Theoretical and Computational Molecular Science

X. LU, H. NIKAWA, L. FENG, T. TSUCHIYA, Y. MAEDA, T. AKASAKA, N. MIZOROGI, Z. SLANINA and S. NAGASE, "Location of the Y atoms in $Y@C_{82}$ and Its Influence on the Reactivity of Cage Carbons," *J. Am. Chem. Soc.* **131**, 12066–12607 (2009).

X. GAO, Y. OHTSUKA, K. ISHIMURA and S. NAGASE, "Mechanism and Dynamic Correlation Effects in Cycloaddition Reactions of Singlet Difluorocarbene to Alkenes and Disilene," *J. Phys. Chem. A* **113**, 9582–9860 (2009).

M. YAMADA, N. MIZOROGI, T. TSUCHIYA, T. AKASAKA and S. NAGASE, "Synthesis and Characterization of the D_{5h} Isomer of the Endohedral Dimetallofullerene $Ce_2@C_{80}$: Two-Dimensional Circulation of Encapsulated Metal Atoms inside a Fullerene Cage," *Chem. –Eur. J.* **15**, 9486–9493 (2009).

M. YAMADA, M. OKAMURA, S. SATO, C. I. SOMEYA, N. MIZOROGI, T. TSUCHIYA, T. AKASAKA, T. KATO and S. NAGASE, "Two Regioisomers of Endohedral Pyrrolidinodimetallofullerene $M_2@I_h$-$C_{80}(CH_2)_2$NTrt (M = La, Ce; Trt = trityl): Control of Metal Atom Positions by Addition Positions," *Chem. –Eur. J.* **15**, 10533–10542 (2009).

M. SAITO, M. SHIRATAKE, T. TAJIMA, J. -D. GUO and S. NAGASE, "Synthesis and Structure of the Dithienostannole Anion," *J. Organomet. Chem.* **694**, 4056–4061 (2009).

Y. PENG, J. -D. GUO, B. D. ELLIS, Z. ZHU, J. C. FETTINGER, S. NAGASE and P. P. POWER, "Reaction of Hydrogen or Ammonia with Unsaturated Germanium or Tin Molecules under Ambient Conditions: Oxidative Addition versus Arene Elimination," *J. Am. Chem. Soc.* **131**, 16272–16282 (2009).

X. LU, H. NIKAWA, T. TSUCHIYA, T. AKASAKA, M. TOKI, H. SAWA, N. MIZOROGI and S. NAGASE, "Nitrated Benzyne Derivatives of $La@C_{82}$: Addition of NO_2 and Its Positional Directing Effect on the Subsequent Addition of Benzynes," *Angew. Chem., Int. Ed.* **49**, 594–597 (2010).

H. NIKAWA, Y. ARAKI, Z. SLANINA, T. TSUCHIYA, T. AKASAKA, T. WADA, O. ITO, K. -P. DINSE, M. ATA, T. KATO and S. NAGASE, "The Effect of Atomic Nitrogen on the C_{60} Cage," *Chem. Commun.* **46**, 631–633 (2010).

M. SAITO, T. TANIKAWA, T. TAJIMA, J. -D. GUO and S. NAGASE, "Synthesis and Structures of Heterasumanenes Having Different Heteroatom Functionalities," *Tetrahedron Lett.* **51**, 672–675 (2010).

X. GAO, J. JANG and S. NAGASE, "Hydrazine and Thermal Reduction of Graphene Oxide: Reaction Mechanisms, Product Structures, and Reaction Design," *J. Phys. Chem. C* **114**, 832–842 (2010).

M. YAMADA, T. AKASAKA and S. NAGASE, "Endohedral Metal Atoms in Pristine and Functionalized Fullerene Cages," *Acc. Chem. Res.* **43**, 92–102 (2010).

Y. OHTSUKA and S. NAGASE, "Projector Monte Carlo Method Based on Slater Determinants. Test Application to Singlet Excited States of H_2O and LiF," *Chem. Phys. Lett.* **485**, 367–370 (2010).

N. KANO, H. MIYAKE, K. SASAKI, T. KAWASHIMA, N. MIZOROGI and S. NAGASE, "Dianionic Species with a Bond Consisting of Two Pentacoordinated Silicon Atoms," *Nat. Chem.* **2**, 112–116 (2010).

Y. MAEDA, S. SATO, K. INADA, H. NIKAWA, M. YAMADA, N. MIZOROGI, T. HASEGAWA, T. TSUCHIYA, T. AKASAKA, T. KATO, Z. SLANINA and S. NAGASE, "Regioselective Exohedral Functionalization of $La@C_{82}$ and Its 1,2,3,4,5-Pentamethylcyclopentadiene and Adamantylidene Adducts," *Chem. –Eur. J.* **16**, 2193–2197 (2010).

Y. MAEDA, T. KATO, T. HASEGAWA, M. KAKO, T. AKASAKA, J. LU and S. NAGASE, "Two-Step Alkylation of Single-Walled Carbon Nanotubes: Substituent Effect on Sidewall Functionalization," *Org. Lett.* **12**, 996–999 (2010).

T. TSUCHIYA, T. AKASAKA and S. NAGASE, "New Vistas in Fullerene Endohedrals: Functionalization with Compounds from Main Group Elements," *Pure Appl. Chem.* **82**, 505–521 (2010).

T. SASAMORI, J. S. HAN, K. HIRONAKA, N. TAKAGI, S. NAGASE and N. TOKITOH, "Synthesis and Structure of Stable 1,2-Diaryldisilyne," *Pure Appl. Chem.* **82**, 603–612 (2010).

M. SAITO, T. TANIKAWA, T. TAJIMA, J. -D. GUO and S. NAGASE, "Arching a Bay Area of Triphenyleno[1,12-*bcd*]thiophene with Group 14 Functionalities: Synthesis of the First Triphenylene Derivatives Having Thiophene and Metallafluorenen Moieties," *J. Organomet. Chem.* **695**, 1035–1041 (2010).

K. TAKEUCHI, M. ICHINOHE, A. SEKIGUCHI, J. -D. GUO and S. NAGASE, "Reactivity of the Disilyne RSi≡SiR (R = $Si^iPr[CH(SiMe_3)_2]_2$) toward Bis(silylcyanide) Forming a 1,4-Diaza-2,3-disilabenzene Analog," *J. Phys. Org. Chem.* **23**, 390–394 (2010).

