIDA, K. SUMIDA, E. F. SCHWIER, M. YE, Z. S. ALIEV, M. B. BABANLY, I. R. AMIRASLANOV, E. V. CHULKOV, K. A. KOKH, O. E. TERESHCHENKO, K. SHIMADA, S. SHIN and A. KIMURA, "Topologically Nontrivial Phase-Change Compound GeSb<sub>2</sub>Te<sub>4</sub>," *ACS Nano* **14**, 9059–9065 (2020).
- P. SINGH, M. ALAM, S. KUMAR, K. ANAND, V. K. GANGWAR, S. GHOSH, M. SAWADA, K. SHIMADA, R. K. SINGH, A. K. GHOSH and S. CHATTERJEE, "Roles of Re-Entrant Cluster Glass State and Spin-Lattice Coupling in Magneto-Dielectric Behavior of Giant Dielectric Double Perovskite La<sub>1.8</sub>Pr<sub>0.2</sub>CoFeO<sub>6</sub>," *J. Phys.: Condens. Matter* **32**, 445801 (9 pages) (2020).
- P. E. EVANS, T. KOMESU, E. F. SCHWIER, S. KUMAR, K. SHIMADA and P. A. DOWBEN, "The Band Shifts in MoS<sub>2</sub>(0001) and WSe<sub>2</sub>(0001) Induced by Palladium Adsorption," *J. Phys.: Condens. Matter* **32**, 465001 (7 pages) (2020).

- C. M. LAURIO, H. KATSUKI and H. YANAGI, "Numerical Simulations on Strong Coupling of Bloch Surface Waves and Excitons in Dielectric-Organic Multilayer Structures," *J. Phys.: Condens. Matter* **32**, 415003 (11 pages) (2020).
- H. OKOCHI, H. KATSUKI, M. TSUBOUCHI, R. ITAKURA and H. YANAGI, "Photon Energy Dependent Ultrafast Photoinduced Terahertz Response in a Microcrystalline Film of CH<sub>3</sub>NH<sub>3</sub>PbBr<sub>3</sub>," *J. Phys. Chem. Lett.* **11**, 6068–6076 (2020).
- H. MIZUNO, T. JINJYO, C. LAURIO, H. KATSUKI, I. HIROMITSU, F. SASAKI and H. YANAGI, "Fabrication and Characterization of Vertical Microcavities Containing a Submicron Particle Film of 5,5'-di(4-biphenyl)-2,2'-bithiophene," *Jpn. J. Appl. Phys.* **59**, SDDA14 (5 pages) (2020).
- T. AKAZAWA, F. SASAKI, K. BANDO, H. MIZUNO, H. KATSUKI and H. YANAGI, "Fabrication of Low-Dimensional Microstructures with Distyrylbenzene Derivatives," *Jpn. J. Appl. Phys.* **59**, SDDA07 (5 pages) (2020).

## Materials Molecular Science

- A. ISHIHARA, T. NAGAI, K. UKITA, M. ARAO, M. MATSUMOTO, L. YU, T. NAKAMURA, O. SEKIZAWA, Y. TAKAGI, K. MATSUZAWA, T. NAPPORN, S. MITSUSHIMA, T. URUGA, T. YOKOYAMA, Y. IWASAWA, H. IMAI and K. OTA, "Emergence of Oxygen Reduction Activity in Zirconium Oxide-Based Compounds in Acidic Media: Creation of Active Sites for Oxygen Reduction Reaction," *J. Phys. Chem. C* **123**, 18150–18159 (2019).
- T. NAKAMURA, Y. TAKAGI, S. CHAVEANGHONG, T. URUGA, M. TADA, Y. IWASAWA and T. YOKOYAMA, "Quick Operando Ambient Pressure Hard X-Ray Photoelectron Spectroscopy for Reaction Kinetic Measurements of Polymer Electrolyte Fuel Cells," *J. Phys. Chem. C* **124**, 17520–17527 (2020).
- K. KAWAGUCHI, T. MIYAMACHI, T. IIMORI, Y. TAKAHASHI, T. HATTORI, T. YOKOYAMA, M. KOTSUGI and F. KOMORI, "Realizing Large Out-of-Plane Magnetic Anisotropy in L10-FeNi Films Grown by Nitrogen-Surfactant Epitaxy on Cu(001)," *Phys. Rev. Mater.* **4**, 054403 (7 pages) (2020).
- Y. SONG, Q. SUN, T. YOKOYAMA, H. ZHU, Q. LI, R. HUANG, Y. REN, Q. HUANG, X. XING and J. CHEN, "Transforming Thermal Expansion from Positive to Negative: The Case of Cubic Magnetic Compounds of (Zr,Nb)Fe<sub>2</sub>," *J. Phys. Chem. Lett.* **11**, 1954–1961 (2020).
- Y. WAKISAKA, D. KIDO, H. UEHARA, Q. YUAN, F. E. FEITEN, S. MUKAI, S. TAKAKUSAGI, Y. UEMURA, T. YOKOYAMA, T. WADA, M. UO, O. SEKIZAWA, T. URUGA, Y. IWASAWA and K. ASAKURA, "Development of Surface Fluorescence X-Ray Absorption Fine Structure Spectroscopy Using a Laue-Type Monochromator," *Chem. Rec.* **19**, 1157–1165 (2019).
- S. IKEMOTO, X. HUANG, S. MURATSUGU, S. NAGASE, T. KOITAYA, H. MATSUI, G. YOKOTA, T. SUDOH, A. HASHIMOTO, Y. TAN, S. YAMAMOTO, J. TANG, I. MATSUDA, J. YOSHINOBU, T. YOKOYAMA, S. KUSAKA, R. MATSUDA and M. TADA, "Reversible Low-Temperature Redox Activity and Selective Oxidation Catalysis Derived from the Concerted Activation of Multiple Metal Species on Cr and Rh-Incorporated Ceria Catalysts," *Phys. Chem. Chem. Phys.* **21**, 20868–20877 (2019).

