

# PUBLICATIONS

## DIVISION OF SYNTHETIC CHEMISTRY

### — Organoelement Chemistry —

Jin, S.; Vu, H. T.; Hioki, K.; Noda, N.; Yoshida, H.; Shimane, T.; Ishizuka, S.; Takashima, I.; Mizuhata, Y.; Beverly, Pe K.; Ogawa, T.; Nishimura, N.; Packwood, D.; Tokitoh, N.; Kurata, H.; Yamasaki, S.; Ishii, K. J.; Uesugi M., Discovery of Self-Assembling Small Molecules as Vaccine Adjuvants, *Angew. Chem. Int. Ed. Engl.*, **60**, 961-969 (2021).

Iwai, K.; Mizuhata, Y.; Tokitoh, N., Alkali-Metal-Ion-Centered Sandwich Structures of 4-Bromophenyl[tris(pentafluorophenyl)] Borates and Their Synthetic Utility, *Organometallics*, **40**, 570-577 (2021).

Murai, T.; Lu, W.; Kuribayashi, T.; Morisaki, K.; Ueda, Y.; Hamada, S.; Kobayashi, Y.; Sasamori, T.; Tokitoh, N.; Kawabata, T.; Furuta, T., Conformational Control in Dirhodium (II) Paddlewheel Catalysts Supported by Chalcogen-Bonding Interactions for Stereoselective Intramolecular C-H Insertion Reactions, *ACS Catal.*, **11**, 595-607 (2021).

Omatsu, Y.; Mizuhata, Y.; Tokitoh, N., Easily Separable Cyclic Oligosilanes with *p*-Methoxyphenyl Groups and Their Stereoselective Functionalization, *Eur. J. Inorg. Chem.*, **2021**, 1005-1012 (2021).

Hyakutake, R.; Yoshimura, T.; Sasamori, T.; Tokitoh, N.; Morisaki, K.; Kawabata, T., Decisive Effects of *c-n* Axial Chirality of Intermediary Enolates on the Stereochemical Course of  $\beta$ -Lactam Formation from  $\beta$ -Branched  $\alpha$ -Amino Acid Derivatives via Memory of Chirality, *Heterocycles*, **103(2)**, 995-1010 (2021).

Yanagisawa, T.; Mizuhata, Y.; Tokitoh, N., A Novel Reactivity of Phosphanylaluminum (>P-Al<): Reversible Addition of a Saturated Interelement Bond to Olefins, *Chem. Eur. J.*, **27**, 11273-11278 (2021).

Nagata, M.; Min, H.; Watanabe, E.; Fukumoto, H.; Mizuhata, Y.; Tokitoh, N.; Agou, T.; Yasuda, T., Fused-Nonacyclic Multi-Resonance Delayed Fluorescence Emitter Based on Ladder-Thiaborin Exhibiting Narrowband Sky-Blue Emission with Accelerated Reverse Intersystem Crossing, *Angew. Chem. Int. Ed. Engl.*, **60**, 20280-20285 (2021).

Garcia, J. A.; Yukimoto, M.; Mizuhata, Y.; Tokitoh, N., A Unique 1,4-Silyl Group Migration from Carbon to Carbon: Formation of Benzylic Silane in the Reaction of Sterically Hindered Benzylic Telluride with Alkylolithium, *J. Organomet. Chem.*, **956**, 122119 (2021).

Nagata, M.; Oshiro, T.; Mizuhata, Y.; Tokitoh, N.; Hosoya, T.; Yamada, S.; Konno, T.; Fukumoto, H.; Kubota, T.; Agou, T., Synthesis of Carbazole-Fused Azaborines via a Pd-Catalyzed C-H Activation-Cyclization Reaction, *Bull. Chem. Soc. Jpn.*, **94(1)**, 21-23, (2021).

### — Structural Organic Chemistry —

Zhang, S.; Hashikawa, Y.; Murata, Y., Cage-Expansion of Fullerenes, *J. Am. Chem. Soc.*, **143**, 12450-12454 (2021).

Suárez, M.; Makowski, K.; Lemos, R.; Almagro, L.; Rodríguez, H.; Herranz, M. Á.; Molero, D.; Ortiz, O.; Maroto, E.; Albericio, F.; Murata, Y.; Martín, N., An Androsterone-H<sub>2</sub>@C<sub>60</sub> hybrid: Synthesis, Properties and Molecular Docking Simulations with SARS-Cov-2, *ChemPlusChem*, **86**, 972-981 (2021).

Hashikawa, Y.; Kizaki, K.; Murata, Y., Pressure-Induced Annulative Orifice Closure of a Cage-Opened C<sub>60</sub> derivative, *Chem. Commun. (Camb)*, **57**, 5322-5325 (2021).

Hashikawa, Y.; Hasegawa, S.; Murata, Y., Photochemical Orifice Expansion of a Cage-Opened C<sub>60</sub> Derivative, *Org. Lett.*, **23**, 3854-3858 (2021).

Hashikawa, Y.; Li, H.; Murata, Y., Reactions of C<sub>60</sub> with Pyridazine and Phthalazine, *Chem. Eur. J.*, **27**, 7507-7511 (2021).

Horii, Y.; Suzuki, H.; Miyazaki, Y.; Nakano, M.; Hasegawa, S.; Hashikawa, Y.; Murata, Y., Dynamics and Magnetic Properties of NO Molecules Encapsulated in Open-Cage Fullerene Derivatives Evidenced by Low Temperature Heat Capacity, *Chem. Phys.*, **23**, 10251-10256 (2021).

Hashikawa, Y.; Li, J.; Okamoto, S.; Murata, Y., Reactions on a 1,2-Dicarbonyl Moiety of a Fullerene Skeleton, *Chem. Eur. J.*, **27**, 7235-7238 (2021).

Shugai, A.; Nagel, U.; Murata, Y.; Li, Y.; Mamone, S.; Krachmalnicoff, A.; Alom, S.; Whitby, R. J.; Levitt, M. H.; Rõm, T., Infrared Spectroscopy of an Endohedral Water in Fullerene, *J. Chem. Phys.*, **154**, 124311 (2021).

Hashikawa, Y.; Okamoto, S.; Murata, Y., Nonclassical Abramov Products Formed on Orifices of Cage-Opened C<sub>60</sub> Derivatives, *Chem. Eur. J.*, **27**, 4864-4868 (2021).

Hashikawa, Y.; Hasegawa, S.; Murata, Y., Precise Fixation of an NO Molecule inside Carbon Nanopores: A Long-Range Electron-Nuclear Interaction, *Angew. Chem. Int. Ed. Engl.*, **60**, 2866-2870 (2021).

Hashikawa, Y.; Murata, Y., Water-Mediated Thermal Rearrangement of a Cage-Opened C<sub>60</sub> Derivative, *ChemPlusChem*, **86**, 1559-1562 (2021).

Sakamaki, D.; Tanaka, S.; Tanaka, K.; Takino, M.; Gon, M.; Tanaka, K.; Hirose, T.; Hirobe, D.; Yamamoto, H. M.; Fujiwara, H., Double Heterohelices Composed of Benzo[b]- and Dibenzo[b,i]phenoxazine: A Comprehensive Comparison of Their Electronic and Chiroptical Properties, *J. Phys. Chem. Lett.*, **12**, 9283-9292 (2021).

Fukushima, T.; Tamaki, K.; Isobe, A.; Hirose, T.; Shimizu, N.; Takagi, H.; Haruki, R.; Adachi, S.-I.; Hollamby, M. J.; Yagai, S., Diethylene-Powered Light-Induced Folding of Supramolecular Polymers, *J. Am. Chem. Soc.*, **143**, 5845-5854 (2021).

Kubo, H.; Hirose, T.; Shimizu, D.; Matsuda, K., Donor-Acceptor Type [5]Helicene Derivative with Strong Circularly Polarized Luminescence, *Chem. Lett.*, **50**, 804-807 (2021).

Kato, S.-I.; Kumagai, R.; Abe, T.; Higuchi, C.; Shiota, Y.; Yoshizawa, K.; Takahashi, N.; Yamamoto, K.; Hossain, M. Z.; Hayashi, K.; Hirose, T.; Nakamura, Y., Arylene-Hexaynylene and -Octaynylene Macrocycles: Extending the Polyyne Chains Drives Self-Association by Enhanced Dispersion Force, *Chem. Commun. (Camb)*, **57**, 576-579 (2021).

Kubo, H.; Hirose, T.; Nakashima, T.; Kawai, T.; Hasegawa, J.-Y.; Matsuda, K., Tuning Transition Electric and Magnetic Dipole Moments: [7]Helicenes Showing Intense Circularly Polarized Luminescence, *J. Phys. Chem. Lett.*, **12**, 686-695 (2021).

Shimizu, A.; Ishizaki, Y.; Horiuchi, S.; Hirose, T.; Matsuda, K.; Sato, H.; Yoshida, J.-I., HOMO-LUMO Energy-Gap Tuning of  $\pi$ -Conjugated Zwitterions Composed of Electron-Donating Anion and Electron-Accepting Cation, *J. Org. Chem.*, **86**, 770-781 (2021).

Ohmura, T.; Morimasa, Y.; Ichino, T.; Miyake, Y.; Murata, Y.; Sugimoto, M.; Tajima, K.; Taketsugu, T.; Maeda, S., Mechanism of 2,6-Dichloro-4,4'-Bipyridine-Catalyzed Diboration of Pyrazines Involving a Bipyridine-Stabilized Boryl Radical, *Bull. Chem. Soc. Jpn.*, **94**, 1894-1902 (2021).

Hashikawa, Y.; Sadai S.; Murata, Y., Reductive Decarbonylation of a Cage-Opened C<sub>60</sub> Derivative, *Org. Lett.*, **23**, 9495-9499 (2021).

Du S.; Hashikawa Y.; Ito H.; Hashimoto K.; Murata Y.; Hirayama Y.; Hirakawa K., Inelastic Electron Transport and Ortho-Para Fluctuation of Water Molecule in H<sub>2</sub>O@C<sub>60</sub> Single Molecule Transistors, *Nano Lett.*, **21**, 10346-10353 (2021).

Hashikawa Y.; Murata Y., Synthesis and Oligomerization of CpM(CO)<sub>2</sub>, *ACS Omega*, **6**, 34137-34141 (2021).

Hashikawa, Y.; Sadai S.; Murata, Y., Amino-Functionalized Cage-Opened C<sub>60</sub> Derivatives, *Org. Lett.*, **23**, 9586-9590 (2021).

#### — Synthetic Organic Chemistry —

Imayoshi, A.; Lakshmi, B. V.; Ueda, Y.; Yoshimura, T.; Matayoshi, A.; Furuta, T.; Kawabata, T., Enantioselective Preparation of Mechanically Planar Chiral Rotaxanes by Kinetic Resolution Strategy, *Nat. Commun.*, **12**, 404 (2021).

Chen, G.; Arai, K.; Morisaki, K.; Kawabata, T.; Ueda, Y., Dirhodium-Catalyzed Chemo- and Site-Selective C-H Amidation of *N*, *N*-Dialkylanilines, *Synlett*, **32**, 728-732 (2021).

Shibayama, H.; Ueda, Y.; Tanaka, T.; Kawabata, T., Seven-Step Stereodivergent Total Syntheses of Punicafolin and Macaranginin, *J. Am. Chem. Soc.*, **143**, 1428-1434 (2021).

Murai, T.; Lu, W.; Kuribayashi, T.; Morisaki, K.; Ueda, Y.; Hamada, S.; Kobayashi, Y.; Sasamori, T.; Tokitoh, N.; Kawabata, T.; Furuta, T., Conformational Control in Dirhodium(II) Paddlewheel Catalysts Supported by Chalcogen-Bonding Interactions for Stereoselective Intramolecular C-H Insertion Reactions, *ACS Catal.*, **11**, 595-607 (2021).

Xing, Y.; Nikaido, M.; Murai, T.; Hamada, S.; Kobayashi, Y.; Sasamori, T.; Kawabata, T.; Furuta, T., Concise Synthesis of an Amide-Functionalized [7]Helicene-Like Molecule via Intramolecular Amidation, *Heterocycles*, **103**, 544-553 (2021).

Hyakutake, R.; Yoshimura, T.; Sasamori, T.; Tokitoh, N.; Morisaki, K.; Kawabata, T., Decisive Effects of C-N Axial Chirality of Intermediary Enolates on the Stereochemical Course of  $\beta$ -Lactam Formation from  $\beta$ -Branched  $\alpha$ -Amino Acid Derivatives via Memory of Chirality, *Heterocycles*, **103**, 995-1010 (2021).

Ueda, Y., Site-Selective Molecular Transformation: Acylation of Hydroxy Groups and C-H Amination, *Chem. Pharm. Bull. (Tokyo)*, **69**, 931-944 (2021).

Hamada, S.; Yano, K.; Kobayashi, Y.; Kawabata, T.; Furuta, T., Oxidation of Cyclic Benzylic Ethers by an Electronically Tuned Nitroxyl Radical, *Tetrahedron Lett.*, **83**, 153404 (2021).

#### — Advanced Inorganic Synthesis —

Yumoto, G.; Hirori, H.; Sekiguchi, F.; Sato, R.; Saruyama, M.; Teranishi, T.; Kanemitsu, Y., Strong Spin-Orbit Coupling Inducing Autler-Townes Effect in Lead Halide Perovskite Nanocrystals, *Nat. Commun.*, **12**, 3026 (2021).

Zhang, J.; Sakai, H.; Suzuki, K.; Hasobe, T.; Tkachenko, N. V.; Chang, I.-Y.; Hyeon-Deuk, K.; Kaji, H.; Teranishi, T.; Sakamoto, M., Near-Unity Singlet Fission on a Quantum Dot Initiated by Resonant Energy Transfer, *J. Am. Chem. Soc.*, **143**, 17388-17394 (2021).

Cho, K.; Yamada, T.; Tahara, H.; Tadano, T.; Suzuura, H.; Saruyama, M.; Sato, R.; Teranishi, T.; Kanemitsu, Y., Luminescence Fine Structures in Single Lead Halide Perovskite Nanocrystals: Size Dependence of the Exciton-Phonon Coupling, *Nano Lett.*, **21**, 7206-7212 (2021).

Li, Z.; Saruyama, M.; Asaka, T.; Tatetsu, Y.; Teranishi, T., Determinants of Crystal Structure Transformation of Ionic Nanocrystals in Cation Exchange Reactions, *Science*, **373**, 332-337 (2021).

Wang, L.; Takeda, S.; Sato, R.; Sakamoto, M.; Teranishi, T.; Tamai, N., Morphology-Dependent Coherent Acoustic Phonon Vibrations and Phonon Beat of Au Nanopolyhedrons, *ACS Omega*, **6**, 5485-5489 (2021).

Saruyama, M.; Sato, R.; Teranishi, T., Transformations of Ionic Nanocrystals via Full and Partial Ion Exchange Reactions, *Acc. Chem. Res.*, **54**, 765-775 (2021).

Isozaki, K.; Ueno, R.; Ishibashi, K.; Nakano, G.; Yin, H.; Iseri, K.; Sakamoto, M.; Takaya, H.; Teranishi, T.; Nakamura, M., Gold Nanocluster Functionalized with Peptide Dendron Thiolates: Acceleration of the Photocatalytic Oxidation of an Amino Alcohol in a Supramolecular Reaction Field, *ACS Catal.*, **11**, 13180-13187 (2021).

Nakagawa, K.; Hirori, H.; Sanari, Y.; Sekiguchi, F.; Sato, R.; Saruyama, M.; Teranishi, T.; Kanemitsu, Y., Interference Effects in High-Order Harmonics from Colloidal Perovskite Nanocrystals Excited by an Elliptically Polarized Laser, *Phys. Rev. Mater.*, **5**, 16001 (2021).