X. GAO, L. LIU, S. IRLE and S. NAGASE, "Carbon Spiral Helix: A Nanoarchitecture Derived from Monovalency Defects in Graphene," *Angew. Chem., Int. Ed.* **49**, 3200–3202 (2010).

M. YAMADA, T. TSUCHIYA, T. AKASAKA and S. NAGASE, "In-Depth Understanding of π-Electron Systems: New Vistas in Fullerene Endohedrals," *Pure Appl. Chem.* **82**, 757–767 (2010).

M. SAITO, M. SAKAGUCHI, T. TAJIMA, K. ISHIMURA, S. NAGASE and M. HADA, "Dilithioplumbole: A Lead-Bearing Aromatic Cyclopentadinyl Analog," *Science* **328**, 339–342 (2010).

J. ZHOU, H. LI, J. LU, G. LUO, L. LAI, R. QIN, L. WANG, S. NAGASE, Z. GAO, W. MEI, G. LI, D. YU and S. SANVITO, "Selection of Single-Walled Carbon Nanotubes According to Both Their Diameter and Chirality via Nanotweezers," *Nano Res.* **3**, 296–306 (2010).

X. LU, Z. SLANINA, T. AKASAKA, T. TSUCHIYA, N. MIZOROGI and S. NAGASE, "$Yb@C_{2n}$ (n = 40, 41, 42): New Fullerene Allotropes with Unexpected Electrochemical Properties," *J. Am. Chem. Soc.* **132**, 5896–5905 (2010).

Y. TAKANO, M. A. HERRANZ, N. MARTIN, S. G. RADHAKRISHNAN, D. M. GULDI, T. TSUCHIYA, S. NAGASE and T. AKASAKA, "Donor–Acceptor Conjugates of Lanthanum Endohedral Metallofullerene and π-Extended Tetrathiafulvalene," *J. Am. Chem. Soc.* **132**, 8048–8055 (2010).

M. SAITO, M. SAKAGUCHI, T. TAJIMA, K. ISHIMURA and S. NAGASE, "Synthesis, Structures, and Properties of Plumboles," *Phosphorus, Sulfur Silicon Relat. Elem.* **185**, 1068–1076 (2010).

M. O. ISHITUKA, H. ENOKI, T. TSUCHIYA, Z. SLANINA, N. MIZOROGI, S. NAGASE, M. T. H. LIU and T. AKASAKA, "Chemical Modification of Endohedtral Metallofullertene La@C_{82} with 3-Chloro-3-phenyldiazirine," *Phosphorus, Sulfur Silicon Relat. Elem.* **185**, 1124–1130 (2010).

X. WANG, Y. PENG, Z. XHU, J. C. FETTINGER, P. P. POWER, J. GUO and S. NAGASE, "Synthesis and Characterization of Two of the Three Isomers of a Germanium-Substituted Bicyclo[2.2.0]hexane Diradicaloid: Stretching the Ge–Ge Bond," *Angew. Chem., Int. Ed.* **49**, 4593–4597 (2010).

D. M. GULDI, L. FENG, S. G. RADHAKRISHNAN, H. NIKAWA, M. YAMADA, N. MIZOROGI, T. TSUCHIYA, T. AKASAKA, S. NAGASE, M. A. HERRANZ and N. MARTIN, "A Molecular $Ce_2@I_h$-C_{80} Switch—Unprecedented Oxidative Pathway in Photoinduced Charge Transfer Reactivity," *J. Am. Chem. Soc.* **132**, 9078–9086 (2010).

M. SAITO, T. KUWABARA, C. KAMBAYASHI, M. YOSHIOKA, K. ISHIMURA and S. NAGASE, "Synthesis, Structure, and Reaction of Tetraethyldilithiostannole," *Chem. Lett.* **39**, 700–701 (2010).

A. P. RAHALKAR, M. KATOUDA, S. R. GADRE and S. NAGASE, "Molecular Tailoring Approach in Conjugation with MP2 and RI-MP2 Codes: A Comparison with Fragment Molecular Orbital Method," *J. Comput. Chem.* **31**, 2405–2418 (2010).

M. SAITO, T. KUWABARA, K. ISHIMURA and S. NAGASE, "Synthesis and Structures of Lithium Salts of Stannole Anions," *Bull. Chem. Soc. Jpn.* **83**, 825–827 (2010).

T. IWASA and K. NOBUSADA, "Nonuniform Light-Matter Interaction Theory for Near-Field-Induced Electron Dynamics," *Phys. Rev. A* **80**, 043409 (11 pages) (2009).

Y. KUBOTA and K. NOBUSADA, "Applicability of Site-Basis Time-Evolution Equation for Thermalization of Exciton States in a Quantum Dot Array," *J. Phys. Soc. Jpn.* **78**, 114603 (7 pages) (2009).

Y. KAWASHITA , K. YABANA, M. NODA, K. NOBUSADA and T. NAKATSUKASA, "Oscillator Strength Distribution of C_{60} in the Time-Dependent Density Functional Theory," *THEOCHEM* **914**, 130–135 (2009).

Y. NEGISHI, W. KURASHIGE, Y. NIIHORI, T. IWASA and K. NOBUSADA, "Isolation, Structure, and Stability of a Dodecanethiolate-Protected Pd_1Au_{24} Cluster," *Phys. Chem. Chem. Phys.* **12**, 6219–6225 (2010).

W. MIZUKAMI, Y. KURASHIGE, M. EHARA, T. YANAI and T. ITOH, "Ab Initio Study of the Excited Singlet States of All *trans* α,ω-Diphenylpolyenes with One to Seven Polyene Double Bonds: Simulation of the Spectral Data within Franck–Condon Approximation," *J. Chem. Phys.* **131**, 174313 (10 pages) (2009).

T. YANAI, Y. KURASHIGE, E. NEUSCAMMAN and G. K.-L. CHAN, "Multireference Quantum Chemistry through a Joint Density Matrix Renormalisation Group and Canonical Transformation Theory," *J. Chem. Phys.* **132**, 024105 (9 pages) (2010).

E. NEUSCAMMAN, T. YANAI and G. K.-L. CHAN, "Strongly Contracted Canonical Transformation Theory," *J. Chem. Phys.* **132**, 024106 (13 pages) (2010).

T. IMAI, K. ODA, A. KOVALENKO, F. HIRATA and A. KIDERA, "Ligand Mapping on Protein Surfaces by the 3D-RISM Theory; Toward Computational Fragment-Based Drug Design," *J. Am.Chem. Soc.* **131**, 12430–12440 (2009).