## LIST OF PUBLICATIONS

- K. YAMAMOTO, S. E. MOUSSAOUI, Y. HIRATA, S. YAMAMOTO, Y. KUBOTA, S. OWADA, M. YABASHI, T. SEKI, K. TAKANASHI, I. MATSUDA and H. WADATI**, “Element-Selective Tracking Ultrafast Demagnetization Process in Co/Pt Multilayer Thin Films by the Resonant Magneto-Optical Kerr Effect,” *Appl. Phys. Lett.* **116**, 172406 (5 pages) (2020).
- T. SUGIMOTO and Y. MATSUMOTO**, “Orientational Ordering in Heteroepitaxial Water Ice on Metal Surfaces,” *Phys. Chem. Chem. Phys.* **29**, 16435–17012 (2020).
- F. KATO, T. SUGIMOTO and Y. MATSUMOTO**, “Direct Experimental Evidence for Markedly Enhanced Surface Proton Activity Inherent to Water Ice,” *J. Phys. Chem. Lett.* **11**, 2524–2529 (2020).
- K. HARADA, T. SUGIMOTO, F. KATO, K. WATANABE and Y. MATSUMOTO**, “Thickness Dependent Homogeneous Crystallization of Ultrathin Amorphous Solid Water Films,” *Phys. Chem. Chem. Phys.* **22**, 1963–1973 (2020).
- Y. OTSUKI, K. WATANABE, T. SUGIMOTO and Y. MATSUMOTO**, “Enhanced Structural Disorder at a Nanocrystalline Ice Surface,” *Phys. Chem. Chem. Phys.* **21**, 20442–20453 (2019).
- M. KIKUCHI, S. IZAWA, N. RAI and M. HIRAMOTO**, “Very Low Activation Energy for Carrier Generation of Surface Doped Organic Single Crystals Observed by Hall Effects,” *Appl. Phys. Lett.* **115**, 113301 (4 pages) (2019).
- H. UENO, I. JEON, H. LIN, A. THOTE, T. NAKAGAWA, H. OKADA, S. IZAWA, M. HIRAMOTO, S. MARUYAMA and Y. MATSUO**, “Li@C<sub>60</sub> Endohedral Fullerene as Supramolecular Dopant for C<sub>60</sub> Electron-transporting Layer Promoting Efficiency in Perovskite Solar Cells,” *Chem. Commun.* **55**, 11837–11839 (2019).
- S. IZAWA, N. SHINTAKU, M. KIKUCHI and M. HIRAMOTO**, “Importance of Interfacial Crystallinity to Reduce Open-Circuit Voltage Loss in Organic Solar Cells,” *Appl. Phys. Lett.* **115**, 153301 (4 pages) (2019).
- K. FUJIMOTO, S. IZAWA, Y. ARIKAI, S. SUGIMOTO, H. OUE, T. INUZUKA, N. UEMURA, M. SAKAMOTO, M. HIRAMOTO and M. TAKAHASHI**, “Regioselective Bay-Functionalization of Perylenes toward Tailor-Made Synthesis of Acceptor Materials for Organic Photovoltaics,” *ChemPlusChem* **85**, 285–293 (2020).
- M. KATAYAMA, T. KAJI, S. NAKAO and M. HIRAMOTO**, “Ultra-Thick Organic Pigment Layer up to 10 μm Activated by Crystallization in Organic Photovoltaic Cells,” *Front. Energy Res. Section Solar Energy* **8**, 1–12 (2019).
- J. LEE, A. PERROT, M. HIRAMOTO and S. IZAWA**, “Photoconversion Mechanism at *pn*-Homojunction Interface in Single Organic Semiconductor,” *Materials* **13**, 1727 (8 pages) (2020).
- Y. NAKAMURA, M. IWASHITA, M. KIKUCHI, R. TSURUTA, K. YOSHIDA, Y. GUNJO, Y. YABARA, T. HOSOKAI, T. KOGANEZAWA, S. IZAWA and M. HIRAMOTO**, “Electronic and Crystallographic Examinations of the Homoepitaxially-Grown Rubrene Single Crystals,” *Materials* **13**, 1978 (11 pages) (2020).
- Y. YABARA, S. IZAWA and M. HIRAMOTO**, “Donor/Acceptor Photovoltaic Cells Fabricated on *p*-Doped Organic Single-Crystal Substrates,” *Materials* **13**, 2068 (8 pages) (2020).
- K. FUJIMOTO, M. TAKAHASHI, S. IZAWA and M. HIRAMOTO**, “Development of Perylene-Based Non-Fullerene Acceptors,” *Materials* **13**, 1978 (11 pages) (2020).
- H. NAWAZ, T. TAKEIRI, A. KUWABARA, M. YONEMURA and G. KOBAYASHI**, “Synthesis and H<sup>+</sup> Conductivity of a New Oxyhydride Ba<sub>2</sub>YHO<sub>3</sub> with Anion-Ordered Rock-Salt Layers,” *Chem. Commun.* **56**, 10373–10376 (2020).
- J. YANAGISAWA, T. HIRAKO, F. KAOBAYASHI, D. SAITO, M. YOSHIDA, M. KATO, F. TAKEIRI, G. KOBAYASHI, M. OHBA, L. F. LINDOY, R. OHTANI and S. HAYAMI**, “Luminescent Ionic Liquid Formed from a Melted Rhodium(V) Cluster,” *Chem. Commun.* **56**, 7957–7960 (2020).
- Y. MATSUDA, K. FUNAKOSHI, R. SEBE, G. KOBAYASHI, M. YONEMURA, N. IMANICHI, D. MORI and S. HIGASHIMOTO**, “Arrangement of Water Molecules and High Proton Conductivity of Tunnel Structure Phosphates, KMg<sub>1-x</sub>H<sub>2x</sub>(PO<sub>4</sub>)<sub>3-y</sub>H<sub>2</sub>O,” *RSC Adv.* **10**, 7803–7811 (2020).
- F. TAKEIRI, T. YAJIMA, S. HOSOKAWA, Y. MATSUSHITA and H. KAGEYAMA**, “Topochemical Anion Insertion into One-Dimensional Bi Channels in Bi<sub>2</sub>PdO<sub>4</sub>,” *J. Solid State Chem.* **286**, 121273 (2020).
- H. UBUKATA, T. BROUX, F. TAKEIRI, K. SHITARA, H. YAMASHITA, A. KUWABARA, G. KOBAYASHI and H. KAGEYAMA**, “Hydride Conductivity in an Anion-Ordered Fluorite Structure LnHO with an Enlarged Bottleneck,” *Chem. Mater.* **31**, 7360–7366 (2019).
- D. YOSHIZAWA, Y. SAWADA, Y. KOUSAKA, J. KISHINE, Y. TOGAWA, M. MITO, K. INOUE, J. AKIMITSU, T. NAKANO, Y. NOZUE and M. HAGIWARA**, “Anomalous Spiked Structures in ESR Signals from the Chiral Helimagnet CrNb<sub>3</sub>S<sub>6</sub>,” *Phys. Rev. B* **100**, 104413 (6 pages) (2019).
- I. G. BOSTREM, E. G. EKOMASOV, J. KISHINE, A. S. OVCHINNIKOV and V. E. SINITSYN**, “Discrete Magnetic Breathers in Monoaxial Chiral Helimagnet,” *Chelyabinsk Phys. Math. J.* **5(2)**, 194–201 (2020).
- A. INUI, R. AOKI, Y. NISHIUE, K. SHIOTA, Y. KOUSAKA, H. SHISHIDO, D. HIROBE, M. SUDA, J. OHE, J. KISHINE, H. M. YAMAMOTO and Y. TOGAWA**, “Chirality-Induced Spin-Polarized State of a Chiral Crystal CrNb<sub>3</sub>S<sub>6</sub>,” *Phys. Rev. Lett.* **124**, 166602 (6 pages) (2020).
- G. W. PATERSON, A. A. TERESHCHENKO, S. NAKAYAMA, Y. KOUSAKA, J. KISHINE, S. MCVITIE, A. S. OVCHINNIKOV, I. PROSKURIN and Y. TOGAWA**, “Tensile Deformations of the Magnetic Chiral Soliton Lattice Probed by Lorentz Transmission Electron Microscopy,” *Phys. Rev. B* **101**, 184424 (12 pages) (2020).
- J. KISHINE and A. S. OVCHINNIKOV**, “Magnetic Response of a Highly Nonlinear Soliton Lattice in a Monoaxial Chiral Helimagnet,” *Phys. Rev. B* **101**, 184425 (12 pages) (2020).
- T. TAJIRI, M. MITO, Y. KOUSAKA, J. AKIMITSU, J. KISHINE and K. INOUE**, “Spontaneous Magnetostriction Effects in the Chiral Magnet CrNb<sub>3</sub>S<sub>6</sub>,” *Phys. Rev. B* **102**, 014446 (7 pages) (2020).