Trinh, T. T.; Kim, J.; Sato, R.; Matsumoto, K.; Teranishi, T., Synthesis of Mesoscopic Particles of Multi-Component Rare Earth Permanent Magnet Compounds, *Sci. Technol. Adv. Mater.*, **22**, 37-54 (2021).

Kawawaki, T.; Kataoka, Y.; Hirata, M.; Akinaga, Y.; Takahata, R.; Wakamatsu, K.; Fujiki, Y.; Kataoka, M.; Kikkawa, S.; Alotabi, A. S.; Hossain, S.; Osborn, D. J.; Teranishi, T.; Andersson, G. G.; Metha, G. F.; Yamazoe, S.; Negishi, Y., Creation of High-Performance Heterogeneous Photocatalysts by Controlling Ligand Desorption and Particle Size of Gold Nanocluster, *Angew. Chem. Int. Ed. Engl.*, **60**, 21340-21350 (2021).

Oshime, N.; Ohwada, K.; Sugawara, K.; Abe, T.; Yamauchi, R.; Ueno, T.; MacHida, A.; Watanuki, T.; Ueno, S.; Fujii, I.; Wada, S.; Sato, R.; Teranishi, T.; Yamauchi, M.; Ishii, K.; Toyokawa, H.; Momma, K.; Kuroiwa, Y., Bragg Coherent Diffraction Imaging Allowing Simultaneous Retrieval of Three-Dimensional Shape and Strain Distribution for 40-500 nm Particles, *Jpn. J. Appl. Phys.*, **60**, SFFA07 (2021).

## DIVISION OF MATERIALS CHEMISTRY — Chemistry of Polymer Materials —

Miyazaki, M.; Nakano, K.; Tadokoro, C.; Vlădescu, S.-C.; Reddyhoff, T.; Sasaki, S.; Tsujii, Y., Enhancing Durability of Concentrated Polymer Brushes Using Microgrooved Substrates, *Wear*, **482-483**, 203984 (2021).

Watanabe, S.; Kodama, E.; Tadokoro, C.; Sakakibara, K.; Nakano, K.; Sasaki, S.; Tsujii, Y., Durability Improvement of Concentrated Polymer Brushes by Multiscale Texturing, *Tribol. Lett.*, **69**, 99 (2021).

Nakanishi, Y.; Sakakibara, K.; Nakamichi, K.; Ohno, K.; Morinaga, T.; Sato, T.; Sagawa, T.; Tsujii, Y., Concentrated-Polymer-Brush-Modified Silica Nanoparticles Self-Assembled in Ionic Liquid Containing Iodide/Triiodide (I-/I<sub>3</sub>-)-Redox System as Quasi-Solid Electrolytes for Dye-Sensitized Solar Cells, *ACS Appl. Nano Mater.*, **4**, 6620-6628 (2021).

Sakakibara, K.; Ishida, H.; Kinose, Y.; Tsujii, Y., Regioselective Synthesis of Cellulosic Janus Bottlebrushes with Polystyrene and Poly ( $\epsilon$ -Caprolactone) Side Chains and Their Solid-State Microphase Separation, *Cellulose*, **28**, 6857-6868 (2021).

Yoshikawa, C.; Sakakibara, K.; Nonsuwan, P.; Yamazaki, T.; Tsujii, Y., Nonbiofouling Coatings Using Bottlebrushes with Concentrated Polymer Brush Architecture, *Biomacromolecules*, **22**, 2505-2514 (2021).

Kinose, Y.; Sakakibara, K.; Sato, O.; Tsujii, Y., Near-Zero Azimuthal Anchoring of Liquid Crystals Assisted by Viscoelastic Bottlebrush Polymers, *ACS Appl. Polym. Mater.*, **3**, 2618-2625 (2021).

Shomura, R.; Sakakibara, K.; Marukane, S.; Nakamichi, K.; Morinaga, T.; Tsujii, Y.; Sato, T., Novel Use of a Pyridinium Salt to Form a Solid Electrolyte Interphase (SEI) on High Voltage Lithium-Excess Layered Positive Active Material, *Bull. Chem. Soc. Jpn.*, **94**, 1594-1601 (2021).

Watanabe, S.; Kodama, E.; Sakakibara, K.; Sasaki, S.; Tsujii, Y., Effect of Surface Texturing on the Durability of Concentrated Polymer Brushes, *Tribol. Int.*, **155**, 106668 (2021).

Sakakibara, K.; Maeda, K.; Yoshikawa, C.; Tsujii, Y., Water Lubricating and Biocompatible Films of Bacterial Cellulose Nanofibers Surface-Modified with Densely Grafted, Concentrated Polymer Brushes, *ACS Appl. Nano Mater.*, **4**, 1503-1511 (2021).

Maguire, S. M.; Krook, N. M.; Kulshreshtha, A.; Bilchak, C. R.; Brosnan, R.; Pana, A.-M.; Rannou, P.; Maréchal, M.; Ohno, K.; Jayaraman, A.; Composto, R. J., Interfacial Compatibilization in Ternary Polymer Nanocomposites: Comparing Theory and Experiments, *Macromolecules*, **54**, 797-811 (2021).

Maguire, S. M.; Boyle, M. J.; Bilchak, C. R.; Demaree, J. D.; Keller, A. W.; Krook, N. M.; Ohno, K.; Kagan, C. R.; Murray, C. B.; Rannou, P.; Composto, R. J., Grafted Nanoparticle Surface Wetting during Phase Separation in Polymer Nanocomposite Films, *ACS Appl. Mater. Interfaces*, **13**, 37628-37637 (2021).

Rakotondravao, H. M.; Ishizuka, N.; Sakakibara, K.; Wada, R.; Ichihashi, E.; Takahashi, R.; Takai, T.; Horiuchi, J.-I.; Kumada, Y., Characterization of a Macroporous Epoxy-Polymer Based Resin for the Ion-Exchange Chromatography of Therapeutic Proteins, *J. Chromatogr. A*, **1656**, 462503 (2021).

Kinose, Y., Structure and Function of Bottlebrush Polymer: [I] Control of Confirmation by Stiff Main Chain and [II] Anchoring Properties of Liquid Crystal Determined by Mobility of Side Chain, *J. Fiber Sci. Technol.*, **77**, 170-177 (2021).

## — Polymer Controlled Synthesis —

Imamura, Y.; Yamago, S., Role of Lewis Acids in Preventing the Degradation of Dithioester-Dormant Species in the RAFT Polymerization of Acrylamides in Methanol to Enable the Successful Dual Control of Molecular Weight and Tacticity, *Polym. Chem.*, **12**, 5336-5341 (2021).

Murata, R.; Wang, Z.; Miyazawa, Y.; Antol, I.; Yamago, S.; Abe, M., SOMO-HOMO Conversion in Triplet Carbenes, *Org. Lett.*, **23**, 4955-4959 (2021).

Li, X.; Ogihara, T.; Kato, T.; Nakamura, Y.; Yamago, S., Evidence for Polarity- and Viscosity-Controlled Pathways in the Termination Reaction in the Radical Polymerization of Acrylonitrile, *Macromolecules*, **54**, 4497-4506 (2021).

Miyazawa, Y.; Wang, Z.; Matsumoto, M.; Hatano, S.; Antol, I.; Kayahara, E.; Yamago, S.; Abe, M., 1,3-Diradicals Embedded in Curved Paraphenylene Units: Singlet Versus Triplet State and In-Plane Aromaticity, *J. Am. Chem. Soc.*, **143**, 7426-7439 (2021).

Park, B.; Tosaka, M.; Yamago, S., Crystallization of Isotactic Poly(*N,N*-Diethyl Acrylamide) Synthesized by Ytterbium Triflate/H<sub>2</sub>O-Catalyzed Stereoselective Radical Polymerization, *Polym. J.*, **53**, 533-538 (2021).

Park, B.; Imamura, Y.; Yamago, S., Stereocontrolled Radical Polymerization of Acrylamides by Ligand-Accelerated Catalysis, *Polym. J.*, **53**, 515-521 (2021).

Li, X.; Kato, T.; Nakamura, Y.; Yamago, S., The Effect of Viscosity on the Coupling and Hydrogen-Abstraction Reaction between Transient and Persistent Radicals, *Bull. Chem. Soc. Jpn.*, **94**, 966-972 (2021).

Matsuki, H.; Okubo, K.; Takaki, Y.; Niihori, Y.; Mitsui, M.; Kayahara, E.; Yamago, S.; Kobayashi, K., Synthesis and Properties of a Cyclohexa-2,7-Anthrylene Ethynylene Derivative, *Angew. Chem. Int. Ed. Engl.*, **60**, 998-1003 (2021).

Jiang, Y.; Fan, W.; Tosaka, M.; Cunningham, M. F.; Yamago, S., Fabrication of Structurally Controlled Poly(*n*-Butyl Acrylate) Particles by *ab initio* Emulsion Organotellurium-Mediated Radical Polymerization. Synthesis of High Molecular Weight Homo and Block Copolymers, *Macromolecules*, **54**, 10691-10699 (2021).

[Others]

Yamago, S., Practical Synthesis of Dendritic Hyperbranched Polymers by Reversible Deactivation Radical Polymerization, *Polym. J.*, **53**, 847-864 (2021).

Yamago, S.; Lu, Y., Recent Developments in Reversible Deactivation Radical Polymerization, *Science of Synthesis*, **5**, 575-606 (2021).

Tosaka, M., Basic Knowledge of Wide-Angle X-Ray Diffraction, *Nippon Gomu Kyokaishi*, **94**(4), 130-135 (2021).

Tosaka, M., X-Ray Analysis of Fiber and Polymer Structures, *Journal of The Society of Fiber Science and Technology, Japan*, **76**(12), 521-528 (2021).

Yamago, S.; Lu, Y., Photocatalytic Living Radical Polymerization, in *Catalytic Reactions for Modern Organic Synthesis 101, The Society of Synthetic Organic Chemistry, Japan, Ed., Tokyo Kagaku Doujin*, pp. 190-191 (2021).

Yamago, S., Living Radical Polymerization by Representative Element Catalysts, in *Catalytic Reactions for Modern Organic Synthesis 101, The Society of Synthetic Organic Chemistry, Japan, Ed., Tokyo Kagaku Doujin*, pp. 188-189 (2021).

#### — Inorganic Photonics Materials —

Hallböck, K. J.; Yamaguchi, T.; Matsuzaki, Y.; Watanabe, H.; Mizuochi, N.; Ishi-Hayase, J., Wide-Field AC Magnetic Field Imaging Using Continuous-Wave Optically Detected Magnetic Resonance of Nitrogen-Vacancy Centers in Diamond, *Proc. SPIE Int. Soc. Opt. Eng.*, **11700**, 117004A (2021).

Nebel, C. E.; Aharonovich, I.; Mizuochi, N.; Hatano, M., Diamond for Quantum Applications Part 2, *Semiconductors and Semimetals*, **104**, 2-259 (2021).

Makino, Y.; Mahiko, T.; Liu, M.; Tsurui, A.; Yoshikawa, T.; Nagamachi, S.; Tanaka, S.; Hokamoto, K.; Ashida, M.; Fujiwara, M.; Mizuochi, N.; Nishikawa, M., Straightforward Synthesis of Silicon Vacancy (SiV) Center-Containing Single-Digit Nanometer Nanodiamonds via Detonation Process, *Diam. Relat. Mater.*, **112**, 108248 (2021).

Herbschleb, E. D.; Kato, H.; Makino, T.; Yamasaki, S.; Mizuochi, N., Ultra-High Dynamic Range Quantum Measurement Retaining Its Sensitivity, *Nat. Commun.*, **12**, 306 (2021).

Kurita, T.; Shimotsuma, Y.; Fujiwara, M.; Fujie, M.; Mizuochi, N.; Shimizu, M.; Miura, K., Direct Writing of High-Density Nitrogen-Vacancy Centers Inside Diamond by Femtosecond Laser Irradiation, *Appl. Phys. Lett.*, **118**, 214001 (2021).

Watanabe, A.; Nishikawa, T.; Kato, H.; Fujie, M.; Fujiwara, M.; Makino, T.; Yamasaki, S.; Herbschleb, E. D.; Mizuochi, N., Shallow NV Centers Augmented by Exploiting n-Type Diamond, *Carbon N. Y.*, **178**, 294-300 (2021).

Matsumoto, K. T.; Kobayashi, M.; Morioka, N.; Hiraoka, K., Specific Heat of Cu Substituted GdNiSi, *Jpn. J. Appl. Phys.*, **60**, 43001 (2021).

Miyashita, K.; Segawa, T. F.; Takeda, K.; Ohki, I.; Onoda, S.; Ohshima, T.; Abe, H.; Takashima, H.; Takeuchi, S.; Shames, A. I.; Morita, K.; Wang, Y.; So, F. T.-K.; Terada, D.; Igarashi, R.; Kagawa, A.; Kitagawa, M.; Mizuochi, N.; Shirakawa, M.; Negoro, M., Room-Temperature Hyperpolarization of Polycrystalline Samples with Optically Polarized Triplet Electrons: Pentacene or Nitrogen-Vacancy Center in Diamond?, *Magn. Reson. (Gott)*, **2**(1), 33-48 (2021).

Morioka, N.; Babin, C.; Nagy, R.; Gediz, I.; Hesselmeier, E.; Liu, D.; Joliffe, M.; Niethammer, M.; Dasari, D.; Vorobyov, V.; Kolesov, R.; Stöhr, R.; Ul-Hassan, J.; Son, N. T.; Ohshima, T.; Udvarhelyi, P.; Thiering, G.; Gali, A.; Wrachtrup, J.; Kaiser, F., Author Correction: Spin-Controlled Generation of Indistinguishable and Distinguishable Photons from Silicon Vacancy Centres in Silicon Carbide, *Nat. Commun.*, **12**, 5978 (2021).

Babin, C.; Stöhr, R.; Morioka, N.; Linkewitz, T.; Steidl, T.; Wörnle, R.; Liu, D.; Hesselmeier, E.; Vorobyov, V.; Denisenko, A.; Hentschel, M.; Gobert, C.; Berwian, P.; Astakhov, G. V.; Knolle, W.; Majety, S.; Saha, P.; Radulaski, M.; Son, N. T.; Ul-Hassan, J.; Kaiser, F.; Wrachtrup, J., Fabrication and Nanophotonic Waveguide Integration of Silicon Carbide Colour centres with Preserved Spin-Optical Coherence, *Nat. Mater.*, **21**, 67-73 (2021).

Prananto, D.; Kainuma, Y.; Hayashi, K.; Mizuochi, N.; Uchida, K. -I.; An, T., Probing Thermal Magnon Current via Nitrogen-Vacancy Centers in Diamond, *Phys. Rev. Appl.*, **16**, 064058 (2021).

Kainuma, Y.; Hayashi, K.; Tachioka, C.; Ito, M.; Makino, T.; Mizuochi, N.; An, T., Scanning Diamond NV Center Magnetometry Probe Fabricated by Laser Cutting and Focused Ion Beam Milling, *J. Appl. Phys.*, **130**, 243903 (2021).

#### — Nanospintronics —

Hung, Y. M.; Shiota, Y.; Hisatomi, R.; Moriyama, T.; Ono, T., High Thermal Stability and Low Driven Current Achieved by Vertical Domain Wall Motion Memory with Artificial Ferromagnet, *Appl. Phys. Express.*, **14**, 23001 (2021).

Ando, F.; Kawarazaki, R.; Naritsuka, M.; Kasahara, Y.; Miyasaka, Y.; Narita, H.; Kan, D.; Shiota, Y.; Moriyama, T.; Shimakawa, Y.; Matsuda, Y.; Ono, T., Investigation of the Upper Critical Field in Artificially Engineered Nb/V/Ta Superlattices, *Jpn. J. Appl. Phys.*, **60**, 60902 (2021).