T. YUI, H. SHIIBA, Y. TSUTSUMI, S. HAYASHI, T. MIYATA and F. HIRATA, "Systematic Docking Study of Carbohydrate Binding Module Protein of Cel7A with Cellulose Iα Crystal Model," *J. Phys. Chem. B* **114**, 49–58 (2009).

R. ISHIZUKA and F. HIRATA, "The Dynamics of Solvent around a Solute: Generalized Langevin Theory," *Phys. Rev. E* **81**, 011202 (7 pages) (2010).

Y. MARUYAMA, N. YOSHIDA and F. HIRATA, "Revisiting the Salt-Induced Conformational Change of DNA with 3D-RISM Theory," *J. Phys. Chem. B* **114**, 6464–6471 (2010).

S. PHONGPHONPHANEE, N. YOSHIDA and F. HIRATA, "Molecular Selectivity in Aquaporin Channels Studied by the 3D-RISM Theory," *J. Phys. Chem. B* **114**, 7967–7973 (2010).

S. PHONGPHONPHANEE, T. RUNGROMONGKOL, N. YOSHIDA, S. HANNONGBUA and F. HIRATA, "Proton Transport through the Influenza A M2 Channel: 3D-RISM Study," *J. Am. Chem. Soc.* **132**, 9782–9788 (2010).

T. MIYATA, Y. IKUTA and F. HIRATA, "Free Energy Calculation Using Molecular Dynamics Simulation Combined with Three Dimensional Reference Interaction Site Model (3D-RISM) Theory. I. Free Energy Perturbation and Thermodynamic Integration along Coupling Parameter," *J. Chem. Phys.* **133**, 044114 (15 pages) (2010).

Y. TANAKA and K. YONEMITSU, "Growth Dynamics of Photoinduced Domains in Two-Dimensional Charge-Ordered Conductors Depending on Stabilization Mechanisms," *J. Phys. Soc. Jpn.* **79**, 024712 (8 pages) (2010).

N. MAESHIMA, K. YONEMITSU and K. HINO, "Photoinduced Dynamics in the One-Dimensional Two-Orbital Degenerate Hubbard Model," *J. Phys.: Conf. Series* **200**, 012109 (4 pages) (2010).

S. MIYASHITA, Y. TANAKA, S. IWAI and K. YONEMITSU, "Charge, Lattice, and Spin Dynamics in Photoinduced Phase Transitions from Charge-Ordered Insulator to Metal in Quasi-Two-Dimensional Organic Conductors," *J. Phys. Soc. Jpn.* **79**, 034708 (9 pages) (2010).

Y. TANAKA and K. YONEMITSU, "Theory of I–V Characteristics for Two-Dimensional Charge-Ordered Electron Systems at Quarter Filling," *Physica B* **405**, S211–S213 (2010).

K. YONEMITSU, S. MIYASHITA and Y. TANAKA, "Frustration and Lattice Effects on Photoinduced Melting of Charge Orders in Quasi-Two-Dimensional Organic Conductors," *Physica B* **405**, S369–S372 (2010).

T. YAGASAKI and S. SAITO, "Molecular Dynamics Simulation of Nonlinear Spectroscopies of Intermolecular Motions in Liquid Water," *Acc. Chem. Res.* **42**, 1250–1258 (2009).

T. YAGASAKI, J. ONO and S. SAITO, "Ultrafast Energy Relaxation and Anisotropy Decay of the Librational Motion in Liquid Water: A Molecular Dynamics Study," *J. Chem. Phys.* **131**, 164511 (11 pages) (2009).
K. KIM, K. MIYAZAKI and S. SAITO, "Slow Dynamics in Random Media: Crossover from Glass to Localization Transition," *Europhys. Lett.* **88**, 36002 (5 pages) (2009).
J. TAYAMA, A. ISHIHARA, M. BANNO, K. OHTA, S. SAITO and K. TOMINAGA, "Temperature Dependence of Vibrational Frequency Fluctuation of N_3^- in D_2O," *J. Chem. Phys.* **133**, 014505 (11 pages) (2010).
K. KIM and S. SAITO, "Multi-Time Density Correlation Functions in Glass-Forming Liquids: Probing Dynamical Heterogeneity and Its Lifetime," *J. Chem. Phys.* **133**, 044511 (10 pages) (2010).

M. TASHIRO, M. EHARA and K. UEDA, "Double Core-Hole Electron Spectroscopy for Open-Shell Molecules: Theoretical Perspective," *Chem. Phys. Lett.* **496**, 217–222 (2010).
R. CAMMI, R. FUKUDA, M. EHARA and H. NAKATSUJI, "Symmetry-Adapted Cluster and Symmetry-Adapted Cluster-Configuration Interaction Method in the Polarizable Continuum Model-Theory for Solvent Effect on Electronic Excitation of Molecules in Solution," *J. Chem. Phys.* **133**, 024104 (24 pages) (2010).
M. TASHIRO, M. EHARA, H. FUKUZAWA, K. UEDA, C. BUTH, N.V. KRYZHEVOI and L. S. CEDERBAUM, "Molecular Double Core-Hole Electronic Spectroscopy for Chemical Analysis," *J. Chem. Phys.* **132**, 184302 (11 pages) (2010).
R. FUKUDA, M. EHARA, H. NAKATSUJI, N. KISHIMOTO and K. OHNO, "Valence Ionized States of Iron Pentacarbonyl and η^5-Cyclopentadienyl Cobalt Dicarbonyl Studied by the SAC-CI Calculation and Collision-Energy Resolved Penning Ionization Electron Spectroscopy," *J. Chem. Phys.* **132**, 084302 (12 pages) (2010).
M. EHARA and K. UEDA, "Vibrational Spectra and Geometry Relaxation in Core-Electronic Processes of N_2O and CO_2," *J. Phys. Conf. Series* **235**, 012020 (9 pages) (2010).
R. R. LUCCHESE, R. MONTUORO, K. KOTSIS, M. TASHIRO, M. EHARA, J. D. BOZEK, A. DAS and E. D. POLIAKOFF, "The Effect of Vibrational Motion on the Dynamics of Shape Resonant Photoionization of BF_3 Leading to the E^2A_1' State of BF_3^+," *Mol. Phys.* **108**, 1055–1067 (2010).
W. MIZUKAMI, Y. KURASHIGE, M. EHARA, T. YANAI and T. ITOH, "Ab Initio Study of the Excited Singlet States of All *trans* α,ω-Diphyenylpolyenes with One to Seven Polyene Double Bonds: Simulation of the Spectral Data within Franck–Condon Approximation," *J. Chem. Phys.* **131**, 174313 (10 pages) (2009).
M. EHARA, "High-Precision Ab Initio Core-Level Spectroscopy," *J. Phys.: Conf. Series* **194**, 012006 (8 pages) (2009).
Y. LU and M. EHARA, "Electronic Structure and Optical Properties of Chelating Hetero-Atomic Conjugated Molecules: A SAC-CI Study," *Theor. Chem. Acc.* **124**, 395–408 (2009).
M. PROMKATWAEW, S. SURAMITR, T. K. KARPKIRD, S. NAMUANGRUK, M. EHARA and S. HANNONGBUA, "Absorption and Emission Spectra of UVB Blocking Methoxy Substituted Cinnamates Investigated by the SAC-CI Method," *J. Chem. Phys.* **131**, 224306 (10 pages) (2009).
R. FUKUDA, S. HAYAKI and H. NAKATSUJI, "Valence Ionization Spectra of Group Six Metal Hexacarbonyls Studied by the Symmetry-Adapted Cluster-Configuration Interaction Method," *J. Chem. Phys.* **131**, 174303 (10 pages) (2009).