**B. ADINARAYANA, D. SHIMIZU, K. FURUKAWA and A. OSUKA**, "Stable Radical versus Reversible  $\sigma$ -Bond Formation of (Porphyrinyl) Dicyanomethyl Radicals," *Chem. Sci.* **10**, 6007–6012 (2019).

**K. SUDOH, Y. SATOH, K. FURUKAWA, H. NAKANO and Y. MATANO**, "Synthesis and Optical, Magnetic, and Electrochemical Properties of 5,10,15,20-Tetraaryl-5,15-diazaporphyrin-tertiary Amine Conjugates," *J. Porphyrins Phthalocyanines* **24**, 286–297 (2020).

**B. ADINARAYANA, K. KATO, D. SHIMIZU, T. TANAKA, K. FURUKAWA and A. OSUKA**, "Cyclophane-Type Chlorin Dimers from Dynamic Covalent Chemistry of 2,18-Porphyrinyl Dicyanomethyl Diradicals," *Angew. Chem., Int. Ed.* **59**, 4320–4323 (2020).

**K. GOTO, M. ASADA, T. NAKAMURA and F. TANI**, "Switching Photomechanical Response by Structural Phase Transition and Evaluating Responsivity from Relaxation," *ChemPhotoChem* **4**, 1–7 (2020).

**T. INOUE, M. SHIBUTA, T. SUZUKI and A. NAKAJIMA**, "Occupied and Unoccupied Levels of Half-Fluorinated and Perfluorinated Rubrene Thin Films Probed by One- and Two-Photon Photoemission," *J. Phys. Chem. C* **124**, 12409–12416 (2020).