Nishimura, T.; Kim, D.-Y.; Kim, D.-H.; Nam, Y.-S.; Park, Y.-K.; Kim, N.-H.; Shiota, Y.; You, C.-Y.; Min, B.-C.; Choe, S.-B.; Ono, T., Interfacial Dzyaloshinskii-Moriya Interaction and Damping-like Spin-Orbit Torque in [Co/Gd/Pt]<sub>N</sub> Magnetic Multilayers, *Phys. Rev. B*, **103**, 104409 (2021).

Miyasaka, Y.; Kawarazaki, R.; Narita, H.; Ando, F.; Ikeda, Y.; Hisatomi, R.; Daido, A.; Shiota, Y.; Moriyama, T.; Yanase, Y.; Ono, T., Observation of Nonreciprocal Superconducting Critical Field, *Appl. Phys. Express*, **14**, 73003 (2021).

Kobayashi, Y.; Ikebuchi, T.; Shiota, Y.; Ono, T.; Moriyama, T., Estimation of Magnetic Domain Size in Chiral Antiferromagnet Mn<sub>3</sub>Ir by the Anomalous Hall Measurements, *Journal of the Magnetism Society of Japan*, **45**, 75-78 (2021).

Hung, Y. M.; Shiota, Y.; Yamada, S.; Ohta, M.; Shibata, T.; Sasaki, T.; Hisatomi, R.; Moriyama, T.; Ono, T., Positive Correlation between Interlayer Exchange Coupling and the Driving Current of Domain Wall Motion in a Synthetic Antiferromagnet, *Appl. Phys. Lett.*, **119**, 32407 (2021).

Hayashi, K.; Yamada, K.; Shima, M.; Ohya, Y.; Ono, T.; Moriyama, T., Control of Antiferromagnetic Resonance and the Morin Temperature in Cation Doped  $\alpha$ -Fe<sub>2-x</sub>M<sub>x</sub>O<sub>3</sub> (M = Al, Ru, Rh, and In), *Appl. Phys. Lett.*, **119**, 32408 (2021).

Taga, K.; Hisatomi, R.; Ohnuma, Y.; Sasaki, R.; Ono, T.; Nakamura, Y.; Usami, K., Optical Polarimetric Measurement of Surface Acoustic Waves, *Appl. Phys. Lett.*, **119**, 181106 (2021).

Shiota, Y.; Hisatomi, R.; Moriyama, T.; Samardak, A. S.; Ono, T., Inhomogeneous Magnetic Properties Characterized by Simultaneous Electrical and Optical Detection of Spin-Torque Ferromagnetic Resonance, *Appl. Phys. Lett.*, **119**, 192409 (2021).

Ikebuchi, T.; Kobayashi, Y.; Sugiura, I.; Shiota, Y.; Ono, T.; Moriyama, T., Long-Distance Spin Current Transmission in Single-Crystalline NiO Thin Films, *Appl. Phys. Express.*, **14**, 123001 (2021).

Murayama, H.; Ishida, K.; Kurihara, R.; Ono, T.; Sato, Y.; Kasahara, Y.; Watanabe, H.; Yanase, Y.; Cao, G.; Mizukami, Y.; Shibauchi, T.; Matsuda, Y.; Kasahara, S., Bond Directional Anapole Order in a Spin-Orbit Coupled Mott Insulator  $\text{Sr}_2(\text{Ir}_{1-x}\text{Rh}_x)\text{O}_4$ , *Phys. Rev. X*, **11**, 11021 (2021).

## DIVISION OF BIOCHEMISTRY

### — Biofunctional Design-Chemistry —

Iwata, T.; Hirose, H.; Sakamoto, K.; Hirai, Y.; Arafiles, J. V. V.; Akishiba, M.; Imanishi, M.; Futaki, S., Liquid Droplet Formation and Facile Cytosolic Translocation of IgG in the Presence of Attenuated Cationic Amphiphilic Lytic Peptides, *Angew. Chem. Int. Ed. Engl.*, **60**, 19804-19812 (2021).

Hirai, Y.; Hirose, H.; Imanishi, M.; Asai, T.; Futaki, S., Cytosolic Protein Delivery Using pH-Responsive, Charge-Reversible Lipid Nanoparticles, *Sci. Rep.*, **11**, 19896 (2021).

Sakamoto, K.; Michibata, J.; Hirai, Y.; Ide, A.; Ikitoh, A.; Takatani-Nakase, T.; Futaki, S., Potentiating the Membrane Interaction of an Attenuated Cationic Amphiphilic Lytic Peptide for Intracellular Protein Delivery by Anchoring with Pyrene Moiety, *Bioconjug. Chem.*, **32**, 950-957 (2021).

Arafiles, J. V. V.; Hirose, H.; Hirai, Y.; Kuriyama, M.; Sakyamah, M. M.; Nomura, W.; Sonomura, K.; Imanishi, M.; Otaka, A.; Tamamura, H.; Futaki, S., Discovery of a Macropinocytosis-Inducing Peptide Potentiated by Medium-Mediated Intramolecular Disulfide Formation, *Angew. Chem. Int. Ed. Engl.*, **60**, 11928-11936 (2021).

Sakamoto, K.; Morishita, T.; Aburai, K.; Ito, D.; Imura, T.; Sakai, K.; Abe, M.; Nakase, I.; Futaki, S.; Sakai, H., Direct Entry of Cell-Penetrating Peptide Can Be Controlled by Maneuvering the Membrane Curvature, *Sci. Rep.*, **11**, 31 (2021).

Futaki, S., Functional Peptides that Target Biomembranes: Design and Modes of Action, *Chem. Pharm. Bull. (Tokyo)*, **69**, 601-607 (2021).

Kuroki, K.; Sakai, T.; Masuda, T.; Kawano, K.; Futaki, S., Membrane Anchoring of a Curvature-Inducing Peptide, EpN18, Promotes Membrane Translocation of Octaarginine, *Bioorg. Med. Chem. Lett.*, **43**, 128103 (2021).

Nakata, E.; Hirose, H.; Gerelbaatar, K.; Arafiles, J. V. V.; Zhang, Z.; Futaki, S.; Morii, T., A Facile Combinatorial Approach to Construct a Ratiometric Fluorescent Sensor: Application for the Real-Time Sensing of Cellular pH Changes, *Chem. Sci.*, **12**, 8231-8240 (2021).

Arafiles, J. V. V.; Futaki, S., Chemical Passports to Cross Biological Borders, *Nat. Chem.*, **13**, 517-519 (2021).

Sakamoto, K.; Akishiba, M.; Iwata, T.; Arafiles, J.V.V.; Imanishi, M.; Futaki, S., Use of Homoarginine to Obtain Attenuated Cationic Membrane Lytic Peptides, *Bioorg. Med. Chem. Lett.*, **40**, 127925 (2021).

Ida, H.; Takahashi, Y.; Kumatani, A.; Shiku, H.; Murayama, T.; Hirose, H.; Futaki, S.; Matsue, T., Nanoscale Visualization of Morphological Alteration of Live-Cell Membranes by the Interaction with Oligoarginine Cell-Penetrating Peptides, *Anal. Chem.*, **93**, 5383-5393 (2021).

Nakase, I.; Ueno, N.; Matsuzawa, M.; Noguchi, K.; Hirano, M.; Omura, M.; Takenaka, T.; Sugiyama, A.; Bailey Kobayashi, N.; Hashimoto, T.; Takatani-Nakase, T.; Yuba, E.; Fujii, I.; Futaki, S.; Yoshida, T., Environmental pH Stress Influences Cellular Secretion and Uptake of Extracellular Vesicles, *FEBS Open Bio*, **11**, 753-767 (2021).

Szabó, I.; Illien, F.; Dókus, L. E.; Yousef, M.; Baranyai, Z.; Bősze, S.; Ise, S.; Kawano K.; Sagan, S.; Futaki, S.; Hudecz, F.; Bánóczy, Z., Influence of the DabcyL Group on the Cellular Uptake of Cationic Peptides: Short Oligoarginines as Efficient Cell-Penetrating Peptides, *Amino Acids*, **53**, 1033-1049 (2021).

Kawano, K.; Yokoyama, F.; Kamasaka, K.; Kawamoto, J.; Ogawa, T.; Kurihara, T.; Futaki, S., Design of the N-Terminus Substituted Curvature-Sensing Peptides that Exhibit Highly Sensitive Detection Ability of Bacterial Extracellular Vesicles, *Chem. Pharm. Bull. (Tokyo)*, **69**, 1075-1082 (2021).

### — Chemistry of Molecular Biocatalysts —

Yoda, A.; Mori, N.; Akiyama, K.; Kikuchi, M.; Xie, X.; Miura, K.; Yoneyama, K.; Sato-Izawa, K.; Yamaguchi, S.; Yoneyama, K.; Nelson, D. C.; Nomura, T., Strigolactone Biosynthesis Catalyzed by Cytochrome P450 and Sulfotransferase in Sorghum, *New Phytol.*, **232**, 1999-2010 (2021).

Mashiguchi, K.; Seto, Y.; Yamaguchi, S., Strigolactone Biosynthesis, Transport and Perception, *Plant J.*, **105**, 335-350 (2021).

Akiyama, R.; Watanabe, B.; Nakayasu, M.; Lee, H. J.; Kato, J.; Umemoto, N.; Muranaka, T.; Saito, K.; Sugimoto, Y.; Mizutani, M., The Biosynthetic Pathway of Potato Solanidanes Diverged from That of Spirosolananes Due to Evolution of a Dioxygenase, *Nat. Commun.*, **12**, [1300-1]-[1300-10] (2021).

Nakayasu, M.; Umemoto, N.; Akiyama, R.; Ohyama, K.; Lee, H. J.; Miyachi, H.; Watanabe, B.; Muranaka, T.; Saito, K.; Sugimoto, Y.; Mizutani, M., Characterization of C-26 Aminotransferase, Indispensable for Steroidal Glycoalkaloid Biosynthesis, *Plant J.*, **108**, 81-92 (2021).

Watanabe, B.; Makino, K.; Mizutani, M.; Takaya, H., Synthesis and Structural Confirmation of Calibagenin and Saxosterol, *Tetrahedron*, **91**, [132194-1]-[132194-15] (2021).

Watanabe, B.; Nishitani, S.; Koeduka, T., Synthesis of Deuterium-Labeled Cinnamic Acids: Understanding the Volatile Benzenoid Pathway in the Flowers of the Japanese Loquat *Eriobotrya japonica*, *J. Labelled Comp. Radiopharm.*, **64**, 403-416 (2021).

### — Molecular Biology —

Kuroda, R.; Kato, M.; Tsuge, T.; Aoyama, T., Arabidopsis Phosphatidylinositol 4-Phosphate 5-Kinase Genes PIP5K7, PIP5K8, and PIP5K9 Are Redundantly Involved in Root Growth Adaptation to Osmotic Stress, *Plant J.*, **106**, 913-927 (2021).

Aki, S. S.; Yura, K.; Aoyama, T.; Tsuge, T., SAP130 and CSN1 Interact and Regulate Male Gametogenesis in *Arabidopsis thaliana*, *J Plant Res.*, **134**, 279-289 (2021).

Shimamura, R.; Ohashi, Y.; Taniguchi, Y. Y.; Kato, M.; Tsuge, T.; Aoyama, T., Arabidopsis PLD $\zeta_1$  and PLD $\zeta_2$  Localize to Post-Golgi Membrane Compartments in a Partially Overlapping Manner, *Plant Mol. Biol.*, doi: 10.1007/s11103-021-01205-0 (2021).

— **Chemical Biology** —

Takemoto, Y.; Kadota, S.; Minami, I.; Otsuka, S.; Okuda, S.; Abo, M.; Punzalan, L. L.; Shen, Y.; Shiba, Y.; Uesugi, M., Chemical Genetics Reveals a Role of Squalene Synthase in TGF $\beta$  Signaling and Cardiomyogenesis, *Angew. Chem. Int. Ed. Engl.*, **60**, 21824-21831 (2021).

Nakashima, M.; Uesugi, M., Asian Chemical Biology Initiative (ACBI): Bringing Together Chemical Biologists Within Asia, *Chembiochem*, **22**, 2738-2740 (2021).

Kaufmann, M.; Schlingmann, K.-P.; Berezin, L.; Molin, A.; Sheftel, J.; Vig, M.; Gallagher, J. C.; Nagata, A.; Masoud, S. S.; Sakamoto, R.; Nagasawa, K.; Uesugi, M.; Kottler, M. L.; Konrad, M.; Jones, G., Differential Diagnosis of Vitamin D-Related Hypercalcemia Using Serum Vitamin D Metabolite Profiling, *J. Bone Miner. Res.*, **36**, 1340-1350 (2021).

Long, T.; Liu, L.; Tao, Y.; Zhang, W.; Quan, J.; Zheng, J.; Hegemann, J. D.; Uesugi, M.; Yao, W.; Tian, H.; Wang, H., Light-Controlled Tyrosine Nitration of Proteins, *Angew. Chem. Int. Ed. Engl.*, **60**, 13414-13422 (2021).

Kawagoe, F.; Mendoza, A.; Hayata, Y.; Asano, L.; Kotake, K.; Mototani, S.; Kawamura, S.; Kurosaki, S.; Akagi, Y.; Takemoto, Y.; Nagasawa, K.; Nakagawa, H.; Uesugi, M.; Kittaka, A., Discovery of a Vitamin D Receptor-Silent Vitamin D Derivative That Impairs Sterol Regulatory Element-Binding Protein In Vivo, *J. Med. Chem.*, **64**, 5689-5709 (2021).

Li, Q.; Meissner, T. B.; Wang, F.; Du, Z.; Ma, S.; Kshirsagar, S.; Tilburgs, T.; Buenostro, J. D.; Uesugi, M.; Strominger, J. L., ELF3 Activated by a Superenhancer and an Autoregulatory Feedback Loop is Required for High-Level HLA-C Expression on Extravillous Trophoblasts, *Proc. Natl. Acad. Sci. U. S. A.*, **118**, e2025512118 (2021).

Hakariya, H.; Takashima, I.; Takemoto, M.; Noda, N.; Sato, S.-I.; Uesugi, M., Non-Genetic Cell-Surface Modification with a Self-Assembling Molecular Glue, *Chem. Commun.*, **57**, 1470-1473 (2021).

Jin, S.; Vu, H. T.; Hioki, K.; Noda, N.; Yoshida, H.; Shimane, T.; Ishizuka, S.; Takashima, I.; Mizuhata, Y.; Beverly Pe, K.; Ogawa, T.; Nishimura, N.; Packwood, D.; Tokitoh, N.; Kurata, H.; Yamasaki, S.; Ishii, K. J.; Uesugi, M., Discovery of Self-Assembling Small Molecules as Vaccine Adjuvants, *Angew. Chem. Int. Ed. Engl.*, **60**, 961-969 (2021).

Nishio, T.; Yoshikawa, Y.; Yoshikawa, K.; Sato, S., Longer DNA Exhibits Greater Potential for Cell-Free Gene Expression, *Sci Rep.*, **11**, 11739 (2021).

Hagihara, M.; Shiroto, S.; Igarashi, S.; Sato, S., Guanine-Tethered Oligonucleotides Restore Abnormal Protein Synthesis with a SNP Mutation in a 5'-UTR G-Quadruplex of Human MSH2, *Chem. Lett.*, **50**, 1806-1809 (2021).

Isor, A.; Chartier, B. V.; Abo, M.; Currens, E. R.; Weerapana, E.; McCulla, R. D., Identifying Cysteine Residues Susceptible to Oxidation by Photoactivatable Atomic Oxygen Precursors Using a Proteome-Wide Analysis, *RSC Chem. Biol.*, **2**, 577-591 (2021).

Beverly Alog Pe, K.; Yatsuzuka, K.; Hakariya, H.; Kida, T.; Katsuda, Y.; Fukuda, M.; Sato, S., RNA-Based Cooperative Protein Labeling That Permits Direct Monitoring of the Intracellular Concentration Change of an Endogenous Protein, *Nucleic Acids Res.*, **49**, 22 (2021).