S. G. ITOH, H. OKUMURA and Y. OKAMOTO, "Replica-Exchange Method in Parameter Space: Overcoming Steric Restrictions for Biomolecules," *J. Chem. Phys.* **132**, 134105 (8 pages) (2010).
H. OKUMURA, E. GALLICCHIO and R. M. LEVY, "Conformational Populations of Ligand-Sized Molecules by Replica Exchange Molecular Dynamics and Temperature Reweighting," *J. Comput. Chem.* **31**, 1357–1367 (2010).

H. HIRATE, Y. SAITO, I. NAKAYA, H. SAWAI, H. YUKAWA, M. MORINAGA, T. BABA and H. NAKAI, "Quantitative Approach to the Understanding of Catalytic Effect of Metal Oxides on the Desorption Reaction of MgH_2," *Int. J. Quantum Chem.* **109**, 2793–2800 (2009).
T. AKAMA, M. KOBAYASHI and H. NAKAI, "Electronic Temperature in Divide-and-Conquer Electronic Structure Calculation Revisited: Assessment and Improvement of Self-Consistent Field Convergence," *Int. J. Quantum Chem.* **109**, 2706–2713 (2009).
Y. IMAMURA, Y. TSUKAMOTO, H. KIRYU and H. NAKAI, "Extension of Density Functional Theory to Nuclear Orbital Plus Molecular Orbital Theory: Self-Consistent Field Calculations with the Colle-Salvetti Electron–Nucleus Correlation Functional," *Bull. Chem. Soc. Jpn.* **82**, 1133–1139 (2009).
M. KOBAYASHI and H. NAKAI, "Divide-and-Conquer-Based Linear-Scaling Approach for Traditional and Renormalized Coupled Cluster Methods with Single, Double, and Noniterative Triple Excitations," *J. Chem. Phys.* **131**, 114108 (9 pages) (2009).
T. SATO and H. NAKAI, "Density Functional Method Including Weak Interactions: Dispersion Coefficients Based on the Local Response Approximation," *J. Chem. Phys.* **131**, 224104 (12 pages) (2009).
M. HOJO, T. UEDA, M. IKE, K. OKAMURA, T. SUGIYAMA, M. KOBAYASHI and H. NAKAI, "Observation by UV-Visible and NMR Spectroscopy and Theoretical Confirmation of 4-Isopropyltropolonate Ion, 4-Isopropyltropolone (hinokitiol), and Protonated 4-Isopropyltropolone in Acetonitrile," *J. Chem. Eng. Data* **55**, 1986–1989 (2010).
T. TOUMA, M. KOBAYASHI and H. NAKAI, "Time-Dependent Hartree-Fock Frequency-Dependent Polarizability Calculation Applied to Divide-and-Conquer Electronic Structure Method," *Chem. Phys. Lett.* **485**, 247–252 (2010).
T. AKAMA and H. NAKAI, "Short-Time Fourier Transform Analysis of Real-Time Time-Dependent Hartree-Fock and Time-Dependent Density Functional Theory Calculations with Gaussian Basis Functions," *J. Chem. Phys.* **132**, 054104 (11 pages) (2010).
Y. IMAMURA, A. TAKAHASHI, T. OKADA, T. OHNO and H. NAKAI, "Extension of Energy Density Analysis to Periodic-Boundary-Condition Calculations with Plane-Wave Basis Functions," *Phys. Rev. B* **81**, 115136 (7 pages) (2010).
T. ATSUMI, T. ABE, K.-Y. AKIBA and H. NAKAI, "Theoretical Study on Bond-Switching in 1,6-Dihydro-6a-thia-1,6-diazapentalene (10-S-3) Systems Compared with Corresponding Oxygen Analogues," *Bull. Chem. Soc. Jpn.* **83**, 520–529 (2010).

T. AKAMA, Y. IMAMURA and H. NAKAI, "Application of Real-Time Time-Dependent Density Functional Theory with the CV-B3LYP Functional to Core Excitations," *Chem. Lett.* **39**, 407–409 (2010).
T. ATSUMI and H. NAKAI, "Acceleration of Self-Consistent-Field Convergence in *Ab Initio* Molecular Dynamics and Monte Carlo Simulations and Geometry Optimization," *Chem. Phys. Lett.* **490**, 102–108 (2010).
M. KOBAYASHI, A. SZABADOS, H. NAKAI and P. SURJAN, "Generalized Møller-Plesset Partioning in Multiconfiguration Perturbation Theory," *J. Chem. Theory Comput.* **6**, 2024–2033 (2010).

M. TANAKA and Y. TANIMURA, "Multistate Electron Transfer Dynamics in the Condensed Phase: Exact Calculations from the Reduced Hierarchy Equations of Motion Approach," *J. Chem. Phys.* **132**, 214502 (11 pages) (2010).
A. G. DIJKSTRA and Y. TANIMURA, "Non-Markovian Entanglement Dynamics in the Presence of System-Bath Coherence," *Phys. Rev. Lett.* **104**, 250401 (4 pages) (2010).