## Life and Coordination-Complex Molecular Science

**N. MURAKI, K. ISHII, S. UCHIYAMA, S. G. ITOH, H. OKUMURA and S. AONO**, "Structural Characterization of HypX Responsible for CO Biosynthesis in the Maturation of NiFe-Hydrogenase," *Commun. Biol.* **2**, 385 (12 pages) (2019).

**N. MURAKI, C. KITATSUJI, Y. OKAMOTO, T. UCHIDA, K. ISHIMORI and S. AONO**, "Structural Basis for Heme Transfer Reaction in Heme Uptake Machinery from Corynebacteria," *Chem. Commun.* **55**, 13864–13867 (2019).

**R. INOUE, T. NAKAGAWA, K. MORISHIMA, N. SATO, A. OKUDA, R. URADE, R. YOGO, S. YANAKA, M. YAGI-UTSUMI, K. KATO, K. OMOTO, K. ITO and M. SUGIYAMA**, "Newly Developed Laboratory-Based Size Exclusion Chromatography Small-Angle X-Ray Scattering System (La-SSS)," *Sci. Rep.* **9**, 12610 (12 pages) (2019).

**R. MURAKAMI, Y. YUNOKI, K. ISHII, K. TERAUCHI, S. UCHIYAMA, H. YAGI and K. KATO**, "Cooperative Binding of KaiB to the KaiC Hexamer Ensures Accurate Circadian Clock Oscillation in Cyanobacteria," *Int. J. Mol. Sci.* **20**, 4550 (10 pages) (2019).

**C. CHO, J. JANG, Y. KANG, H. WATANABE, T. UCHIHASHI, S. J. KIM, K. KATO, J. Y. LEE and J.-J. SONG**, "Structural Basis of Nucleosome Assembly by the Abol AAA+ATPase Histone Chaperone," *Nat. Commun.* **10**, 5764 (13 pages) (2019).

**M. L. A. DE LEOZ, D. L. DUEWER, A. FUNG, L. LIU, H. K. YAU, O. POTTER, G. O. STAPLES, K. FURUKI, R. FRENKEL, Y. HU, Z. SOSIC, P. ZHANG, F. ALTMANN, C. GRUBER, C. SHAO, J. ZAIA, W. EVERES, S. PANGELLEY, D. SUCKAU, A. WIECHMANN, A. RESEMANN, W. JABS, A. BECK, J. W. FROEHLICH, C. HUANG, Y. LI, Y. LIU, S. SUN, Y. WANG, Y. SEO, H. J. AN, N. C. REICHARDT, J. E. RUIZ, S. ARCHER-HARTMANN, P. AZADI, L. BELL, Z. LAKOS, Y. AN, J. F. CIPOLLO, M. PUČIĆ-BAKOVIĆ, J. ŠTAMBUK, G. LAUC, X. LI, P. G. WANG, A. BOCK, R. HENNIG, E. RAPP, M. CRESKEY, T. CYR, M. NAKANO, T. SUGIYAMA, P. A. LEUNG, P. LINK-LENCZOWSKI, J. JAWOREK, S. J. YANG, H. ZHANG, T. KELLY, S. KLAPOETKE, R. CAO, J. Y. KIM, H. K. LEE, J. LEE, J. S. YOO, S. R. KIM, S. K. SUH, N. DE HAAN, D. FALCK, G. S. M. LAGEVEEN-KAMMEIJER, M. WUHRER, R. J. EMERY, R. P. KOZAK, L. P. LIEW, L. ROYLE, P. A. URBANOWICZ, N. PACKER, X. SONG, A. EVEREST-DASS, E. LATTOVÁ, S. CAJIC, K. ALAGESAN, D. KOLARICH, T. KASALI, V. LINDO, Y. CHEN, K. GOSWAMI, B. GAU, R. AMUNUGAMA, R. JONES, C. J. M. STROOP, K. KATO, H. YAGI, S. KONDO, C. T. YUEN, A. HARAZONO, X. SHI, P. MAGNELLI, B. T. KASPER, L. K. MAHAL, D. J. HARVEY, R. M. O'FLAHERTY, P. RUDD, R. SALDOVA, E. S. HECHT, D. C. MUDDIMAN, J. KANG, P. BHOSKAR, D. MENARD, A. SAATI, C. MERLE, S. MAST, S. TEP, J. TRUONG, T. NISHIKAZE, S. SEKIYA, A. SHAFER, S. FUNAOKA, M. TOYODA, P. DE VREUGD, C. CARON, P. PRADHAN, N. C. TAN, Y. MECHREF, S. PATIL, J. S. ROHRER, R. CHAKRABARTI, D. DADKE, M. LAHORI, C. ZOU, C. W. CAIRO, B. REIZ, R. M. WHITTAL, C. LEBRILLA, L. D. WU, A. GUTTMAN, M. SZIGETI, B. G. KREMKOW, K. LEE, C. SIHLBOM, B. ADAMCZYK, C. JIN, N. G. KARLSSON, J. ÖRNROS, G. LARSON, J. NILSSON, B. MEYER, A. WIEGANDT, E. KOMATSU, H. PERREAU, E. D. BODNAR, N. SAID, Y. N. FRANCOIS, E. LEIZE-WAGNER, S. MAIER, A. ZECK, A. J. R. HECK, Y. YANG, R. HASELBERG, Y. Q. YU, W. ALLEY, J. W. LEONE, H. YUAN and S. E. STEIN**, "NIST Interlaboratory Study on Glycosylation Analysis of Monoclonal Antibodies: Comparison of Results from Diverse Analytical Methods," *Mol. Cell. Proteomics* **19**, 11–30 (2020).