Mendoza, A.; Takemoto, Y.; Cruzado, K. T.; Masoud, S. S.; Nagata, A.; Tantipanjanorn, A.; Okuda, S.; Kawagoe, F.; Sakamoto, R.; Odagi, M.; Mototani, S.; Togashi, M.; Kawatani, M.; Aono, H.; Osada, H.; Nakagawa, H.; Higashi, T.; Kittaka, A.; Nagasawa, K.; Uesugi, M., Controlled Lipid  $\beta$ -Oxidation and Carnitine Biosynthesis by a Vitamin D Metabolite, *Cell Chem. Biol.*, doi: 10.1016/j.chembiol.2021.08.008 (2021).

**DIVISION OF ENVIRONMENTAL CHEMISTRY**

— **Molecular Materials Chemistry** —

Wada, Y.; Nakagawa, H.; Kaji, H., Acceleration of Reverse Intersystem Crossing using Different Types of Charge Transfer States, *Chem. Asian J.*, **16**, 1073-1076 (2021).

Visbal, H.; Omura, T.; Nagashima, K.; Itoh, T.; Ohwaki, T.; Imai, H.; Ishigaki, T.; Maeno, A.; Suzuki, K.; Kaji, H.; Hirao, K., Exploring the Capability of Mayenite (12CaO $\cdot$ 7Al $_2$ O $_3$ ) as Hydrogen Storage Material, *Sci. Rep.*, **11**, 6278 (2021).

Zhang, J.; Sakai, H.; Suzuki, K.; Hasobe, T.; Tkachenko, N. V.; Chang, I.-Y.; Hyeon-Deuk, K.; Kaji, H.; Teranishi, T.; Sakamoto, M., Near-Unity Singlet Fission on a Quantum Dot Initiated by Resonant Energy Transfer, *J. Am. Chem. Soc.*, **143**, 17388-17394 (2021).

Shizu, K.; Kaji, H., Theoretical Determination of Rate Constants from Excited States: Application to Benzophenone, *J. Phys. Chem. A.*, **125**, 9000-9010 (2021).

Tsuchiya, Y.; Diesing, S.; Bencheikh, F.; Wada, Y.; dos Santos, P. L.; Kaji, H.; Zysman-Colman, E.; Samuel, I. D. W.; Adachi, C., Exact Solution of Kinetic Analysis for Thermally Activated Delayed Fluorescence Materials, *J. Phys. Chem. A.*, **125**, 8074-8089 (2021).

Chen, D.; Kusakabe, Y.; Ren, Y.; Sun, D.; Rajamalli, P.; Wada, Y.; Suzuki, K.; Kaji, H.; Zysman-Colman, E., Multichromophore Molecular Design for Thermally Activated Delayed-Fluorescence Emitters with Near-Unity Photoluminescence Quantum Yields, *J. Org. Chem.*, **86**, 11531-11544 (2021).

Ren, Y.; Wada, Y.; Suzuki, K.; Kusakabe, Y.; Geldsetzer, J.; Kaji, H., Efficient Blue Thermally Activated Delayed Fluorescence Emitters Showing Very Fast Reverse Intersystem Crossing, *Appl. Phys. Express.*, **14**, 71003 (2021).

Wada, Y.; Shizu, K.; Kaji, H., Molecular Vibration Accelerates Charge Transfer Emission in a Highly Twisted Blue Thermally Activated Delayed Fluorescence Material, *J. Phys. Chem. A.*, **125**, 4534-4539 (2021).

Wada, Y.; Wakisaka, Y.; Kaji, H., Efficient Direct Reverse Intersystem Crossing between Charge Transfer-Type Singlet and Triplet States in a Purely Organic Molecule, *Chemphyschem*, **22**, 621 (2021).

Wada, Y.; Wakisaka, Y.; Kaji, H., Efficient Direct Reverse Intersystem Crossing between Charge Transfer-Type Singlet and Triplet States in a Purely Organic Molecule, *Chemphyschem*, **22**, 625-632 (2021).

- Mamada, M.; Goushi, K.; Nakamura, R.; Kaji, H.; Adachi, C., Synthesis and Characterization of 5,5-Bitetracene, *Chem. Lett.*, **50**, 800-803 (2021).
- Ito, H.; Shimizu, T.; Wada, Y.; Kaji, H.; Fukagawa, H., Comprehensive Study on Operational Lifetime of Organic Light-Emitting Diodes: Effects of Molecular Structure and Energy Transfer, *Jpn. J. Appl. Phys.*, **60**, 40902 (2021).
- Shizu, K.; Adachi, C.; Kaji, H., Correlated Triplet Pair Formation Activated by Geometry Relaxation in Directly Linked Tetracene Dimer (5,5'-Bitetracene), *ACS Omega*, **6**, 2638-2643 (2021).
- Kaji, H., Multiscale Charge Transport Simulation and in Silico Material Design for Highly-Efficient OLEDs, *Dig. Tech. Pap.*, **52**, 308-311 (2021).
- Ishida, K.; Higashino, T.; Wada, Y.; Kaji, H.; Saeki, A.; Imahori, H., Thiophene-Fused Naphthodiphospholes: Modulation of the Structural and Electronic Properties of Polycyclic Aromatics by Precise Fusion of Heteroles, *Chempluschem*, **86**, 130-136 (2021).
- Ishida, K.; Higashino, T.; Wada, Y.; Kaji, H.; Saeki, A.; Imahori, H., Thiophene-Fused Naphthodiphospholes: Modulation of the Structural and Electronic Properties of Polycyclic Aromatics by Precise Fusion of Heteroles, *Chempluschem*, **86(1)**, 130-136 (2021).
- Imahori, H.; Kobori, Y.; Kaji, H., Manipulation of Charge-Transfer States by Molecular Design: Perspective from "Dynamic Exciton", *Acc. Mater. Res.*, **2(7)**, 501-514 (2021).
- Chen, D.; Kusakabe, Y.; Ren, Y.; Sun, D.; Rajamalli, P.; Wada, Y.; Suzuki, K.; Kaji, H.; Zysman-Colman, E., Multichromophore Molecular Design for Efficient Thermally Activated Delayed Fluorescence Emitters with Near-Unity Photoluminescence Quantum Yields, *J. Org. Chem.*, **86(17)**, 11531-11544 (2021).
- Shibano, M.; Suzuki, K.; Kaji, H.; Takano, T., N-Adamantylphthalimide-Based Thermally Activated Delayed Fluorescence Emitter for Solution-Processed Organic Light-Emitting Diodes, *Chem. Lett.*, **50**, 1953-1955 (2021).
- Crovini, E.; Zhang, Z.; Kusakabe, Y.; Ren, Y.; Wada, Y.; Naqvi, B. A.; Sahay, P.; Matulaitis, T.; Dising, S.; Samuel, I. D. W.; Brütting, W.; Suzuki, K.; Kaji, H.; Bräse, S.; Zysman-Colman, E., Effect of a Twin-Emitter Design Strategy on a Previously Reported Thermally Activated Delayed Fluorescence Organic Light-Emitting Diode, *Beilstein J. Org. Chem.*, **17**, 2894-2905 (2021).
- [Others]
- Shizu, K.; Adachi, C.; Kaji, H., Quantitative Prediction of Internal Conversion Rate Constant for the Screening of Singlet Fission Materials, *The 13th Asian Conference on Organic Electronics (A-COE2021)*, Online (2021).
- Suzuki, K.; Kaji, H., Solid-State NMR Analysis of Materials in Organic Semiconductors, *The 11th International Conference on Flexible and Printed Electronics (ICFPE 2021)*, Online (2021).
- Ren, Y.; Wada, Y.; Suzuki, K.; Kusakabe, Y.; Geldsetzer, J.; Kaji, H., A Molecular Design Achieving Very Fast Reverse Intersystem Crossing, *The 13th Asian Conference on Organic Electronics (A-COE2021)*, Online (2021).
- Kusakabe, Y.; Wada, Y.; Nakagawa, H.; Shizu, K.; Kaji, H., A New Molecular Design Realizing Very Fast Reverse Intersystem Crossing, *The 13th Asian Conference on Organic Electronics (A-COE2021)*, Online (2021).
- Shizu, K.; Kaji, H., Low-Cost and Quantitative Prediction of Rate Constants: Application to Decay Mechanism of Benzophenone, *The 13th Asian Conference on Organic Electronics (A-COE2021)*, Online (2021).
- Suzuki, K., Structural Analysis of Organic Semiconducting Materials Using Solid-State NMR, *239th ECS Meeting*, Online (2021).
- Shizu, K.; Adachi, C.; Kaji, H., Quantitative Prediction of Singlet Fission Rates and Molecular Design of Singlet Fission Materials, *The 101st CSJ Annual Meeting* (2021).
- **Hydrospheric Environment Analytical Chemistry** —
- Takano, S.; Tsuchiya, M.; Imai, S.; Yamamoto, Y.; Fukami, Y.; Suzuki, K.; Sohrin, Y., Isotopic Analysis of Nickel, Copper, and Zinc in Various Freshwater Samples for Source Identification, *Geochem. J.*, **55(3)**, 171-183 (2021).
- Liao, W.-H.; Takano, S.; Tian, H.-A.; Chen, H.-Y.; Sohrin, Y.; Ho, T.-Y., Zn Elemental and Isotopic Features in Sinking Particles of the South China Sea: Implications for its Sources and Sinks, *Geochim. Cosmochim. Acta*, **314**, 68-84 (2021).
- Zheng, L.; Minami, T.; Takano, S.; Ho, T.-Y.; Sohrin, Y., Sectional Distribution Patterns of Cd, Ni, Zn, and Cu in the North Pacific Ocean: Relationships to Nutrients and Importance of Scavenging, *Global Biogeochem. Cycles*, **35**, e2020GB006558 (2021).
- Nakaguchi, Y.; Ikeda, Y.; Sakamoto, A.; Zheng, L.; Minami, T.; Sohrin, Y., Distribution and Stoichiometry of Al, Mn, Fe, Co, Ni, Cu, Zn, Cd, and Pb in the East China Sea, *J. Oceanogr.*, **77**, 463-485 (2021).
- Sakata, K.; Takahashi, Y.; Takano, S.; Matsuki, A.; Sakaguchi, A.; Tanimoto, H., First X-Ray Spectroscopic Observations of Atmospheric Titanium Species: Size Dependence and the Emission Source, *Environ. Sci. Technol.*, **55**, 10975-10986 (2021).
- **Chemistry for Functionalized Surfaces** —
- Tomita, K.; Shioya, N.; Shimoaka, T.; Okudaira, K. K.; Yoshida, H.; Koganezawa, T.; Hasegawa, T., Substrate-Independent Control of Polymorphs in Tetraphenylporphyrin Thin Films by Varying the Solvent Evaporation Time Using a Simple Spin-Coating Technique, *Cryst. Growth. Des.*, **21**, 5116-5125 (2021).
- Wakioka, M.; Yamashita, N.; Mori, H.; Murdey, R.; Shimoaka, T.; Shioya, N.; Wakamiya, A.; Nishihara, Y.; Hasegawa, T.; Ozawa, F., Formation of Trans-Poly(thienylenevinylene) Thin Films by Solid-State Thermal Isomerization, *Chem. Mater.*, **33**, 5631-5638 (2021).
- Shioya, N.; Fujiwara, R.; Tomita, K.; Shimoaka, T.; Okudaira, K. K.; Yoshida, H.; Koganezawa, T.; Hasegawa, T., Monitoring of Crystallization Process in Solution-Processed Pentacene Thin Films by Chemical Conversion Reactions, *J. Phys. Chem. C*, **125**, 2437-2445 (2021).
- Nagasawa, T.; Sato, R.; Hasegawa, T.; Numadate, N.; Shioya, N.; Shimoaka, T.; Hasegawa, T.; Hama, T., Absolute Absorption Cross Section and Orientation of Dangling OH Bonds in Water Ice, *Astrophys. J. Lett.*, **923**, L3 (2021).

— Molecular Microbial Science —

Yokoyama, F.; Imai, T.; Aoki, W.; Ueda, M.; Kawamoto, J.; Kurihara, T., Identification of a Putative Sensor Protein Involved in Regulation of Vesicle Production by a Hypervesiculating Bacterium, *Shewanella vesiculosa* HM13, *Front. Microbiol.*, **12**, 629023 (2021).

Shimizu, A.; Tobe, R.; Aono, R.; Inoue, M.; Hagita, S.; Kiriyama, K.; Toyotake, Y.; Ogawa, T.; Kurihara, T.; Goto, K.; Prakash, N. T.; Mihara, H., Initial Step of Selenite Reduction via Thioredoxin for Bacterial Selenoprotein Biosynthesis, *Int. J. Mol. Sci.*, **22(20)**, 10965 (2021).

Kawano, K.; Yokoyama, F.; Kamasaka, K.; Kawamoto, J.; Ogawa, T.; Kurihara, T.; Futaki, S., Design of the N-Terminus Substituted Curvature-Sensing Peptides That Exhibit Highly Sensitive Detection Ability of Bacterial Extracellular Vesicles, *Chem. Pharm. Bull. (Tokyo)*, **69(11)**, 1075-1082 (2021).

Di Guida, R.; Casillo, A.; Stellavato, A.; Di Meo, C.; Kawai, S.; Kawamoto, J.; Ogawa, T.; Kurihara, T.; Schiraldi, C.; Corsaro, M. M., Complete Lipooligosaccharide Structure from *Pseudoalteromonas nigrifaciens* Sq02-Rif<sup>r</sup> and Study of Its Immunomodulatory Activity, *Mar. Drugs*, **19(11)**, 646 (2021).

[Others]

Kurihara, T., Mechanism of Protein Loading onto Extracellular Membrane Vesicles Discovered in a Novel Bacterial Strain, *SEIKAGAKU*, **93(2)**, 252-256 (2021).

Kurihara, T., Elucidation of the Mechanism of Selective Protein Transport to Bacterial Extracellular Membrane Vesicles and its Application to the Construction of Extracellular Protein Production Platform, *IFO Research Communications*, **35**, 11-25 (2021).

Ogawa, T., Analysis of the Bacterial Conversion of  $\omega$ -3 Polyunsaturated Fatty Acids and Studies on its Application, *IFO Research Communications*, **35**, 135 (2021).

**DIVISION OF MULTIDISCIPLINARY CHEMISTRY**

— Polymer Materials Science —

Jinnai, H.; Takenaka, M.; Shibayama, M.; Han, C. C.; Cheng, S. Z. D., Tribute to Takeji Hashimoto, *Polymer*, **222**, 123676 (2021).

Takenaka, M.; Nishitsuji, S.; Watanabe, Y.; Yamaguchi, D.; Koizumi, S., Analyses of Hierarchical Structures in Vulcanized SBR Rubber by Using Contrast-Variation USANS and SANS, *J. Appl. Crystallogr.*, **54**, 949-956 (2021).

Kimura, Y.; Imai, S.; Takenaka, M.; Terashima, T., Amphiphilic Random Cyclopolymers as Versatile Scaffolds for Ring-Functionalized and Self-Assembled Materials, *Macromolecules*, **54**, 3987-3998 (2021).

Pournaghshband Isfahani, A.; Shahrooz, M.; Yamamoto, T.; Muchtar, A.; Ito, M. M.; Yamaguchi, D.; Takenaka, M.; Sivaniah, E.; Ghalei, B., Influence of Microstructural Variations on Morphology and Separation Properties of Polybutadiene-Based Polyurethanes, *RSC Advances*, **11**, 15449-15456 (2021).

Nakanishi, Y.; Mita, K.; Yamamoto, K.; Ichino, K.; Takenaka, M., Effects of Mixing Process on Spatial Distribution and Coexistence of Sulfur and Zinc in Vulcanized EPDM Rubber, *Polymer*, **218**, 123486 (2021).

Imai, S.; Ommura, Y.; Watanabe, Y.; Ogawa, H.; Takenaka, M.; Ouchi, M.; Terashima, T., Amphiphilic Random and Random Block Terpolymers with PEG, Octadecyl, and Oleyl Pendants for Controlled Crystallization and Microphase Separation, *Polym. Chem.*, **12**, 1439-1447 (2021).