K. NISHIYAMA, T. HANAMOTO, H. SHIGEMATSU, K. KITADA, K. IKETAKI, T. KAJI and M. HIRAMOTO, "Morphology of Rare-Earth (Y, Sm) Nanostructures Synthesized by the Surfactant-Assembled Method," *Chem. Lett.* **39**, 974–975 (2010).

Photo-Molecular Science

H. HASEGAWA and Y. OHSHIMA, "Coherent Rotational Dynamics of Molecules Induced by Intense Ultrafast Laser Fields," *J. Phys.: Conf. Series* **185**, 012014 (4 pages) (2009).
K. KITANO, H. HASEGAWA and Y. OHSHIMA, "Ultrafast Angular-Momentum Orientation by Linearly Polarized Laser Fields," *Phys. Rev. Lett.* **103**, 223003 (4 pages) (2009).

K. HOSAKA, H. SHIMADA, H. CHIBA, H. KATSUKI, Y. TERANISHI and K. OHMORI, "Ultrafast Fourier Transform with a Femtosecond Laser Driven Molecule," *Phys. Rev. Lett.* **104**, 180501 (4 pages) (2010).
H. GOTO, H. KATSUKI and K. OHMORI, "Optical Modification of the Vibrational Distribution of the Iodine Molecule," *Chem. Phys. Lett.* **493**, 170–172 (2010).

M. NAGASAKA, T. HATSUI, T. HORIGOME, Y. HAMAMURA and N. KOSUGI, "Development of a Liquid Flow Cell to Measure Soft X-Ray Absorption in Transmission Mode: A Test for Liquid Water," *J. Electron Spectrosc. Relat. Phenom.* **177**, 130–134 (2010).
E. OTERO, N. KOSUGI and S. G. URQUHART, "Strong Double Excitation and Open-Shell Features in the Near-Edge X-Ray Absorption Fine Structure Spectroscopy of Ferrocene and Ferrocenium Compounds," *J. Chem. Phys.* **113**, 114313 (8 pages) (2009).
C. MIRON, V. KIMBERG, P. MORIN, C. NICOLAS, N. KOSUGI, S. GAVRILYUK and F. GEL'MUKHANOV, "Vibrational Scattering Anisotropy Generated by Multichannel Quantum Interference," *Phys. Rev. Lett.* **105**, 093002 (4 pages) (2010).
H. YAMANE, A. GERLACH, S. DUHM, Y. TANAKA, T. HOSOKAI, Y. Y. MI, J. ZEGENHAGEN, N. KOCH, K. SEKI and F. SCHREIBER, "Site-Specific Geometric and Electronic Relaxations at Organic–Metal Interfaces," *Phys. Rev. Lett.* **105**, 046103 (4 pages) (2010).
W.-J. HUA, H. YAMANE, B. GAO, J. JIANG, S.-H. Li, H. S. KATO, M. KAWAI, T. HATSUI, Y. LUO, N. KOSUGI and H. ÅGREN, "A Systematic Study of Soft-X-Ray Spectra of Poly(dG)poly(dC) and Poly(dA)poly(dT) DNA Duplexes," *J. Phys. Chem. B* **114**, 7016–7021 (2010).
H. YAMANE, K. KANAI, Y. OUCHI, N. UENO and K. SEKI, "Impact of Interface Geometric Structure on Organic–Metal Interface Energetics and Subsequent Films Electronic Structure," *J. Electron Spectrosc. Relat. Phenom.* **174**, 28–34 (2009).
H. S. KATO, R. HIRAKAWA, F. YAMAUCHI, T. MINATO, M. KAWAI, T. HATSUI and N. KOSUGI, "Electronic State Observation of Inner Organic Thin Films beneath Electrodes: Fluorescence-Yield X-Ray Absorption Spectra of Pentacene Derivative Films," *J. Electron Spectrosc. Relat. Phenom.* **174**, 93–99 (2009).
M. NAGASAKA, H. KONDOH, K. AMEMIYA, I. NAKAI, T. SHIMADA, R. YOKOTA and T. OHTA, "Mechanism of Ammonia Formation on Rh(111) Studied by Dispersive Near-Edge X-Ray Absorption Fine Structure Spectroscopy," *J. Phys. Chem. C* **114**, 2164–2170 (2010).
I. NAKAI, H. KONDOH, T. SHIMADA, M. NAGASAKA, R. YOKOTA, T. KATAYAMA, K. AMEMIYA, H. ORITA and T. OHTA, "Mechanism of N Plus NO Reaction on Rh(111) Surfaces: A Precursor-Mediated Reaction," *J. Phys. Chem. C* **113**, 13257–13265 (2009).
T. IWAHASHI, T. NISHI, H. YAMANE, T. MIYAMAE, K. KANAI, K. SEKI, D. KIM and Y. OUCHI, "Surface Structural Study on Ionic Liquids Using Metastable Atom Electron Spectroscopy," *J. Phys. Chem. C* **113**, 19237–19243 (2009).

Y. POO-ARPORN, V. VAILIKHIT, D. BASHYAL, K. NAKAJIMA, P. SONGSIRIRITTHIGUL and K. MITSUKE, "Preparation and Evaluation of High Efficiency Dye-Sensitized Solar Cells," *Proceedings of Pure and Applied Chemistry International Conference* PACCON2010, 424–426 (2010).
H. KATAYANAGI, B. P. KAFLE, C. HUANG, MD. S. I. PRODHAN, H. YAGI and K. MITSUKE, "Feasibility Study on the Mass-Selected Velocity Map Imaging of Polyatomic Molecules and Fullerenes," *Proceedings of Pure and Applied Chemistry International Conference* PACCON2010, 941–944 (2010).
K. NAKAJIMA, K. OHTA, H. KATAYANAGI and K. MITSUKE, "Azo Dyes as Photosensitizers for Organic Solar Cells," *Proceedings of Pure and Applied Chemistry International Conference* PACCON2010, 967–970 (2010).
H. KATAYANAGI and K. MITSUKE, "Mass-Analyzed Velocity Map Imaging of Thermal Photofragments from C_{60}," *J. Chem. Phys. (Communication)* **133**, 081101 (4 pages) (2010).

C. EVAIN, C. SZWAJ, S. BIELAWSKI, M. HOSAKA, A. MOCHIHASHI, M. KATOH and M.-E. COUPRIE, "Shifted Feedback Suppression of Turbulent Behavior in Advection-Diffusion Systems," *Phys. Rev. Lett.* **102**, 134501 (4 pages) (2009).