**S. YANAKA, R. YOGO, H. WATANABE, Y. TANIGUCHI, T. SATOH, N. KOMURA, H. ANDO, H. YAGI, N. YUKI, T. UCHIHASHI and K. KATO**, "On-Membrane Dynamic Interplay between Anti-GM1 IgG Antibodies and Complement Component C1q," *Int. J. Mol. Sci.* **21**, 147 (12 pages) (2020).

**M. YAGI-UTSUMI, A. SIKDAR, C. SONG, J. PARK, R. INOUE, H. WATANABE, R. N. BURTON-SMITH, T. KOZAI, T. SUZUKI, A. KODAMA, K. ISHII, H. YAGI, T. SATOH, S. UCHIYAMA, T. UCHIHASHI, K. JOO, J. LEE, M. SUGIYAMA, K. MURATA and K. KATO**, "Supramolecular Tholos-Like Architecture Constituted by Archaeal Proteins without Functional Annotation," *Sci. Rep.* **10**, 1540 (10 pages) (2020).

**G. GEORGE, S. NINAGAWA, H. YAGI, T. SAITO, T. ISHIKAWA, T. SAKUMA, T. YAMAMOTO, K. IMAMI, Y. ISHIHAMA, K. KATO, T. OKADA and K. MORI**, "EDEM2 Stably Disulfide-Bonded to TXNDC11 Catalyzes the First Mannose Trimming Step in Mammalian Glycoprotein ERAD," *eLife* **9**, e53455 (19 pages) (2020).

**H. YAGI, M. YAGI-UTSUMI, R. HONDA, Y. OHTA, T. SAITO, M. NISHIO, S. NINAGAWA, K. SUZUKI, T. ANZAI, Y. KAMIYA, K. AOKI, M. NAKANISHI, T. SATOH and K. KATO**, "Improved Secretion of Glycoproteins Using an N-Glycan-Restricted Passport Sequence Tag Recognized by Cargo Receptor," *Nat. Commun.* **11**, 1368 (9 pages) (2020).

**K. YAMADA, Y. YAMAGUCHI, Y. UEKUSA, K. AOKI, I. SHIMADA, T. YAMAGUCHI and K. KATO**, "Solid-State  $^{17}\text{O}$  NMR Analysis of Synthetically  $^{17}\text{O}$ -Enriched D-Glucosamine," *Chem. Phys. Lett.* **749**, 137455 (5 pages) (2020).

**T. SATOH, M. NISHIO, K. SUZUKI, M. YAGI-UTSUMI, Y. KAMIYA, T. MIZUSHIMA and K. KATO**, "Crystallographic Snapshots of the EF-Hand Protein MCFD2 Complexed with the Intracellular Lectin ERGIC-53 Involved in Glycoprotein Transport," *Acta Crystallogr., Sect. F: Struct. Biol. Commun.* **76**, 216–221 (2020).