Ikami, T.; Kimura, Y.; Takenaka, M.; Ouchi, M.; Terashima, T., Design Guide of Amphiphilic Crystalline Random Copolymers for Sub-10 nm Microphase Separation, *Polym. Chem.*, **12**, 501-510 (2021).

Ogawa, H.; Takenaka, M.; Miyazaki, T., Molecular Weight Effect on the Transition Processes of a Symmetric PS-*b*-P2VP during Spin-Coating, *Macromolecules*, **54**, 1017-1029 (2021).

Aoki, H.; Ogawa, H.; Takenaka, M., Neutron Reflectometry Tomography for Imaging and Depth Structure Analysis of Thin Films with In-Plane Inhomogeneity, *Langmuir*, **37**, 196-203 (2021).

Lazim, N. H.; Hidzir, N. M.; Hamzah, N. S.; Mikihiro, T.; Shamsudin, S. A., The Effects of the Cross-Linking Mechanism of Low Doses of Gamma Irradiation on the Mechanical, Thermal, and Viscoelastic Properties of the Natural Rubber Latex/poly(styrene-*block*-isoprene-*block*-styrene) Block Copolymer Blend, *Polym. Eng. Sci.*, doi: 10.1002/pen.25843 (2021).

Ikami, T.; Watanabe, Y.; Ogawa, H.; Takenaka, M.; Yamada, N. L.; Ouchi, M.; Aoki, H.; Terashima, T., Multilayered Lamellar Materials and Thin Films by Instant Self-Assembly of Amphiphilic Random Copolymers, *ACS Macro Lett.*, **10**, 1524-1528 (2021).

Shimokita, K.; Yamamoto, K.; Miyata, N.; Nakanishi, Y.; Ogawa, H.; Takenaka, M.; Yamada, N. L.; Miyazaki, T., Investigation of Interfacial Water Accumulation between Polypropylene Thin Film and Si Substrate by Neutron Reflectivity, *Langmuir*, **37**, 14550-14557 (2021).

— Molecular Rheology —

Shimada, R.; Urakawa, O.; Inoue, T.; Watanabe, H., Phase Equilibrium and Dielectric Relaxation in Mixture of 5CB with Dilute Dimethyl Phthalate: Effect of Coupling between Orientation and Composition Fluctuations on Molecular Dynamics in Isotropic One-Phase State, *Soft Matter*, **17**, 6259-6272 (2021).

Sato, T.; Kwon, Y.; Matsumiya, Y.; Watanabe, H., A Constitutive Equation for Rouse Model Modified for Variations of Spring Stiffness, Bead Friction, and Brownian Force Intensity under Flow, *Phys. Fluids*, **33**, 63106 (2021).

Watanabe, H.; Matsumiya, Y.; Sato, T., Revisiting Nonlinear Flow Behavior of Rouse Chain: Roles of FENE, Friction-Reduction, and Brownian Force Intensity Variation, *Macromolecules*, **54**, 3700-3715 (2021).

Liu, S.; Zhang, Z.; Chen, Q.; Matsumiya, Y.; Watanabe, H., Nonlinear Rheology of Telechelic Ionomers Based on Sodium Sulfonate and Carboxylate, *Macromolecules*, **54**, 9724-9738 (2021).

Matsumiya, Y.; Watanabe, H.; Sukhonthamethirat, N.; Vao-Soongnern, V., Viscoelastic and Dielectric Behavior of Polyisoprene Monofunctionally Head-Modified with Associative Metal-Carboxylate Group, *Nihon Reoroji Gakkaishi*, **49**, 189-197 (2021).

Matsumiya, Y.; Watanabe, H., Non-Universal Features in Uniaxially Extensional Rheology of Linear Polymer Melts and Concentrated Solutions: A Review, *Prog. Polym. Sci.*, **112**, 101325 (2021).



Hamada, Y.; Sato, T.; Taniguchi, T., Multiscale Simulation of a Polymer Melt Flow between Two Coaxial Cylinders under Nonisothermal Conditions, *Math. Eng.*, **3**, (2021).

Sato, T.; Taniguchi, T., Multiscale Simulation of the Flows of a Bidisperse Entangled Polymer Melt, *Nihon Reoraji Gakkaishi*, **49**, 87-95 (2021).

Sato, T.; Moghadam, S.; Tan, G.; Larson, R. G., Erratum: A Slip-Spring Simulation Model for Predicting Linear and Nonlinear Rheology of Entangled Wormlike Micellar Solutions, *J. Rheol.*, **65**, 73 (2021).

#### — Molecular Aggregation Analysis —

Hu, S.; Truong, M. A.; Otsuka, K.; Handa, T.; Yamada, T.; Nishikubo, R.; Iwasaki, Y.; Saeki, A.; Murdey, R.; Kanemitsu, Y.; Wakamiya, A., Mixed Lead-Tin Perovskite Films with >7  $\mu\text{s}$  Charge Carrier Lifetimes Realized by Maltol Post-Treatment, *Chem. Sci.*, **12**, 13513-13519 (2021).

Cho, Y.; Bing, J.; Kim, H. D.; Li, Y.; Zheng, J.; Tang, S.; Green, M. A.; Wakamiya, A.; Huang, S.; Ohkita, H.; Ho-Baillie, A. W. Y., Immediate and Temporal Enhancement of Power Conversion Efficiency in Surface-Passivated Perovskite Solar Cells, *ACS Appl. Mater. Interfaces*, **13**, 39178-39185 (2021).

Wakioka, M.; Yamashita, N.; Mori, H.; Murdey, R.; Shimoaka, T.; Shioya, N.; Wakamiya, A.; Nishihara, Y.; Hasegawa, T.; Ozawa, F., Formation of trans-Poly(thienylenevinylene) Thin Films by Solid-State Thermal Isomerization, *Chem. Mater.*, **33**, 5631-5638 (2021).

Cho, Y.; Kim, H. D.; Zheng, J.; Bing, J.; Li, Y.; Zhang, M.; Green, M. A.; Wakamiya, A.; Huang, S.; Ohkita, H.; Ho-Baillie, A. W. Y., Elucidating Mechanisms behind Ambient Storage-Induced Efficiency Improvements in Perovskite Solar Cells, *ACS Energy Lett.*, **6**, 925-933 (2021).

Yang, F.; Wang, S.; Dai, P.; Chen, L.; Wakamiya, A.; Matsuda, K., Progress in Recycling Organic-Inorganic Perovskite Solar Cells for Eco-Friendly Fabrication, *J. Mater. Chem. A Mater.*, **9**, 2612-2627 (2021).

Truong, M. A.; Lee, H.; Shimazaki, A.; Mishima, R.; Hino, M.; Yamamoto, K.; Otsuka, K.; Handa, T.; Kanemitsu, Y.; Murdey, R.; Wakamiya, A., Near-Ultraviolet Transparent Organic Hole-Transporting Materials Containing Partially Oxygen-Bridged Triphenylamine Skeletons for Efficient Perovskite Solar Cells, *ACS Appl. Energy Mater.*, **4**, 1484-1495 (2021).

Zhang, Z.; Hirori, H.; Sekiguchi, F.; Shimazaki, A.; Iwasaki, Y.; Nakamura, T.; Wakamiya, A.; Kanemitsu, Y., Ultrastrong Coupling between THz Phonons and Photons Caused by an Enhanced Vacuum Electric Field, *Phys. Rev. Res.*, **3**, L032021 (2021).

Sekiguchi, F.; Hirori, H.; Yumoto, G.; Shimazaki, A.; Nakamura, T.; Wakamiya, A.; Kanemitsu, Y., Enhancing the Hot-Phonon Bottleneck Effect in a Metal Halide Perovskite by Terahertz Phonon Excitation, *Phys. Rev. Lett.*, **126**, 77401 (2021).

#### ADVANCED RESEARCH CENTER FOR BEAM SCIENCE — Particle Beam Science —

Nagae, D.; Abe, Y.; Okada, S.; Omika, S.; Wakayama, K.; Hosoi, S.; Suzuki, S.; Moriguchi, T.; Amano, M.; Kamioka, D.; Ge, Z.; Naimi, S.; Suzuki, F.; Tadano, N.; Igosawa, R.; Inomata, K.; Arakawa, H.; Nishimuro, K.; Fujii, T.; Mitsui, T.; Yanagisawa, Y.; Baba, H.; Michimasa, S.; Ota, S.; Lorusso, G.; Litvinov, Y. A.; Ozawa, A.; Uesaka, T.; Yamaguchi, T.; Yamaguchi, Y.; Wakasugi, M., Development and Operation of an Electrostatic Time-of-Flight Detector for the Rare RI Storage Ring, *Nucl. Instrum. Methods Phys. Res. A*, **986**, 164713 (2021).

Baba, K.; Kusumoto, T.; Okada, S.; Ogawara, R.; Kodaira, S.; Raffy, Q.; Barillon, R.; Ludwig, N.; Galindo, C.; Peaupardin, P.; Ishikawa, M., Quantitative Estimation of Track Segment Yields of Water Radiolysis Species under Heavy Ions around Bragg Peak Energies using Geant4-DNA, *Sci. Rep.*, **11**, 1524 (2021).

Kusumoto, T.; Ogawara, R.; Igawa, K.; Baba, K.; Konishi, T.; Furusawa, Y.; Kodaira, S., Scaling Parameter of the Lethal Effect of Mammalian Cells Based on Radiation-Induced OH Radicals: Effectiveness of Direct Action in Radiation Therapy, *J. Radiat. Res.*, **62**, 86-93 (2021).

Jang, J.; Kikunaga, H.; Sekimoto, S.; Inagaki, M.; Kawakami, T.; Ohtsuki, T.; Kashiwagi, S.; Takahashi, K.; Tsukada, K.; Tatenuma, K.; Uesaka, M., Design and Testing of a W-MoO<sub>3</sub> Target System for Electron Linac Production of <sup>99</sup>Mo/<sup>99m</sup>Tc, *Nucl. Instrum. Methods Phys. Res. A*, **987**, 164815 (2021).

Gogami, T.; Chen, C.; Kawama, D.; Achenbach, P.; Ahmidouch, A.; Albayrak, I.; Androic, D.; Asaturyan, A.; Asaturyan, R.; Ates, O.; Baturin, P.; Badui, R.; Boeglin, W.; Bono, J.; Brash, E.; Carter, P.; Chiba, A.; Christy, E.; Danagoulian, S.; De Leo, R.; Doi, D.; Elaasar, M.; Ent, R.; Fujii, Y.; Fujita, M.; Furic, M.; Gabrielyan, M.; Gan, L.; Garibaldi, F.; Gaskell, D.; Gasparian, A.; Han, Y.; Hashimoto, O.; Horn, T.; Hu, B.; Hungerford, E. V.; Jones, M.; Kanda, H.; Kaneta, M.; Kato, S.; Kawai, M.; Khanal, H.; Kohl, M.; Liyanage, A.; Luo, W.; Maeda, K.; Margaryan, A.; Markowitz, P.; Maruta, T.; Matsumura, A.; Maxwell, V.; Meekins, D.; Mkrtchyan, A.; Mkrtchyan, H.; Nagao, S.; Nakamura, S. N.; Narayan, A.; Neville, C.; Niculescu, G.; Niculescu, M. I.; Nunez, A.; Nuruzzaman Okayasu, Y.; Petkovic, T.; Pochodzalla, J.; Qiu, X.; Reinhold, J.; Rodriguez, V. M.; Samanta, C.; Sawatzky, B.; Seva, T.; Shichijo, A.; Tadevosyan, V.; Tang, L.; Taniya, N.; Tsukada, K.; Veilleux, M.; Vulcan, W.; Wesselmann, F. R.; Wood, S. A.; Yamamoto, T.; Ya, L.; Ye, Z.; Yokota, K.; Yuan, L.; Zhamkochyan, S.; Zhu, L., Spectroscopy of A=9 Hyperlithium with the (*e,e'*K<sup>+</sup>) Reaction, *Phys. Rev. C*, **103**, L041301 (2021).

Sakuma, F.; Ajimura, S.; Akaishi, T.; Asano, H.; Bazzi, M.; Beer, G.; Bhang, H.; Bragadireanu, M.; Buehler, P.; Busso, L.; Cargnelli, M.; Choi, S.; Clozza, A.; Curceanu, C.; Enomoto, S.; Fujioka, H.; Fujiwara, Y.; Fukuda, T.; Guaraldo, C.; Hashimoto, T.; Hayano, R. S.; Hiraiwa, T.; Iio, M.; Iliescu, M.; Inoue, K.; Ishiguro, Y.; Ishikawa, T.; Ishimoto, S.; Itahashi, K.; Iwasaki, M.; Iwai, M.; Kanno, K.; Kato, K.; Kato, Y.; Kawasaki, S.; Kienle, P.; Kou, H.; Ma, Y.; Marton, J.; Matsuda, Y.; Miliucci, M.; Mizoi, Y.; Morra, O.; Murayama, R.; Nagae, T.; Noumi, H.; Ohnishi, H.; Okada, S.; Outa, H.; Ozawa, K.; Piscicchia, K.; Sada, Y.; Sakaguchi, A.; Sato, M.; Scordo, A.; Sekimoto, M.; Shi, H.; Shirotori, K.; Simon, M.; Sirghi, D.; Sirghi, F.; Suzuki, S.; Suzuki, T.; Tanida, K.; Tatsuno, H.; Tokuda, M.; Tomono, D.; Toyoda, A.; Tsukada, K.; Doce, O. V.; Widmann, E.; Yamaga, T.; Yamazaki, T.; Yoshida, C.; Zhang, Q.; Zmeskal, J., Recent Results and Future Prospects of Kaonic Nuclei at J-PARC, *Few Body Syst.*, **62**, 103 (2021).

— Laser Matter Interaction Science —

Takenaka, K.; Shinohara, N.; Hashida, M.; Kusaba, M.; Sakagami, H.; Sato, Y.; Masuno, S.-I.; Nagashima, T.; Tsukamoto, M., Delay Times for Ablation Rate Suppression by Femtosecond Laser Irradiation with a Two-Color Double-Pulse Beam, *Appl. Phys. Lett.*, **119**, 231603 (2021).

— Electron Microscopy and Crystal Chemistry —

Sugimoto, Y.; Nakamichi, M.; Kim, J.-H.; Kurata, H.; Haruta, M.; Miyamoto, M., Deuterium and Helium Desorption Behavior and Microstructure Evolution in Beryllium during Annealing, *J. Nucl. Mater.*, **544**, 152686 (2021).

Lai, M.-W.; Kurata, H., Exploring (1 $\bar{1}$ 2)-Related Ordered Structure in Oxidation-Synthesized  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> Nanowhiskers, *J. Mater. Sci.*, **56**, 7286-7297 (2021).

Jin, S.; Vu, H. T.; Hioki, K.; Noda, N.; Yoshida, H.; Shimane, T.; Ishizuka, S.; Takashima, I.; Mizuhata, Y.; Pe, K. B.; Ogawa, T.; Nishimura, N.; Packwood, D.; Tokitoh, N.; Kurata, H.; Yamasaki, S.; Ishii, K. J.; Uesugi, M., Discovery of Self-Assembling Small Molecules as Vaccine Adjuvants, *Angew. Chem. Int. Ed. Engl.*, **60**, 73-80 (2021).

Haruta, M.; Nemoto, T.; Kurata, H., Sub-Picometer Sensitivity and Effect of Anisotropic Atomic Vibrations on Ti L<sub>2,3</sub>-edge spectrum of SrTiO<sub>3</sub>, *Appl. Phys. Lett.*, **119**, 232901 (2021).

Iwashimizu, C.; Haruta, M.; Kurata, H., Electron Orbital Mapping of SrTiO<sub>3</sub> Using Electron Energy-Loss Spectroscopy, *Appl. Phys. Lett.*, **119**, 232902 (2021).