M. SHIMADA, M. KATOH, M. ADACHI, T. TANIKAWA, S. KIMURA, M. HOSAKA, N. YAMAMOTO, Y. TAKASHIMA and T. TAKAHASHI, "Transverse-Longitudinal Coupling Effect in Laser Bunch Slicing," *Phys. Rev. Lett.* **103**, 144802 (4 pages) (2009).

S. KIMURA, T. ITO, M. SAKAI, E. NAKAMURA, N. KONDO, T. HORIGOME, K. HAYASHI, M. HOSAKA, M. KATOH, T. GOTO, T. EJIMA and K. SODA, "SAMRAI: A Novel Variably Polarized Angle-Resolved Photoemission Beamline in the VUV Region at UVSOR-II," *Rev. Sci. Instrum.* **81**, 053104 (7 pages) (2010).

M. SHIMADA, M. KATOH, M. ADACHI, S. KIMURA, T. TANIKAWA, M. HOSAKA, N. YAMAMOTO, Y. TAKASHIMA and T. TAKAHASHI, "Transverse-Longitudinal Coupling Effect in Laser Bunch Slicing," *Phys. Rev. Lett.* **103**, 144802 (4 pages) (2009).

S. R. PARK, W. S. JUNG, C. KIM, D. J. SONG, C. KIM, S. KIMURA, K. D. LEE and N. HUR, "Quasiparticle Scattering and the Protected Nature of the Topological States in a Parent Topological Insulator Bi_2Se_3," *Phys. Rev. B* **81**, 041405(R) (4 pages) (2010).

S. KIMURA, T. MIZUNO and T. IIZUKA, "Synchrotron Terahertz Spectroscopy of Solids under Extreme Conditions," *AIP. Conf. Proc.* **1214**, 71–74 (2010).

J. H. KIM, S. J. KIM, C. I. LEE, M. A. JUNG, H. J. OH, J.-S. RHYEE, Y. JO, H. MITANI, H. MIYAZAKI, S. KIMURA and Y. S. KWON, "Kondo-Like Behavior in Magnetic and Thermal Properties of Single-Crystal $Tm_5Si_2Ge_2$," *Phys. Rev. B* **81**, 104401 (8 pages) (2010).

H. MIYAZAKI, T. ITO, H. J. IM, K. TERASHIMA, T. IIZUKA, S. YAGI, M. KATO, K. SODA and S. KIMURA, "Change of Lattice Constant due to Hybridization Effect of a Ferromagnetic Semiconductor EuO," *J. Phys.: Conf. Series* **200**, 012124 (4 pages) (2010).

T. HIRAHARA, Y. SAKAMOTO, Y. SAISYU, H. MIYAZAKI, S. KIMURA, T. OKUDA, I. MATSUDA, S. MURAKAMI and S. HASEGAWA, "A Topological Metal at the Surface of an Ultrathin $Bi_{1-x}Sb_x$ Alloy Film," *Phys. Rev. B* **81**, 165422 (5 pages) (2010).

Y. SAKAMOTO, T. HIRAHARA, H. MIYAZAKI, S. KIMURA and S. HASEGAWA, "Spectroscopic Evidence of a Topological Quantum Phase Transition in Ultrathin Bi_2Se_3 Films," *Phys. Rev. B* **81**, 165432 (4 pages) (2010).

S. KIMURA, E. NAKAMURA, M. HOSAKA, T. TAKAHASHI and M. KATOH, "Design of Terahertz Pump–Photoemission Probe Spectroscopy Beamline at UVSOR-II," *AIP Conf. Proc.* **1234**, 63–66 (2010).

S. KIMURA, T. ITO, M. SAKAI, E. NAKAMURA, N. KONDO, K. HAYASHI, T. HORIGOME, M. HOSAKA, M. KATOH, T. GOTO, T. EJIMA and K. SODA, "SAMRAI: A Variably Polarized Angle-Resolved Photoemission Beamline in the VUV Region at UVSOR-II," *Rev. Sci. Instrum.* **81**, 053104 (7 pages) (2010).

M. KIMURA, H. FUJIWARA, A. SEKIYAMA, J. YAMAGUCHI, K. KISHIMOTO, H. SUGIYAMA, G. FUNABASHI, S. IMADA, S. IGUCHI, Y. TOKURA, A. HIGASHIYA, M. YABASHI, K. TAMASAKU, T. ISHIKAWA, T. ITO, S. KIMURA and S. SUGA, "Polaronic Behavior of Photoelectron Spectra of Fe_3O_4 Revealed by Both Hard X-Ray and Extremely Low Energy Photons," *J. Phys. Soc. Jpn.* **79**, 064710 (5 pages) (2010).

H. MIYAZAKI, T. ITO, H. J. IM, K. TERASHIMA, S. YAGI, M. KATO, K. SODA and S. KIMURA, "La-Doped EuO: A Rare Earth Ferromagnetic Semiconductor with the Highest Curie Temperature," *Appl. Phys. Lett.* **96**, 232503 (3 pages) (2010).

Y. HIKOSAKA, P. LABLANQUIE, F. PENENT, P. SELLES, T. KANEYASU, E. SHIGEMASA, J. H. D. ELAND and K. ITO, "Probing the Mechanism of Simultaneous Two-Electron Emission on Core-Hole Decay," *Phys. Rev. A* **80**, 031404(R) (4 pages) (2009).

K. ITO, F. PENENT, Y. HIKOSAKA, E. SHIGEMASA, I. H. SUZUKI, J. H. D. ELAND and P. LABLANQUIE, "Application of a Simple Asynchronous Mechanical Light Chopper to Multielectron Coincidence Spectroscopy," *Rev. Sci. Instrum.* **80**, 123101 (9 pages) (2009).

S. SHEINERMAN, P. LABLANQUIE, F. PENENT, Y. HIKOSAKA, T. KANEYASU, E. SHIGEMASA and K. ITO, "PCI Effects in Argon 2p Double Auger Decay Probed by Multielectron Coincidence Methods," *J. Phys. B* **43**, 115001 (9 pages) (2010).

E. SHIGEMASA, T. KANEYASU, T. MATSUSHITA, Y. TAMENORI and Y. HIKOSAKA, "Doppler Effect in Fragment Autoionization Following Core-to-Rydberg Excitations of N_2," *New J. Phys.* **12**, 063030 (9 pages) (2010).