## LIST OF PUBLICATIONS

- K. MORISHIMA, A. OKUDA, R. INOUE, N. SATO, Y. MIYAMOTO, R. URADE, M. YAGI-UTSUMI, K. KATO, R. HIRANO, T. KUJIRAI, H. KURUMIZAKA and M. SUGIYAMA**, “Integral Approach to Biomacromolecular Structure by Analytical-Ultracentrifugation and Small-Angle Scattering,” *Commun. Biol.* **3**, 294 (7 pages) (2020).
- M. YAGI-UTSUMI, S. YANAKA, C. SONG, T. SATOH, C. YAMAZAKI, H. KASAHARA, T. SHIMAZU, K. MURATA and K. KATO**, “Characterization of Amyloid  $\beta$  Fibril Formation under Microgravity Conditions,” *NPJ Microgravity* **6**, 17 (6 pages) (2020).
- M. HIRANYAKORN, S. YANAKA, T. SATOH, T. WILASRI, B. JITYUTI, M. YAGI-UTSUMI and K. KATO**, “NMR Characterization of Conformational Interconversions of Lys48-Linked Ubiquitin Chains,” *Int. J. Mol. Sci.* **21**, 5351 (12 pages) (2020).
- K. OKAZAKI, A. NAKAMURA and R. IINO**, “Chemical-State-Dependent Free Energy Profile from Single-Molecule Trajectories of Biomolecular Motor: Application to Processive Chitinase,” *J. Phys. Chem. B* **124**, 6475–6487 (2020). DOI: 10.1021/acs.jpcb.0c02698
- J. ANDO, T. SHIMA, R. KANAZAWA, R. SHIMO-KON, A. NAKAMURA, M. YAMAMOTO, T. KON and R. IINO**, “Small Stepping Motion of Processive Dynein Revealed by Load-Free High-Speed Single-Particle Tracking,” *Sci. Rep.* **10**, 1080 (11 pages) (2020). DOI: 10.1038/s41598-020-58070-y
- A. VISOOTSAT, A. NAKAMURA, P. VIGNON, H. WATANABE, T. UCHIHASHI and R. IINO**, “Single-Molecule Imaging Analysis Reveals the Mechanism of a High-Catalytic-Activity Mutant of Chitinase A from *Serratia marcescens*,” *J. Biol. Chem.* **295**, 1915–1925 (2020). DOI: 10.1074/jbc.RA119.012078
- J. ANDO, A. NAKAMURA, M. YAMAMOTO, C. SONG, K. MURATA and R. IINO**, “Multicolor High-Speed Tracking of Single Biomolecules with Silver, Gold, Silver-Gold Alloy Nanoparticles,” *ACS Photonics* **6**, 2870–2883 (2019). DOI: 10.1021/acspophotonics.9b00953
- T. IIDA, Y. MINAGAWA, H. UENO, F. KAWAI, T. MURATA and R. IINO**, “Single-Molecule Analysis Reveals Rotational Substeps and Chemo-Mechanical Coupling Scheme of *Enterococcus hirae* V<sub>1</sub>-ATPase,” *J. Biol. Chem.* **294**, 17017–17030 (2019). DOI: 10.1074/jbc.ra119.008947.
- M. MATSUO, Y. HIRATA, K. KURIHARA, T. TOYOTA, T. MIURA, K. SUZUKI and T. SUGAWARA**, “Environment-Sensitive Intelligent Self-Reproducing Artificial Cell with a Modification-Active Lipo-Deoxyribozyme,” *Micromachines* **11**, 606 (18 pages) (2020).
- A. OHTAKA, M. KAWASE, A. USAMI, S. FUKUI, M. YAMASHITA, K. YAMAGUCHI, A. SAKON, T. SHIRAKI, T. ISHIDA, S. NAGATA, Y. KIMURA, G. HAMASAKA, Y. UOZUMI, T. SHINAGAWA, O. SHIMOMURA and R. NOMURA**, “Mechanistic Study on Allylic Arylation in Water with Linear Polystyrene-Stabilized Pd and PdO Nanoparticles,” *ACS Omega* **4**, 15764–15770 (2019).
- G. HAMASAKA, D. ROY, A. TAZAWA and Y. UOZUMI**, “Arylation of Terminal Alkynes by Aryl Iodides Catalyzed by a Parts-per-Million Loading of Palladium Acetate,” *ACS Catal.* **9**, 11640–11646 (2019).
- H. OHTA, K. TOBAYASHI, A. KUROO, M. NAKATSUKA, H. KOBAYASHI, A. FUKUOKA, G. HAMASAKA, Y. UOZUMI, H. MURAYAMA, M. TOKUNAGA and M. HAYASHI**, “Surface Modification of a Supported Pt Catalyst Using Ionic Liquids for Selective Hydrodeoxygenation of Phenols into Arenes under Mild Conditions,” *Chem. –Eur. J.* **25**, 14762–14766 (2019).
- S. ICHII, G. HAMASAKA and Y. UOZUMI**, “The Hiyama Cross-Coupling Reaction at Parts Per Million Levels of Pd: In Situ Formation of Highly Active Spirosilicates in Glycol Solvents,” *Chem. –Asian J.* **14**, 3850–3854 (2019).
- H. HU, H. OTA, H. BAEK, K. SHINOHARA, T. MASE, Y. UOZUMI and Y. M. A. YAMADA**, “Second-Generation meta-Phenolsulfonic Acid–Formaldehyde Resin as a Catalyst for Continuous-Flow Esterification,” *Org. Lett.* **22**, 160–163 (2020).
- T. OSAKO, J. SRISA, K. TORII, G. HAMASAKA and Y. UOZUMI**, “Iterative Preparation of Platinum Nanoparticles in an Amphiphilic Polymer Matrix: Regulation of Catalytic Activity in Hydrogenation,” *Synlett* **31**, 147–152 (2020).
- H. BAEK, K. KASHIMURA, T. FUJII, S. TSUBAKI, Y. WADA, S. FUJIKAWA, T. SATO, Y. UOZUMI and Y. M. A. YAMADA**, “Production of Bio Hydrofined Diesel, Jet Fuel, and Carbon Monoxide from Fatty Acids Using a Silicon Nanowire Array-Supported Rhodium Nanoparticle Catalyst under Microwave Conditions,” *ACS Catal.* **10**, 2148–2156 (2020).
- R. N. DHITAL, A. SEN, T. SATO, H. HU, R. ISHII, D. HASHIZUME, H. TAKAYA, Y. UOZUMI and Y. M. A. YAMADA**, “Activator-Promoted Aryl Halide-Dependent Chemoselective Buchwald–Hartwig and Suzuki–Miyaura Type Cross-Coupling Reactions,” *Org. Lett.* **22**, 4797–4801 (2020).
- S. MIZUNO, H. TSUJI, Y. UOZUMI and M. KAWATSURA**, “Synthesis of  $\alpha$ -Tertiary Amines by the Ruthenium-catalyzed Regioselective Allylic Amination of Tertiary Allylic Esters,” *Chem. Lett.* **49**, 645–647 (2020).
- C. OHDE, T. KUSAMOTO and H. NISHIHARA**, “Effects of Halogen Atom Replacement on the Structure and Magnetic Properties of a Molecular Crystal with Supramolecular Two-Dimensional Network Mediated via Sulfur’s  $\sigma$ -Holes,” *J. Magn. Magn. Mater.* **497**, 165986 (6 pages) (2020).
- H. MAEDA, A. BAJPAYEE, T. KUSAMOTO and H. NISHIHARA**, “Construction of Bis(2,6-bis(1-methylbenzimidazol-2-yl)pyridine)iron(II) Coordination Polymer for Incorporation of Magnetic Function,” *J. Inorg. Organomet. Polym. Mater.* **30**, 147–152 (2020).
- Y. LI, Y. SEGAWA, A. YAGI and K. ITAMI**, “A Nonalternant Aromatic Belt: Methylene-Bridged [6]Cycloparaphenylenes Synthesized from Pillar[6]arene,” *J. Am. Chem. Soc.* **142**, 12850–12856 (2020).
- H. SHUDO, M. KUWAYAMA, Y. SEGAWA and K. ITAMI**, “Synthesis of Cycloptycenes from Carbon Nanobelt,” *Chem. Sci.* **11**, 6775–6779 (2020).
- A. NAKA (FUKAZAWA), S. S. W. OEY (Kyoto University)**, “Diaryldithienophosphorines and Near-Infrared Absorbing Dyes Using These Compounds,” JP2020/036443, 2020.