Autthawong, T.; Promanan, T.; Chayasombat, B.; Yu, A.-S.; Uosaki, K.; Yamaguchi, A.; Kurata, H.; Chairuangri, T.; Sarakonsri, T., Facile Synthesis Sandwich-Structured Ge/NrGO Nanocomposite as Anodes for High-Performance Lithium-Ion Batteries, *Crystals*, **11**, 1582 (2021).

[Others]

Haruta, M.; Kurata, H., Local Electronic State Analysis by Monochromated STEM-EELS, *Kenbikyō*, **56(2)**, 73-80 (2021).

INTERNATIONAL RESEARCH CENTER FOR ELEMENTS SCIENCE

— Synthetic Organotransformation —

Matsuyama, T.; Kikkawa, S.; Fujiki, Y.; Tsukada, M.; Takaya, H.; Yasuda, N.; Nitta, K.; Nakatani, N.; Negishi, Y.; Yamazoe, S., Thermal Stability of Crown-Motif [Au<sub>9</sub>(PPh<sub>3</sub>)<sub>8</sub>]<sup>3+</sup> and [MAu<sub>8</sub>(PPh<sub>3</sub>)<sub>8</sub>]<sup>2+</sup> (M = Pd, Pt) Clusters: Effects of Gas Composition, Single-Atom Doping, and Counter Anions, *J. Chem. Phys.*, **155**, 44307 (2021).

Adak, L.; Jin, M.; Saito, S.; Kawabata, T.; Itoh, T.; Ito, S.; Sharma, A. K.; Gower, N. J.; Cogswell, P.; Geldsetzer, J.; Takaya, H.; Isozaki, K.; Nakamura, M., Iron-Catalysed Enantioselective Carbometalation of Azabicycloalkenes, *Chem. Commun.*, **57**, 6975-6978 (2021).

Adak, L.; Hatakeyama, T.; Nakamura, M., Iron-Catalyzed Cross-Coupling Reactions Tuned by Bulky Ortho-Phenylene Bisphosphine Ligands, *Bull. Chem. Soc. Jpn.*, **94**, 1125-1141 (2021).

Watanabe, B.; Makino, K.; Mizutani, M.; Takaya, H., Synthesis and Structural Confirmation of Calibagenin and Saxosterol, *Tetrahedron*, **91**, (2021).

Isozaki, K.; Ueno, R.; Ishibashi, K.; Nakano, G.; Yin, H.; Iseri, K.; Sakamoto, M.; Takaya, H.; Teranishi, T.; Nakamura, M., Gold Nanocluster Functionalized with Peptide Dendron Thioliates: Acceleration of the Photocatalytic Oxidation of an Amino Alcohol in a Supramolecular Reaction Field, *ACS Catal.*, **11**, 13180-13187 (2021).

Iwasaki, T.; Hirooka, Y.; Takaya, H.; Honma, T.; Nozaki, K., Lithium Hexaphenylrhodate(III) and -Iridate(III): Structure in the Solid State and in Solution, *Organometallics*, **40(15)**, 2489-2495 (2021).

Yamada, Y.; Morita, K.; Sugiura, T.; Toyoda, Y.; Mihara, N.; Nagasaka, M.; Takaya, H.; Tanaka, K.; Koitaya, T.; Nakatani, N.; Ariga-Miwa, H.; Takakusagi, S.; Hitomi, Y.; Kudo, T.; Tsujii, Y.; Yoshizawa, K.; Tanaka, K., Close-Stacking of Iron-Oxo-Based Double-Decker Complex on Graphite Surface Achieved High Catalytic CH<sub>4</sub> Oxidation Activity Comparable to that of Methane Monooxygenases, *ChemRxiv*, doi: org/10.26434/chemrxiv.14728860.v1 (2021).

Tajima, S.; Muranaka, A.; Naito, M.; Taniguchi, N.; Harada, M.; Miyagawa, S.; Ueda, M.; Takaya, H.; Kobayashi, N.; Uchiyama, M.; Tokunaga, Y., Synthesis of a Mechanically Planar Chiral and Axially Chiral [2]Rotaxane, *Org. Lett.*, **23(22)**, 8678-8682 (2021).

Zhao, H.; Isozaki, K.; Taguchi, T.; Yang, S.; Miki, K., Laying Down of Gold Nanorods Monolayers on Solid Surfaces for Surface Enhanced Raman Spectroscopy Applications, *Phys. Chem. Chem. Phys.*, **23**, 26822-26828 (2021).

— Advanced Solid State Chemistry —

Kosugi, Y.; Goto, M.; Tan, Z.; Kan, D.; Isobe, M.; Yoshii, K.; Mizumaki, M.; Fujita, A.; Takagi, H.; Shimakawa, Y., Giant Multiple Caloric Effects in Charge Transition Ferrimagnet, *Sci. Rep.*, **11**, 12682 (2021).

Kloß, S. D.; Haffner, A.; Manuel, P.; Goto, M.; Shimakawa, Y.; Atfield, J. P., Preparation of Iron(IV) Nitridoferrate Ca<sub>4</sub>FeN<sub>4</sub> through Azide-Mediated Oxidation under High-Pressure Conditions, *Nat. Commun.*, **12**, 571 (2021).

Kan, D.; Xie, L.; Shimakawa, Y., Scaling of the Anomalous Hall Effect in Perpendicularly Magnetized Epitaxial Films of the Ferrimagnet, *Phys. Rev. B*, **104**, 134407 (2021).

Takahashi, R.; Tani, Y.; Abe, H.; Yamasaki, M.; Suzuki, I.; Kan, D.; Shimakawa, Y.; Wadati, H., Ultrafast Demagnetization in NiCo<sub>2</sub>O<sub>4</sub> Thin Films Probed by Time-Resolved Microscopy, *Appl. Phys. Lett.*, **119**, 102404 (2021).

Zhang, Z.; Zhang, S.; Jiang, C.; Guo, H.; Qu, F.; Shimakawa, Y.; Yang, M., Integrated Sensing Array of the Perovskite-Type LnFeO<sub>3</sub> (Ln=La, Pr, Nd, Sm) to Discriminate Detection of Volatile Sulfur Compounds, *J. Hazard. Mater.*, **413**, 125380 (2021).

Koizumi, H.; Suzuki, I.; Kan, D.; Inoue, J.-I.; Wakabayashi, Y.; Shimakawa, Y.; Yanagihara, H., Spin Reorientation in Tetragonally Distorted Spinel Oxide Epitaxial Films, *Phys. Rev. B*, **104**, 14422 (2021).

- De Irujo-Labalde, X. M.; Amador, U.; Ritter, C.; Goto, M.; Patino, M. A.; Shimakawa, Y.; Garcíá-Martín, S., 3D to 2D Magnetic Ordering of Fe<sup>3+</sup> Oxides Induced by Their Layered Perovskite Structure, *Inorg. Chem.*, **60**, 8027-8034 (2021).
- Ando, F.; Kawarazaki, R.; Naritsuka, M.; Kasahara, Y.; Miyasaka, Y.; Narita, H.; Kan, D.; Shiota, Y.; Moriyama, T.; Shimakawa, Y.; Matsuda, Y.; Ono, T., Investigation of the Upper Critical Field in Artificially Engineered Nb/V/Ta Superlattices, *Jpn. J. Appl. Phys.*, **60**, 060902 (2021).
- Kosugi, Y.; Goto, M.; Tan, Z.; Fujita, A.; Saito, T.; Kamiyama, T.; Chen, W.-T.; Chuang, Y.-C.; Sheu, H.-S.; Kan, D.; Shimakawa, Y., Colossal Barocaloric Effect by Large Latent Heat Produced by First-Order Intersite-Charge-Transfer Transition, *Adv. Funct. Mater.*, **31**, 2009476 (2021).
- Kan, D.; Suzuki I.; Shimakawa Y., Tuning Magnetic Anisotropy by Continuous Composition-Gradients in a Transition Metal Oxide, *Jpn. J. Appl. Phys.*, **129**, 183902 (2021).
- Injac, S. D. A.; Xu, Y.; Denis Romero, F.; Shimakawa, Y., Pauli-Paramagnetic and Metallic Properties of High Pressure Polymorphs of BaRhO<sub>3</sub> Oxides Containing Rh<sub>2</sub>O<sub>9</sub> Dimers, *Dalton Trans.*, **50**, 4673-4679 (2021).
- Chin, Y.-Y.; Hu, Z.; Shimakawa, Y.; Yang, J.; Long, Y.; Tanaka, A.; Tjeng, L. H.; Lin, H.-J.; Chen, C.-T., Charge and Spin Degrees of Freedom in A-Site Ordered YCu<sub>3</sub>Co<sub>4</sub>O<sub>12</sub> and CaCu<sub>3</sub>Co<sub>4</sub>O<sub>12</sub>, *Phys. Rev. B*, **103**, 115149 (2021).
- Hong, K. H.; Solana-Madruga, E.; Hakala, B. V.; Patino, M. A.; Manuel, P.; Shimakawa, Y.; Attfield, J. P., Substitutional Tuning of Electronic Phase Separation in CaFe<sub>3</sub>O<sub>5</sub>, *Phys. Rev. Mater.*, **5**, 24406 (2021).
- Tan, Z.; Koedtrud, A.; Goto, M.; Iihoshi, M.; Shimakawa, Y., Layered Hexagonal Perovskite Oxides 21R Ba<sub>7</sub>Fe<sub>5</sub>Ge<sub>2</sub>O<sub>20</sub> and 12H Ba<sub>6</sub>Fe<sub>3</sub>Ge<sub>3</sub>O<sub>17</sub>, *Inorg. Chem.*, **60**, 1257-1263 (2021).
- Kim, T.; Sim, S.; Lim, S.; Patino, M. A.; Hong, J.; Lee, J.; Hyeon, T.; Shimakawa, Y.; Lee, S.; Attfield, J. P.; Park, J.-G., Slow Oxidation of Magnetite Nanoparticles Elucidates the Limits of the Verwey Transition, *Nat. Commun.*, **12**, 6356 (2021).
- Shimakawa Y., Novel Materials and Properties in Transition (Rare Earth) Metal Compounds and Oxides, *Funtai Oyobi Fumatsu Yakini/Journal of the Japan Society of Powder and Powder Metallurgy*, **68**, 308 (2021).
- Goto, M.; Oguchi, T.; Shimakawa, Y., Geometrical Spin Frustration and Monoclinic-Distortion-Induced Spin Canting in the Double Perovskites Ln<sub>2</sub>LiFeO<sub>6</sub> (Ln = La, Nd, Sm, and Eu) with Unusually High Valence Fe<sup>5+</sup>, *J. Am. Chem. Soc.*, **143(45)**, 19207-19213 (2021).
- Organometallic Chemistry —
- Solomon, J. B.; Rasekh, M. F.; Hiller, C. J.; Lee, C. C.; Tanifuji, K.; Ribbe, M. W.; Hu, Y., Probing the All-Ferrous States of Methanogen Nitrogenase Iron Proteins, *JACS Au*, **1(2)**, 119-123 (2021).
- Tanifuji, K.; Jasniewski, A. J.; Villarreal, D.; Stiebritz, M. T.; Lee, C. C.; Wilcoxon, J.; Okhi, Y.; Chatterjee, R.; Bogacz, I.; Yano, J.; Kern, J.; Hedman, B.; Hodgson, K. O.; Britt, R. D.; Hu, Y.; Ribbe, M. W., Tracing the Incorporation of the “Ninth Sulfur” into the Nitrogenase Cofactor Precursor with Selenite and Tellurite, *Nat. Chem.*, **13**, 1228-1234 (2021).
- Wakioka, M.; Yamashita, N.; Mori, H.; Murdey, R.; Shimoaka, T.; Shioya, N.; Wakamiya, A.; Nishihara, Y.; Hasegawa, T.; Ozawa, F., Formation of trans-Poly(thienylenevinylene) Thin Films by Solid-State Thermal Isomerization, *Chem. Mater.*, **33**, 5631-5638 (2021).
- Wakioka, M.; Torii, N.; Saito, M.; Osaka, I.; Ozawa, F., Donor-Acceptor Polymers Containing 4,8-Dithienylbenzo[1,2-*b*:4,5-*b'*] dithiophene via Highly Selective Direct Arylation Polymerization, *ACS Appl. Polym. Mater.*, **3**, 830-836 (2021).
- Kang, W.; Rettberg, L. A.; Stiebritz, M. T.; Jasniewski, A. J.; Tanifuji, K.; Lee, C. C.; Ribbe, M. W.; Hu, Y., X-Ray Crystallographic Analysis of Ni<sub>4</sub>B with a Full Complement of Clusters: Structural Insights into the Radical SAM-Dependent Carbide Insertion during Nitrogenase Cofactor Assembly, *Angew. Chem. Int. Ed. Engl.*, **60**, 2364-2370 (2021).
- Liedtke, J.; Lee, C. C.; Tanifuji, K.; Jasniewski, A. J.; Ribbe, M. W.; Hu, Y., Characterization of a Mo-Nitrogenase Variant Containing a Citrate-Substituted Cofactor, *Chembiochem*, **22**, 151-155 (2021).
- Rupnik, K.; Rettberg, L.; Tanifuji, K.; Rebelein, J. G.; Ribbe, M. W.; Hu, Y.; Hales, B. J., An EPR and VTVH MCD Spectroscopic Investigation of the Nitrogenase Assembly Protein Ni<sub>4</sub>B, *J. Biol. Inorg. Chem.*, **26**, 403-410 (2021).
- Kameo, H.; Sakaki, S.; Ohki, Y.; Uehara, N.; Kosukegawa, T.; Suzuki, H.; Takao, T., Four-Electron Reduction of Dioxygen on a Metal Surface: Models of Dissociative and Associative Mechanisms in a Homogeneous System, *Inorg. Chem.*, **60**, 1550-1560 (2021).
- Nanophotonics —
- Ohara, K.; Yamada, T.; Aharen, T.; Tahara, H.; Hirori, H.; Suzuura, H.; Kanemitsu, Y., Impact of Spin-Orbit Splitting on Two-Photon Absorption Spectra in a Halide Perovskite Single Crystal, *Phys. Rev. B*, **103**, L041201 (2021).
- Yoshida, S.; Arashida, Y.; Hirori, H.; Tachizaki, T.; Taninaka, A.; Ueno, H.; Takeuchi, O.; Shigekawa, H., Terahertz Scanning Tunneling Microscopy for Visualizing Ultrafast Electron Motion in Nanoscale Potential Variations, *ACS Photonics*, **8**, 315-323 (2021).
- Sato, S. A.; Hirori, H.; Sanari, Y.; Kanemitsu, Y.; Rubio, A., High-Order Harmonic Generation in Graphene: Nonlinear Coupling of Intraband and Interband Transitions, *Phys. Rev. B*, **103**, L041408 (2021).
- Truong, M. A.; Lee, H.; Shimazaki, A.; Mishima, R.; Hino, M.; Yamamoto, K.; Otsuka, K.; Handa, T.; Kanemitsu, Y.; Murdey, R.; Wakamiya, A., Near-Ultraviolet Transparent Organic Hole-Transporting Materials Containing Partially Oxygen-Bridged Triphenylamine Skeletons for Efficient Perovskite Solar Cells, *ACS Appl. Energy Mater.*, **4**, 1484-1495 (2021).
- Ogawa, Y.; Tahara, H.; Igarashi, N.; Yamada, Y.; Kanemitsu, Y., Spectral Characterization of the Rashba Spin-Split Band in a Lead Halide Perovskite Single Crystal by Photocurrent Heterodyne Interference Spectroscopy, *Phys. Rev. B*, **103**, L081201 (2021).
- Nakagawa, K.; Hirori, H.; Sanari, Y.; Sekiguchi, F.; Sato, R.; Saruyama, M.; Teranishi, T.; Kanemitsu, Y., Interference Effects in High-Order Harmonics from Colloidal Perovskite Nanocrystals Excited by an Elliptically Polarized Laser, *Phys. Rev. Mater.*, **5**, 016001 (2021).