Y. HIKOSAKA, P. LABLANQUIE, F. PENENT, E. SHIGEMASA, J. H. D. ELAND and K. ITO, "Two-Electron Emission on Atomic Photoabsorption Studied by Multi-Electron Coincidence Spectroscopy," *J. Electron Spectrosc. Relat. Phenom.* **181**, 121–124 (2010).

S. HAYASHI, T. SHIBUYA, H. SAKAI, T. TAIRA, C. OTANI, Y. OGAWA and K. KAWASE, "Tunability Enhancement of a Terahertz-Wave Parametric Generator Pumped by a Microchip Nd:YAG Laser," *Appl. Opt.* **48**, 2899–2902 (2009).

M. MIYAZAKI, J. SAIKAWA, H. ISHIZUKI, T. TAIRA and M. FUJII, "Isomer Selective Infrared Spectroscopy of Supersonically Cooled *cis*- and *trans*-*N*-phenylamides in the Region from the Amide Band to NH Stretching Vibration," *Phys. Chem. Chem. Phys.* **11**, 6098–6106 (2009).

P. BRAND, B. BOULANGER, P. SEGONDS, Y. PETIT, C. FELIX, B. MENAERT, T. TAIRA and H. ISHIZUKI, "Angular Quasi-Phase-Matching Experiments and Determination of Accurate Sellmeier Equations for 5%MgO:PPLN," *Opt. Lett.* **34**, 2578–2580 (2009).

H. ISHIZUKI and T. TAIRA, "High Energy Quasi-Phase Matched Optical Parametric Oscillation Using Mg-Doped Congruent $LiTaO_3$ Crystal," *Opt. Express* **18**, 253–258 (2010).

M. TSUNEKANE, T. INOHARA, A. ANDO, N. KIDO, K. KANEHARA and T. TAIRA, "High Peak Power, Passively Q-Switched Microlaser for Ignition of Engines," *IEEE J. Quantum Electron.* **46**, 277–284 (2010).

N. PAVEL, M. TSUNEKANE and T. TAIRA, "Enhancing Performances of a Passively Q-Switched Nd:YAG/Cr^{4+}:YAG Microlaser with a Volume Bragg Grating Output Coupler," *Opt. Lett.* **35**, 1617–1619 (2010).

G. MASADA, T. SUZUDO, Y. SATOH, H. ISHIZUKI, T. TAIRA and A. FURUSAWA, "Efficient Generation of Highly Squeezed Light with Periodically Poled MgO: $LiNbO_3$," *Opt. Express* **18**, 13114–13121 (2010).

T. TAIRA, "High Brightness Microchip Laser and Engine Ignition," *Rev. Laser Eng.* **38**, 576–584 (2010).

T. FUJI, T. SUZUKI, E. E. SEREBRYANNIKOV and A. ZHELTIKOV, "Experimental and Theoretical Investigation of a Multicolor Filament," *Phys. Rev. A* **80**, 063822 (5 pages) (2009).
Y.-I. SUZUKI, T. FUJI, T. HORIO and T. SUZUKI, "Time-Resolved Photoelectron Imaging of Ultrafast Internal Conversion through Conical Intersection in Pyrazine," *J. Chem. Phys.* **132**, 174302 (8 pages) (2010).
P. ZUO, T. FUJI and T. SUZUKI, "Spectral Phase Transfer to Ultrashort UV Pulses through Four-Wave Mixing," *Opt. Express* **18**, 16183–16192 (2010).

Materials Molecular Science

J. NISHIJO, K. JUDAI, S. NUMAO and N. NISHI, "Chromium Acetylide Complex Based Ferrimagnet and Weak Ferromagnet," *Inorg. Chem.* **48**, 9402–9408 (2009).
K. OHASHI, K. INOUE, T. IINO, J. SASAKI, K. JUDAI, N. NISHI and H. SEKIYA, "A Molecular Picture of Metal Ion Solvation: Infrared Spectroscopy of $Cu^+(NH_3)_n$ and $Ag^+(NH_3)_n$ in the Gas Phase," *J. Mol. Liq.* **147**, 71–76 (2009).
Y. HARADA, C. OKABE, T. KOBAYASHI, T. SUZUKI, T. ICHIMURA, N. NISHI and Y.-Z. XU, "Ultrafast Intersystem Crossing of 4-Thiothymidine in Aqueous Solution," *J. Phys. Chem. Lett.* **1**, 480–484 (2010).

H. YOSHIKAWA, S. HAMANAKA, Y. MIYOSHI, Y. KONDO, S. SHIGEMATSU, N. AKUTAGAWA, M. SATO, T. YOKOYAMA and K. AWAGA, "Rechargeable Batteries Driven by Redox Reactions of Mn12 Clusters with Structural Changes: XAFS Analyses of the Charging/Discharging Processes in Molecular Cluster Batteries," *Inorg. Chem.* **48**, 9057–9059 (2009).
Y. TAKAGI, K. ISAMI, I. YAMAMOTO, T. NAKAGAWA and T. YOKOYAMA, "Structure and Magnetic Properties of Iron Nitride Thin Films on Cu(001)," *Phys. Rev. B* **81**, 035422 (8 pages) (2010).
H. IRIE, T. SHIBANUMA, K. KAMIYA, S. MIURA, T. YOKOYAMA and K. HASHIMOTO, "Characterization of Cr(III)-Grafted TiO_2 for Photocatalytic Reaction under Visible Light," *Appl. Catal., B* **96**, 142–147 (2010).
I. YAMAMOTO, T. NAKAGAWA, Y. TAKAGI and T. YOKOYAMA, "Spin Reorientation Transitions of Ni/Pd(111) Films Induced by Fe Deposition," *Phys. Rev. B* **81**, 214442 (7 pages) (2010).