## Research Center of Integrative Molecular Systems

- K. ITO-MIWA, Y. FURUIKE, S. AKIYAMA and T. KONDO, "Tuning the Circadian Period of Cyanobacteria up to 6.6 Days by the Single Amino Acid Substitutions in KaiC," *Proc. Natl. Acad. Sci. U. S. A.* **117**, 20926–20931 (2020). doi.org/10.1073/pnas.2005496117
- I. ANZAI, E. TOKUDA, S. HANDA, H. MISAWA, S. AKIYAMA and Y. FURUKAWA, "Oxidative Misfolding of Cu/Zn-Superoxide Dismutase Triggered by Non-Canonical Intramolecular Disulfide Formation," *Free Radical Biol. Med.* **147**, 187–199 (2020). doi.org/10.1016/j.freeradbiomed.2019.12.017
- Y. KAWAKAMI, T. AMANO, H. OHASHI, H. ITOH, Y. NAKAMURA, H. KISHIDA, T. SASAKI, G. KAWAGUCHI, H. M. YAMAMOTO, K. YAMAMOTO, S. ISHIHARA, K. YONEMITSU and S. IWAI, "Petahertz Non-Linear Current in a Centrosymmetric Organic Superconductor," *Nat. Commun.* **11**, 4138 (6 pages) (2020).
- Y. NABEI, D. HIROBE, Y. SHIMAMOTO, K. SHIOTA, A. INUI, Y. KOUSAKA, Y. TOGAWA and H. M. YAMAMOTO, "Current-Induced Bulk Magnetization of a Chiral Crystal CrNb<sub>3</sub>S<sub>6</sub>," *Appl. Phys. Lett.* **117**, 052408 (5 pages) (2020).
- A. INUI, R. AOKI, Y. NISHIUE, K. SHIOTA, Y. KOUSAKA, H. SHISHIDO, D. HIROBE, M. SUDA, J. OHE, J. KISHINE, H. M. YAMAMOTO and Y. TOGAWA, "Chirality-Induced Spin-Polarized State of a Chiral Crystal CrNb<sub>3</sub>S<sub>6</sub>," *Phys. Rev. Lett.* **124**, 166602 (6 pages) (2020).
- Y. KAWASUGI, K. SEKI, J. PU, T. TAKENOBU, S. YUNOKI, H. M. YAMAMOTO and R. KATO, "Non-Fermi-Liquid Behavior and Doping Asymmetry in an Organic Mott Insulator Interface," *Phys. Rev. B* **100**, 115141 (7 pages) (2019).
- G. KAWAGUCHI and H. M. YAMAMOTO, "Control of Organic Superconducting Field-Effect Transistor by Cooling Rate," *Crystals* **9**, 605 (8 pages) (2019).
- S. OGIKUBO, G. HASHIMOTO, T. UBE, M. SUDA, H. M. YAMAMOTO and T. IKEDA, "Photoinduced Deformation and Isomerization of Azobenzene Liquid-Crystalline Polymer Films at Cryogenic Temperature," *Mol. Cryst. Liq. Cryst.* **676**, 30–35 (2019).
- T. CHOOPPAWA, S. NAMUANGRUK, H. M. YAMAMOTO, V. PROMARAK and P. RASHATASAKHON, "Synthesis, Characterization, and Hole-Transporting Properties of Benzotriazatruxene Derivatives," *J. Mater. Chem. C* **7**, 15035–15041 (2019).
- Y. SHIOMI, J. LUSTIKOVA, S. WATANABE, D. HIROBE, S. TAKAHASHI and E. SAITO, "Spin Pumping from Nuclear Spin Waves," *Nat. Phys.* **15**, 22–26 (2019).
- M. KAMEDA, D. HIROBE, S. DAIMON, Y. SHIOMI, S. TAKAHASHI and E. SAITO, "Microscopic Formulation of Nonlinear Spin Current Induced by Spin Pumping," *J. Magn. Magn. Mater.* **476**, 459–463 (2019).
- N. ITO, T. KIKKAWA, J. BARKER, D. HIROBE, Y. SHIOMI and E. SAITO, "Spin Seebeck Effect in Layered Ferromagnetic Insulators CrSiTe<sub>3</sub> and CrGeTe<sub>3</sub>," *Phys. Rev. B* **100**, 060402(R) (6 pages) (2019).