Sekiguchi, F.; Hirori, H.; Yumoto, G.; Shimazaki, A.; Nakamura, T.; Wakamiya, A.; Kanemitsu, Y., Enhancing the Hot-Phonon Bottleneck Effect in a Metal Halide Perovskite by Terahertz Phonon Excitation, *Phys. Rev. Lett.*, **126**, 077401 (2021).

Tachizaki, T.; Hayashi, K.; Kanemitsu, Y.; Hirori, H., On the Progress of Ultrafast Time-Resolved THz Scanning Tunneling Microscopy, *APL Mater.*, **9**, 060903 (2021).

Yumoto, G.; Hirori, H.; Sekiguchi, F.; Sato, R.; Saruyama, M.; Teranishi, T.; Kanemitsu, Y., Strong Spin-Orbit Coupling Inducing Autler-Townes Effect in Lead Halide Perovskite Nanocrystals, *Nat. Commun.*, **12**, 3026 (2021).

Yamada, Y.; Mino, H.; Kawahara, T.; Oto, K.; Suzuura, H.; Kanemitsu, Y., Polaron Masses in  $\text{CH}_3\text{NH}_3\text{PbX}_3$  Perovskites Determined by Landau Level Spectroscopy in Low Magnetic Fields, *Phys. Rev. Lett.*, **126**, 237401 (2021).

Matsumoto, T.; Nomata, I.; Ohhara, T.; Kanemitsu, Y., Determination of Localized Surface Phonons in Nanocrystalline Silicon by Inelastic Neutron Scattering Spectroscopy and Its Application to Deuterium Isotope Enrichment, *Phys. Rev. Mater.*, **5**, 066003 (2021).

Yamada, T.; Handa, T.; Yamada, Y.; Kanemitsu, Y., Light Emission from Halide Perovskite Semiconductors: Bulk Crystals, Thin Films, and Nanocrystals, *J. Phys. D Appl. Phys.*, **54**, 383001 (2021).

Kimura, T.; Matsumori, K.; Oto, K.; Kanemitsu, Y.; Yamada, Y., Observation of High Carrier Mobility in  $\text{CH}_3\text{NH}_3\text{PbBr}_3$  Single Crystals by AC Photo-Hall Measurements, *Appl. Phys. Express*, **14**, 041009 (2021).

Cho, K.; Yamada, T.; Tahara, H.; Tadano, T.; Suzuura, H.; Saruyama, M.; Sato, R.; Teranishi, T.; Kanemitsu, Y., Luminescence Fine Structures in Single Lead Halide Perovskite Nanocrystals: Size Dependence of the Exciton-Phonon Coupling, *Nano Lett.*, **21**, 7206-7212 (2021).

Zhang, Z.; Hirori, H.; Sekiguchi, F.; Shimazaki, A.; Iwasaki, Y.; Nakamura, T.; Wakamiya, A.; Kanemitsu, Y., Ultrastrong Coupling between THz Phonons and Photons Caused by an Enhanced Vacuum Electric Field, *Phys. Rev. Res.*, **3**, L032021 (2021).

Sanari, Y.; Sekiguchi, F.; Nakagawa, K.; Ishii, N.; Kanemitsu, Y.; Hirori, H., Generation of Wavelength-Tunable Few-Cycle Pulses in the Mid-Infrared at Repetition Rates up to 10 kHz, *Opt. Lett.*, **46**, 5280-5283 (2021).

Hu, S.; Truong, M. A.; Otsuka, K.; Handa, T.; Yamada, T.; Nishikubo, R.; Iwasaki, Y.; Saeki, A.; Murdey, R.; Kanemitsu, Y.; Wakamiya, A., Mixed Lead-Tin Perovskite Films with  $>7 \mu\text{s}$  Charge Carrier Lifetimes Realized by Maltol Post-Treatment, *Chem. Sci.*, **12**, 13513-13519 (2021).

Tachizaki, T.; Sakaguchi, R.; Terada, S.; Kamei, K.-I.; Hirori, H., Response of Human Induced Pluripotent Stem Cells to Terahertz Radiation, *Optics InfoBase Conference Papers*, JM4F.4 (2021).

## BIOINFORMATICS CENTER

### — Chemical Life Science —

Brandão, M. C.; Benedetti, F.; Martini, S.; Soviadan, Y. D.; Irisson, J.-O.; Romagnan, J.-B.; Elineau, A.; Desnos, C.; Jalabert, L.; Freire, A. S.; Picheral, M.; Guidi, L.; Gorsky, G.; Bowler, C.; Karp-Boss, L.; Henry, N.; de Vargas, C.; Sullivan, M. B.; Tara Oceans Consortium Coordinators; Stemmann, L.; Lombard, F., Macroscale Patterns of Oceanic Zooplankton Composition and Size Structure, *Sci. Rep.*, **11**, 15714 (2021).

Kawasaki, T.; Endo, H.; Ogata, H.; Chatchawankanphanich, O.; Yamada, T., The Complete Genomic sequence of the Novel Myovirus RP13 Infecting *Ralstonia Solanacearum*, the Causative agent of Bacterial Wilt, *Arch. Virol.*, **166**, 651-654 (2021).

Sandaa, R.-A.; Saltvedt, M. R.; Dahle, H.; Wang, H.; Våge, S.; Blanc-Mathieu, R.; Steen, I. H.; Grimsley, N.; Edvardsen, B.; Ogata, H.; Lawrence, J., Adaptive evolution of Viruses Infecting Marine Microalgae (haptophytes), from Acute Infections to Stable coexistence, *Biol. Rev. Camb. Philos. Soc.*, doi: 10.1111/brv.12795 (2021).

Cheung, S.; Zehr, J. P.; Xia, X.; Tsurumoto, C.; Endo, H.; Nakaoka, S.-I.; Mak, W.; Suzuki, K.; Liu, H., Gamma4: a Genetically Versatile Gammaproteobacterial nifH Phylotype That is Widely Distributed in the North Pacific Ocean, *Environ. Microbiol.*, **23**, 4246-4259 (2021).

Kijima, S.; Delmont, T. O.; Miyazaki, U.; Gaia, M.; Endo, H.; Ogata, H., Discovery of Viral Myosin Genes with Complex Evolutionary History Within Plankton, *Front. Microbiol.*, **12**, 683294 (2021).

Meng, L.; Endo, H.; Blanc-Mathieu, R.; Chaffron, S.; Hernández-Velázquez, R.; Kaneko, H.; Ogata, H., Quantitative Assessment of Nucleocytoplasmic Large DNA Virus and Host Interactions Predicted by Co-Occurrence Analyses, *mSphere*, **6**, e01298-20 (2021).

Kaneko, H.; Blanc-Mathieu, R.; Endo, H.; Chaffron, S.; Delmont, T. O.; Gaia, M.; Henry, N.; Hernández-Velázquez, R.; Nguyen, C. H.; Mamitsuka, H.; Forterre, P.; Jaillon, O.; de Vargas, C.; Sullivan, M. B.; Suttle, C. A.; Guidi, L.; Ogata, H., Eukaryotic Virus Composition Can Predict the Efficiency of Carbon Export in the Global Ocean, *iScience*, **24**, 102002 (2021).

Yoshida, K.; Zhang, R.; Garcia, K. G.; Endo, H.; Gotoh, Y.; Hayashi, T.; Takemura, M.; Ogata, H., Draft Genome Sequence of Medusavirus stheno, Isolated from the Tatakai River of Uji, Japan, *Microbiol. Resour. Announc.*, **10**, e0132320 (2021).

Yahara, K.; Suzuki, M.; Hirabayashi, A.; Suda, W.; Hattori, M.; Suzuki, Y.; Okazaki, Y., Long-Read Metagenomics Using PromethION Uncovers Oral Bacteriophages and Their Interaction with Host Bacteria, *Nat. Commun.*, **12**, 27 (2021).

Okazaki, Y.; Fujinaga, S.; Salcher, M. M.; Callieri, C.; Tanaka, A.; Kohzu, A.; Oyagi, H.; Tamaki, H.; Nakano, S.-I., Microdiversity and Phylogeographic Diversification of Bacterioplankton in Pelagic Freshwater Systems Revealed through Long-Read Amplicon Sequencing, *Microbiome*, **9**, 24 (2021).

- Acinas, S. G.; Sánchez, P.; Salazar, G.; Cornejo-Castillo, F. M.; Sebastián, M.; Logares, R.; Royo-Llonch, M.; Paoli, L.; Sunagawa, S.; Hingamp, P.; Ogata, H.; Lima-Mendez, G.; Roux, S.; González, J. M.; Arrieta, J. M.; Alam, I. S.; Kamau, A.; Bowler, C.; Raes, J.; Pesant, S.; Bork, P.; Agustí, S.; Gojobori, T.; Vaqué, D.; Sullivan, M. B.; Pedrós-Alió, C.; Massana, R.; Duarte, C. M.; Gasol, J. M., Deep Ocean Metagenomes Provide Insight into the Metabolic Architecture of Bathypelagic Microbial Communities, *Commun. Biol.*, **4**, 604 (2021).
- Yoshikawa, G.; Miyazaki, K.; Ogata, H.; Miyazaki, M., The Evolution of Rag Gene Enhancers and Transcription Factor e and id Proteins in the Adaptive Immune System, *Int. J. Mol. Sci.*, **22**, 5888 (2021).
- Ogawa, S.; Shimidzu, H.; Fukuda, K.; Tsunekawa, N.; Hirano, T.; Sato, F.; Yura, K.; Hasunuma, T.; Ochi, K.; Yamamoto, M.; Sakamoto, W.; Hashimoto, K.; Ogata, H.; Kanao, T.; Nemoto, M.; Inagaki, K.; Tamura, T., Multiple Mutations in RNA Polymerase  $\beta$ -Subunit Gene (*rpoB*) in *Streptomyces incarnatus* NRRL8089 Enhance Production of Antiviral Antibiotic Sinefungin: Modeling rif Cluster region by Density Functional Theory, *Biosci. Biotechnol. Biochem.*, **85**, 1275-1282 (2021).
- Blanc-Mathieu, R.; Dahle, H.; Hofgaard, A.; Brandt, D.; Ban, H.; Kalinowski, J.; Ogata, H.; Sandaa, R.-A., A Persistent Giant Algal Virus, with a Unique Morphology, Encodes an Unprecedented Number of Genes Involved in Energy Metabolism, *J. Virol.*, **95**, e02446 (2021).
- Sakurai, T.; De Velasco, M. A.; Sakai, K.; Nagai, T.; Nishiyama, H.; Hashimoto, K.; Uemura, H.; Kawakami, H.; Nakagawa, K.; Ogata, H.; Nishio, K.; Kudo, M., Integrative Analysis of Gut Microbiome and Host Transcriptomes Reveals Associations between Treatment Outcomes and Immunotherapy-Induced Colitis, *Mol. Oncol.*, doi: 10.1002/1878-0261.13062 (2021).
- Shiozaki, T.; Hashihama, F.; Endo, H.; Ijichi, M.; Takeda, N.; Makabe, A.; Fujiwara, A.; Nishino, S.; Harada, N., Assimilation and Oxidation of Urea-Derived Nitrogen in the Summer Arctic Ocean, *Limnol. Oceanogr.*, doi: 10.1002/lno.11950 (2021).
- Xia, J.; Kameyama, S.; Prodinge, F.; Yoshida, T.; Cho, K.-H.; Jung, J.; Kang, S.-H.; Yang, E.-J.; Ogata, H.; Endo, H., Tight Association between Microbial Eukaryote and Imitervirales Communities in the Pacific Arctic Ocean, *FEMS Microbiol. Ecol.* doi: 10.1101/2021.09.02.458798 (2021).
- Rigonato, J.; Budinich, M.; Murillo, A. A.; Brandão, M. C.; Pierella Karlusich, J. J.; Soviadan, Y. D.; Gregory, A. C.; Endo, H.; Kokoszka, F.; Vik, D.; Henry, N.; Frémont, P.; Labadie, K.; Zayed, A. A.; Dimier, C.; Picheral, M.; Searson, S.; Poulain, J.; Stefanie, K. els; Pesant, S.; Karsenti, E.; Bork, P.; Bowler, C.; Chaffron, S.; de Vargas, C.; Eveillard, D.; Gehlen, M.; Iudicone, D.; Lombard, F.; Ogata, H.; Stemmann, L.; Sullivan, M. B.; Sunagawa, S.; Wincker, P.; Jaillon, O., Insights into Biotic and Abiotic Modulation of Ocean Mesopelagic Communities, *FEMS Microbiol. Ecol.* doi: 10.1101/2021.02.26.433055 (2021).
- Prodinge, F.; Endo, H.; Takano, Y.; Li, Y.; Tominaga, K.; Isozaki, T.; Blanc-Mathieu, R.; Gotoh, Y.; Tetsuya, H.; Taniguchi, E.; Nagasaki, K.; Yoshida, T.; Ogata, H., Year-Round Dynamics of Amplicon Sequence Variant Communities Differ among Eukaryotes, Mimiviridae, and Prokaryotes in a Coastal Ecosystem, *FEMS Microbiol. Ecol.* doi: 10.1101/2021.02.02.429489 (2021).
- Zhang, R.; Endo, H.; Takemura, M.; Ogata, H., RNA Sequencing of Medusavirus Suggests Remodeling of the Host Nuclear Environment at an Early Infection Stage, *Microbiol. Spectr.*, **9**, e00064-21 (2021).
- Royo-Llonch, M.; Sánchez, P.; Ruiz-González, C.; Salazar, G.; Pedrós-Alió, C.; Sebastián, M.; Labadie, K.; Paoli, L. M.; Ibarbalz, F.; Zinger, L.; Churchward, B.; Babin, M.; Bork, P.; Boss, E.; Cochrane, G.; de Vargas, C.; Gorsky, G.; Grimsley, N.; Guidi, L.; Hingamp, P.; Iudicone, D.; Jaillon, O.; Kandels, S.; Not, F.; Ogata, H.; Pesant, S.; Poulton, N.; Raes, J.; Sardet, C.; Speich, S.; Settmann, L.; Sullivan, M. B.; Chaffron, S.; Eveillard, D.; Karsenti, E.; Sunagawa, S.; Wincker, P.; Karp-Boss, L.; Bowler, C.; Acinas, S. G.; Tara Oceans Coordinators., Compendium of 530 Metagenome-Assembled Bacterial and Archaeal Genomes from the Polar Arctic Ocean, *Nat. Microbiol.*, **6**, 1561-1574 (2021).
- [Others]
- Acinas, S. G.; Sánchez, P.; Salazar, G.; Cornejo-Castillo, F. M.; Sebastián, M.; Logares, R.; Royo-Llonch, M.; Paoli, L.; Sunagawa, S.; Hingamp, P.; Ogata, H.; Lima-Mendez, G.; Roux, S.; González, J. M.; Arrieta, J. M.; Alam, I. S.; Kamau, A.; Bowler, C.; Raes, J.; Pesant, S.; Bork, P.; Agustí, S.; Gojobori, T.; Vaqué, D.; Sullivan, M. B.; Pedrós-Alió, C.; Massana, R.; Duarte, C. M.; Gasol, J. M., Deep Ocean Metagenomes Provide Insight into the Metabolic Architecture of Bathypelagic Microbial Communities, *Commun. Biol.*, **4**, 1 (2021).
- Sakurai, T.; De Velasco, M. A.; Sakai, K.; Nagai, T.; Nishiyama, H.; Hashimoto, K.; Uemura, H.; Kawakami, H.; Nakagawa, K.; Ogata, H.; Nishio, K.; Kudo, M., Integrative Analysis of Gut Microbiome and Host Transcriptomes Reveals Associations between Treatment Outcomes and Immunotherapy-Induced Colitis, *Mol. Oncol.*, (2021).
- Zhang, R.; Endo, H.; Takemura, M.; Ogata, H., RNA Sequencing of Medusavirus Suggests Remodeling of the Host Nuclear Environment at an Early Infection Stage, *Microbiol. Spectr.*, (2021).
- Chaffron, S.; Delage, E.; Budinich, M.; Vintache, D.; Henry, N.; Nef, C.; Ardyna, M.; Zayed, A. A.; Junger, P. C.; Galand, P. E.; Lovejoy, C.; Murray, A. E.; Sarmiento, H.; Acinas, S. G.; Babin, M.; Iudicone, D.; Jaillon, O.; Karsenti, E.; Wincker, P.; Karp-Boss, L.; Sullivan, M. B.; Bowler, C.; de Vargas, C.; Eveillard, D., Environmental Vulnerability of the Global Ocean Epipelagic Plankton Community Interactome, *Sci. Adv.*, **7**, 35, eabg1921 (2021).
- Kijima, S.; Delmont, T. O.; Miyazaki, U.; Gaia, M.; Endo, H.; Ogata, H., Myosin Genes in NCLDVs: Their Complex Origins and Putative Functions, *Aquatic Virus Workshop 10* (2021).
- Garcia, K. G.; Yoshida, K.; Aoki, K.; Endo, H.; Takemura, M.; Ogata, H., Recombination between Genomes of Giant Virus Marseilleviridae, *Aquatic Virus Workshop 10* (2021).
- Zia, J.; Kameyama, S.; Prodinge, F.; Yoshida, T.; Cho, K.-H.; Jung, J.; Kang, S.-H.; Yang, E.-J.; Ogata, H.; Endo, H., Characteristics and Association of Microbial Eukaryotic and Mimiviridae Communities in the Beaufort Sea, *Aquatic Virus Workshop 10* (2021).
- Meng, L.; Endo, H.; Blanc-Mathieu, R.; Chaperon, S.; Hernandez-Velazquez, R.; Kaneko, H.; Ogata, H., Who Infects Whom? Assessment of Co-Occurrence Methods for NCLDV-Host Interactions, *Aquatic Virus Workshop 10* (2021).
- Endo, H.; Blanc-Mathieu, R.; Ogata, H., Pole-to-Pole Biogeography of Marine Giant Viruses and Their Role in Biogeochemical Cycles, *Aquatic Virus Workshop 10* (2021).
- Kaneko, H.; Romain, B.-M.; Endo, H.; Ogata, H., The Association of Marine Viruses and Carbon Cycle revealed by a Large Omits Dataset, *Aquatic Virus Workshop 10* (2021).