## Division of Advanced Molecular Science

- Y. TAMURA, H. TAKEZAWA and M. FUJITA, "A Robust Double-Walled Knotted Cage Revealed Guest Binding through Adaptive Portal Expansion," *Chem. Lett.* **49**, 912–914 (2020). DOI: 10.1246/cl.200282
- H. TAKEZAWA, K. SHITOZAWA and M. FUJITA, "Enhanced Reactivity of Twisted Amides Inside a Molecular Cage," *Nat. Chem.* **12**, 574–578 (2020). DOI: 10.1038/s41557-020-0455-y
- Y. MORISHITA, T. SONOHARA, T. TANIGUCHI, K. ADACHI, M. FUJITA and T. ASAI, "Synthetic-Biology-Based Discovery of a Fungal Macrolide from Macrophomina Phaseolina," *Org. Biomol. Chem.* **18**, 2813–2816 (2020). DOI: 10.1039/D0OB00519C
- Y. TAMURA, H. TAKEZAWA and M. FUJITA, "A Double-Walled Knotted Cage for Guest-Adaptive Molecular Recognition," *J. Am. Chem. Soc.* **142**, 5504–5508 (2020). DOI: 10.1021/jacs.0c00459
- I. MORITA, T. MORI, T. MITSUHASHI, S. HOSHINO, Y. TANIGUCHI, T. KIKUCHI, K. NAGAE, N. NASU, M. FUJITA, T. OHWADA and I. ABE, "Exploiting a C–N Bond Forming Cytochrome P450 Monooxygenase for C–S Bond Formation," *Angew. Chem., Int. Ed.* **59**, 3988–3993 (2020). DOI: 10.1002/anie.201916269
- Y. INOMATA, T. SAWADA and M. FUJITA, "Metal-Peptide Torus Knots from Flexible Short Peptides," *Chem* **6**, 294–303 (2020). DOI: 10.1016/j.chempr.2019.12.009
- Y. DOMOTO, M. ABE, T. KIKUCHI and M. FUJITA, "Self-Assembly of Coordination Polyhedra with Highly Entangled Faces Induced by Metal–Acetylene Interactions," *Angew. Chem., Int. Ed.* **59**, 3450–3454 (2020). DOI: 10.1002/anie.201913142
- Y. KANAZAWA, T. MITSUDOME, H. TAKAYA and M. HIRANO, "Pd/Cu-Catalyzed Dehydrogenative Coupling of Dimethyl Phthalate: Synchrotron Radiation Sheds Light on the Cu Cycle Mechanism," *ACS Catal.* **10**, 5909–5919 (2020).

## Division of Research Innovation and Collaboration

- T. KAWASAKI, V. YAHIA and T. TAIRA, "High Brightness Micro-MOPA (Master Oscillator Power Amplifier) with 100-Hz and 100-mJ Operation," *Rev. Laser Eng.* **47(4)**, 221–224 (2019). (in Japanese)
- L. ZHENG, A. KAUSAS and T. TAIRA, ">30 MW Peak Power from Distributed Face Cooling Tiny Integrated Laser," *Opt. Express* **27**, 30217–30224 (2019). DOI: 10.1364/OE.27.030217
- H. H. LIM and T. TAIRA, "High Peak Power Nd:YAG/Cr:YAG Ceramic Microchip Laser with Unstable Resonator," *Opt. Express* **27**, 31307–31315 (2019). DOI: 10.1364/OE.27.031307

## LIST OF PUBLICATIONS

---

- T. SANO, T. EIMURA, A. HIROSE, Y. KAWAHITO, S. KATAYAMA, K. ARAKAWA, K. MASAKI, A. SHIRO, T. SHOBU and Y. SANO**, “Improving Fatigue Performance of Laser-Welded 2024-T3 Aluminum Alloy Using Dry Laser Peening,” *Metals* **9**, 1192 (13 pages) (2019). DOI: 10.3390/met9111192
- H. ISHIZUKI and T. TAIRA**, “Polarity Inversion of Crystal Quartz Using a Quasi-Phase Matching Stamp,” *Opt. Express* **28**, 6505–6510 (2020). DOI: 10.1364/OE.386991
- F. CASSOURET, A. KAUSAS, V. YAHIA, G. AKA, P. LOISEAU and T. TAIRA**, “High Peak-Power Near-MW Laser Pulses by Third Harmonic Generation at 355 nm in Ca<sub>5</sub>(BO<sub>3</sub>)<sub>3</sub>F Nonlinear Single Crystals,” *Opt. Express* **28**, 10524–10530 (2020). DOI: 10.1364/OE.384281
- O. SAITO, E. SEN, Y. OKABE, N. HIGUCHI, H. ISHIZUKI and T. TAIRA**, “Laser Wavelengths Suitable for Generating Ultrasonic Waves in Resin-Coated Carbon Fiber Composites,” *ASME J. Nondestructive Evaluation*, **3**, 031103 (11 pages) (2020). DOI: 10.1115/1.4046719
- K. TAMURA, H. OHBA, M. SAEKI, T. TAGUCHI, H. H. LIM, T. TAIRA and I. WAKAIDA**, “Development of a Laser-Induced Breakdown Spectroscopy System Using a Ceramic Micro-Laser for Fiber-Optic Remote Analysis,” *J. Nucl. Sci. Technol.* **57**, 1189–1198 (2020). DOI: 10.1080/00223131.2020.1776648
- Y. SANO**, “Quarter Century Development of Laser Peening without Coating,” *Metals* **10**, 152 (11 pages) (2020). DOI: 10.3390/met10010152
- Y. SANO, K. AKITA and T. SANO**, “A Mechanism for Inducing Compressive Residual Stresses on a Surface by Laser Peening without Coating,” *Metals* **10**, 816 (12 pages) (2020). DOI: 10.3390/met10060816
- S. TOKITA, H. KOKAWA, S. KODAMA, Y. S. SATO, Y. SANO, Z. LI, K. FENG and Y. WU**, “Suppression of Intergranular Corrosion by Surface Grain Boundary Engineering of 304 Austenitic Stainless Steel Using Laser Peening Plus Annealing,” *Mater. Today Commun.* **25**, 101572 (7 pages) (2020). DOI: 10.1016/j.mtcomm.2020.101572