- Zhang, R.; Endo, H.; Takemura, M.; Ogata, H., RNA-Seq of Medusa Virus Reveals Temporal Viral Gene Expression Profile and Remodeling of the Host Nucleus, *Aquatic Virus Workshop 10* (2021).
- Endo, H.; Ogata, H., Biogeography of Marine Giant Viruses and Their Role in Biogeochemical Cycles, *Institute of Low Temperature Science, Hokkaido University, Joint Research Meeting 2021, Meeting on Biogeochemical Interactions between Atmosphere and Ocean in the Cryosphere*. (2021).
- Ban, H.; Kuwata, A.; Nakamura, Y.; Sato, S.; Yoshikawa, S.; Yamada, K.; Ichinomiya, M.; Ogata, H., Eukaryotic Phytoplankton with Silicified cell Walls: Comparative Genome Analysis of Diatoms and Parmales, *The 45th JSP Annual Meeting -Online Tokyo 2021-* (2021).
- Okazaki, Y., What Freshwater Microbial Ecology Tells Us, *Japanese Society of Microbial Ecology*, **36(2)**, 80-82 (2021).
- **Mathematical Bioinformatics** —
- Wang, Y.; Li, F.; Bharathwaj, M.; Rosas, N. C.; Leier, A.; Akutsu, T.; Webb, G. I.; Marquez-Lago, T. T.; Li, J.; Lithgow, T.; Song, J., DeepBL: A Deep Learning-Based Approach for *in silico* Discovery of Beta-Lactamases, *Brief. Bioinform.*, **22**, bbaa301 (2021).
- Xie, R.; Li, J.; Wang, J.; Dai, W.; Leier, A.; Marquez-Lago, T. T.; Akutsu, T.; Lithgow, T.; Song, J.; Zhang, Y., DeepVF: A Deep Learning-Based Hybrid Framework for Identifying Virulence Factors Using the Stacking Strategy, *Brief. Bioinform.*, **22**, bbaa125 (2021).
- Azam, N. A.; Zhu, J.; Sun, Y.; Shi, Y.; Shurbevski, A.; Zhao, L.; Nagamochi, H.; Akutsu, T., A Novel Method for Inference of Acyclic Chemical Compounds with Bounded Branch-Height Based on Artificial Neural Networks and Integer Programming, *Algorithms. Mol. Biol.*, **16**, 18 (2021).
- Shinzawa, Y.; Akutsu, T.; Nacher, J. C., Uncovering and Classifying the Role of Driven Nodes in Control of Complex Networks, *Sci. Rep.*, **11**, 9627 (2021).
- Li R.; Lin C.-Y.; Guo W.-F.; Akutsu T., Weighted Minimum Feedback Vertex Sets and Implementation in Human Cancer Genes Detection, *BMC Bioinformatics.*, **22**, 143 (2021).
- Liu, P.; Song, J.; Lin, C.-Y.; Akutsu, T., ReCGBM: a Gradient Boosting-Based Method for Predicting Human Dicer Cleavage sites, *BMC Bioinformatics*, **22**, 63 (2021).
- Akutsu, T.; Jansson, J.; Li, R.; Takasu, A.; Tamura, T., New and Improved Algorithms for Unordered Tree Inclusion, *Theor. Comput. Sci.*, **883**, 83-98 (2021).
- Yamaguchi, E.; Akutsu, T.; Nacher, J. C., Probabilistic Critical Controllability Analysis of Protein Interaction Networks Integrating Normal Brain Ageing Gene Expression Profiles, *Int. J. Mol. Sci.*, **22**, 9891 (2021).
- Cheng, X.; Ching, W.-K.; Guo, S.; Akutsu, T., Discrimination of Attractors with Noisy Nodes in Boolean Networks, *Automatica (Oxf)*, **130**, 109630 (2021).
- Zhu, Y.; Li, F.; Xiang, D.; Akutsu, T.; Song, J.; Jia, C., Computational Identification of Eukaryotic Promoters Based on Cascaded Deep Capsule Neural Networks, *Brief. Bioinform.*, **22**, bbaa299 (2021).
- Chen, Z.; Zhao, P.; Li, C.; Li, F.; Xiang, D.; Chen, Y.-Z.; Akutsu, T.; Daly, R. J.; Webb, G. I.; Zhao, Q.; Kurgan, L.; Song, J., ILearnPlus: A Comprehensive and Automated Machine-Learning Platform for Nucleic Acid and Protein Sequence Analysis, Prediction and Visualization, *Nucleic Acids Res.*, **49**, e60 (2021).
- Kajiwarra, M.; Nomura, R.; Goetze, F.; Kawabata, M.; Isomura, Y.; Akutsu, T.; Shimono, M., Inhibitory Neurons Exhibit High Controlling Ability in the Cortical Microconnectome, *PLoS Comput. Biol.*, **17**, e1008846 (2021).
- Shi, Y.; Zhu, J.; Azam, N. A.; Haraguchi, K.; Zhao, L.; Nagamochi, H.; Akutsu, T., An Inverse QSAR Method Based on a Two-Layered Model and Integer Programming, *Int. J. Mol. Sci.*, **22**, 2847 (2021).
- Tanaka, K.; Zhu, J.; Azam, N. A.; Haraguchi, K.; Zhao, L.; Nagamochi, H.; Akutsu, T., An Inverse QSAR Method Based on Decision Tree and Integer Programming, *Lecture Notes in Computer Science (including subseries Lecture Notes in Artificial Intelligence and Lecture Notes in Bioinformatics)*, **12837 LNCS**, 628-644 (2021).
- Zhu, J.; Azam, N. A.; Haraguchi, K.; Zhao, L.; Nagamochi, H.; Akutsu, T., An Improved Integer Programming Formulation for Inferring Chemical Compounds with Prescribed Topological Structures, *Lecture Notes in Computer Science (including subseries Lecture Notes in Artificial Intelligence and Lecture Notes in Bioinformatics)*, **12798 LNAI**, 197-209 (2021).
- Tamura, T., L1 Norm Minimal Mode-Based Methods for Listing Reaction Network Designs for Metabolite Production, *IEICE Trans. Inf. Syst.*, **E104.D**, 679-687 (2021).
- Tamura, T., Efficient Reaction Deletion Algorithms for Redesign of Constraint-Based Metabolic Networks for Metabolite Production with Weak Coupling, *IPSJ Trans. Bioinform.*, **14**, 44551 (2021).
- Mei, S.; Li, F.; Xiang, D.; Ayala, R.; Faridi, P.; Webb, G. I.; Illing, P. T.; Rossjohn, J.; Akutsu, T.; Croft, N. P.; Purcell, A. W.; Song, J., Anthem: A User Customised Tool for Fast and Accurate Prediction of Binding between Peptides and HLA Class I Molecules, *Brief. Bioinform.*, **22**, bbaa415 (2021).
- Nakajima, N.; Hayashi, T.; Fujiki, K.; Shirahige, K.; Akiyama, T.; Akutsu, T.; Nakato, R., Codependency and Mutual Exclusivity for Gene Community Detection from Sparse Single-Cell Transcriptome Data, *Nucleic Acids Res.*, **49**, e104 (2021).
- Ma, Y.; Tamura, T., Dynamic Solution Space Division-Based Methods for Calculating Reaction Deletion Strategies for Constraint-Based Metabolic Networks for Substance Production: DynCubeProd, *Front. Bioinform.*, **1**, doi: 10.3389/fbinf.2021.716112 (2021).
- Tamura, T., Metabolic Network Design for the Production of Useful Substances, *JSBi Bioinformatics Review*, **1(2)**, 37-46 (2021).
- Iqbal, S.; Li, F.; Akutsu, T.; Ascher, D. B.; Webb, G. I.; Song, J., Assessing the Performance of Computational Predictors for Estimating Protein Stability Changes upon Missense Mutations. *Brief. Bioinform.*, **22**, bbab184 (2021).
- Azam, N. A.; Zhu, J.; Haraguchi, K.; Zhao, L.; Nagamochi, H.; Akutsu, T., Molecular Design Based on Artificial Neural Networks, Integer Programming and Grid Neighbor Search, *Proc. 2021 IEEE International Conference on Bioinformatics and Biomedicine*, 360-363 (2021).

Nagamochi, H.; Zhu, J.; Adam, N. A.; Haraguchi, K.; Zhao, L.; Akutsu, T., Integer Linear Programming-Based Methods for Inverse QSAR, *Journal of Computer Chemistry, Japan*, **20**, 106-111 (2021).

[Others]

Akutsu, T., Bioinformatics: An Overview, *The Journal of Information Science and Technology*, **71**, 6, 247-251 (2021).

Nakajima, N.; Akutsu, T.; Nakato, R., Databases for Protein-Protein Interactions, *Methods Mol. Biol.*, **2361**, 229-248 (2021).

#### — Bio-knowledge Engineering —

Cai, M.; Nguyen, C. H.; Mamitsuka, H.; Li, L., XGSEA: CROSS-Species Gene Set Enrichment Analysis via Domain Adaptation, *Brief. Bioinform.*, **22**, bbaa406 (2021).

Nguyen, C. H.; Mamitsuka, H., Learning on Hypergraphs with Sparsity, *IEEE Trans. Pattern. Anal. Mach. Intell.*, **43**, 2710-2722, (2021).

You, R.; Yao, S.; Mamitsuka, H.; Zhu, S., DeepGraphGO: Graph Neural Network for Large-Scale, Multispecies Protein Function Prediction, *Bioinformatics*, **37**, 1262-1271 (2021).

Nguyen, D. H.; Nguyen, C. H.; Mamitsuka, H., Learning Subtree Pattern Importance for Weisfeiler-Lehman Based Graph Kernels, *Mach. Learn.*, **110**, 1585-1607 (2021).

Wimalawarne K.; Mamitsuka H., Reshaped Tensor Nuclear Norms for Higher Order Tensor Completion, *Mach. Learn.*, **110**, 507-531 (2021).

You, R.; Liu, Y.; Mamitsuka, H.; Zhu, S., BERTMeSH: Deep Contextual Representation Learning for Large-Scale High-Performance MeSH Indexing with Full Text, *Bioinformatics*, **37**, 684-692 (2021).

Kaneko, H.; Blanc-Mathieu, R.; Endo, H.; Chaffron, S.; Delmont, T. O.; Gaia, M.; Henry, N.; Hernández-Velázquez, R.; Nguyen, C. H.; Mamitsuka, H.; Forterre, P.; Jaillon, O.; de Vargas, C.; Sullivan, M. B.; Suttle, C. A.; Guidi, L.; Ogata, H., Eukaryotic Virus Composition Can Predict the Efficiency of Carbon Export in the Global Ocean, *iScience*, **24**, 102002 (2021).

Güvençpaltun, B.; Kaski, S.; Mamitsuka, H., DIVERSE: Bayesian Data Integrative Learning for Precise Drug Response Prediction, *IEEE/ACM Trans. Comput. Biol. Bioinform.*, doi: 10.1109/TCBB.2021.3065535 (2021).

Güvenç Paltun, B.; Mamitsuka, H.; Kaski, S., Improving Drug Response Prediction by Integrating Multiple Data sources: Matrix Factorization, Kernel and Network-Based Approaches, *Brief. Bioinform.*, **22**, 346-359 (2021).

Nguyen, D. A.; Nguyen, C. H.; Mamitsuka H., A Survey on Adverse Drug Reaction Studies: Data, Tasks and Machine Learning Methods, *Brief. Bioinform.*, **22**, 164-177 (2021).

Nguyen, D. A.; Ngo, V. L.; Nguyen, K. A.; Nguyen, C. H.; Than, K., Boosting Prior Knowledge in Streaming Variational Bayes, *Neurocomputing*, **424**, 143-159 (2021).

Liu, L.; Mamitsuka, H.; Zhu, S., HPOFiller: Identifying Missing Protein-Phenotype Associations by Graph Convolutional Network, *Bioinformatics*, **37**(19), 3328-3336 (2021).

Güvenç Paltun, B.; Kaski, S.; Mamitsuka, H., Machine Learning Approaches for Drug Combination Therapies, *Brief. Bioinform.*, **22**(6), bbab293 (2021).

Blanc-Mathieu, R.; Kaneko, H.; Endo, H.; Chaffron, S.; Hernandez-Velazquez, R.; Nguyen, C. H.; Mamitsuka, H.; Henry, N.; de Vargas, C.; Sullivan, M. B.; Suttle, C. A.; Guidi, L.; Ogata, H., Viruses of the Eukaryotic Plankton are Predicted to Increase Carbon Export Efficiency in the Global Sunlit Ocean, *iScience*, **24**(1), (2021).

#### HAKUBI PROJECT

##### — Synthesis and Exploration of Novel Charge Transition Oxide Materials for Future Multifunctional Devices —

Injac, S. D. A.; Xu, Y.; Denis Romero, F.; Shimakawa, Y., Pauli-paramagnetic and Metallic Properties of High Pressure Polymorphs of BaRhO<sub>3</sub> Oxides Containing Rh<sub>2</sub>O<sub>9</sub> Dimers, *Dalton Trans.*, **50**, 4673-4679 (2021).

##### — Optoelectronic Energy Recycling and Quantum Cooperative Effects in Semiconductor Nanostructures —

Tahara, H.; Sakamoto, M.; Teranishi, T.; Kanemitsu, Y., Collective Enhancement of Quantum Coherence in Coupled Quantum Dot Films, *Phys. Rev. B*, **104**, L241405 (2021).