K. MOTOKURA, M. TADA and Y. IWASAWA, "Layered Materials with Coexisting Acidic and Basic Sites for Catalytic One-Pot Reaction Sequences," *J. Am. Chem. Soc.* **131**, 7944–7945 (2009).
K. MOTOKURA, M. TOMITA, M. TADA and Y. IWASAWA, "Michael Reactions Catalyzed by Basic Alkylamines and Dialkylaminopyridine Immobilized on Acidic Silica–Alumina Surfaces," *Top. Catal.* **52**, 579–585 (2009).
T. SASAKI, M. TADA and Y. IWASAWA, "Density Functional Theory Study on the Re Cluster/HZSM-5 Catalysis for Direct Phenol Synthesis from Benzene and Molecular Oxygen: Active Re Structure and Reaction Mechanism," *Top. Catal.* **52**, 880–887 (2009).
K. MOTOKURA, S. TANAKA, M. TADA and Y. IWASAWA, "Bifunctional Heterogeneous Catalysis of Silica-Alumina-Supported Tertiary Amines with Controlled Acid-Base Interactions for Efficient 1,4-Addition Reactions," *Chem. –Eur. J.* **15**, 10871–10879 (2009).
H. ARIGA, T. TANIIKE, H. MORIKAWA, M. TADA, B. K. MIN, K. WATANABE, Y. MATSUMOTO, S. IKEDA, K. SAIKI and Y. IWASAWA, "Surface-Mediated Visible-Light Photo-Oxidation on Pure TiO_2(001)," *J. Am. Chem. Soc.* **131**, 14670–14672 (2009).
M. TADA, S. MURATSUGU, M. KINOSHITA, T. SASAKI and Y. IWASAWA, "Alternative Selective Oxidation Pathways for Aldehyde Oxidation and Alkene Epoxidation on a SiO_2-Supported Ru-Monomer Complex Catalyst," *J. Am. Chem. Soc.* **132**, 713–724 (2010).
S. ICHIKAWA, T. SEKI, M. TADA, Y. IWASAWA and T. IKARIYA, "Amorphous Nano-Structured Silicas for High-Performance Carbon Dioxide Confinement," *J. Mater. Chem.* **20**, 3163–3165 (2010).
M. TADA, Y. UEMURA, R. BAL, Y. INADA, M. NOMURA and Y. IWASAWA, "In-Situ Time-Resolved DXAFS for the Determination of Kinetics of Structural Changes of H-ZSM-5-Supported Active Re-Cluster Catalyst in the Direct Phenol Synthesis from Benzene and O_2," *Phys. Chem. Chem. Phys.* **12**, 5701–5706 (2010).
T. TANIIKE, M. TADA, R. COQUET, Y. MORIKAWA, T. SASAKI and Y. IWASAWA, "A Novel Mechanism for Spectator CO-Mediated Reaction with Unique *cis*-$(NO)_2$ Dimer on a Co^{2+}-Dimer/γ-Al_2O_3 (110) Model Catalyst: Density Functional Theory Calculations," *Catal. Today* **154**, 118–126 (2010).
M. TADA, "Surface-Mediated Design and Catalytic Properties of Active Metal Complexes for Advanced Catalysis Creation," *Bull. Chem. Soc. Jpn.* **83**, 855–876 (2010) [Award Accounts].

N. MORINAKA, K. TAKABAYASHI, R. CHIBA, F. YOSHIKANE, S. NIIZEKI, M. TANAKA, K. YAKUSHI, M. KOEDA, M. HEDO, T. FUJIWARA, Y. UWATOKO, Y. NISHIO, K. KAJITA and H. MORI, "Superconductivity Competitive with Checkerboard-Type Charge Ordering in Organic Conductor β-(*meso*-DMBEDT-TTF)$_2PF_6$," *Phys. Rev. B* **80**, 092508 (4 pages) (2009).
R. ŚWIETLIK, A. ŁAPINSKI, M. FOURMIGUÉ and K. YAKUSHI, "Flexibility of Paramagnetic (d^1) Organometallic Dithiolene Complex $[Cp_2Mo(dmit)]^{+\bullet}$ Studied by Raman Spectroscopy," *J. Raman Spectrosc.* **40**, 2092–2098 (2009).
Y. ETO, A. KAWAMOTO, N. MATSUNAGA, K. KUMAGAI, K. YAMAMOTO and K. YAKUSHI, "Evidence for an Exchange Interaction between Donor and Acceptor Layers in β'-(BEDT-TTF)(TCNQ)," *Phys. Rev. B* **80**, 174506 (5 pages) (2009).
H. NAKAYA, K. ITHO, Y. TAKAHASHI, H. ITOH, S. IWAI, S. SAITO, K. YAMAMOTO and K. YAKUSHI, "Terahertz Responses of High-Temperature Metallic Phase and Photoinduced Metallic State in Ferroelectric Charge-Ordered Organic Salt," *Phys. Rev. B* **81**, 15511 (6 pages) (2010).
K. YAMAMOTO, A. KOWALSKA and K. YAKUSHI, "Direct Observation of Ferroelectric Domains Created by Wigner Crystallization of Electrons in α-[Bis(ethylenedithio)tetrathiafulvalene]$_2I_3$," *Appl. Phys. Lett.* **96**, 122901 (3 pages) (2010).

T. MURATA, X. SHAO, Y. NAKANO, H. YAMOCHI, M. URUICHI, K. YAKUSHI, G. SAITO and K. TANAKA, "Tuning of Multi-Instabilities in Organic Alloy, $[(EDO\text{-}TTF)_{1-x}(MeEDO\text{-}TTF)_x]_2PF_6$," *Chem. Mater.* **22**, 3121–3132 (2010).
S. HIROSE, A. KAWAMOTO, N. MATSUNAGA, K. NOMURA, K. YAMAMOTO and K. YAKUSHI, "Reexamination of ^{13}C-NMR in $(TMTTF)_2AsF_6$: Comparison with Infrared Spectroscopy," *Phys. Rev. B* **81**, 205107 (6 pages) (2010).
Y. YUE, K. YAMAMOTO, M. URUICHI, C. NAKANO, K. YAKUSHI, S. YAMADA, T. HIEJIMA and A. KAWAMOTO, "Non-Uniform Site Charge Distribution and Fluctuation of Charge Order in the Metallic State of α-$(BEDT\text{-}TTF)_2I_3$," *Phys. Rev. B* **82**, 075134 (8 pages) (2010).
R. MORGUNOV, A. DMITRIEV, A. CHERNENKAYA, K. YAMAMOTO, K. YAKUSHI and Y. TANIMOTO, "Charge Order–Disorder Phase Transition Detected by EPR in α'-$(BEDT\text{-}TTF)_2IBr_2$," *Physica B* **405**, S138–S140 (2010).
T. HIEJIMA, S. YAMADA, M. URUICHI and K. YAKUSHI, "Infrared and Raman Studies of α-$(BEDT\text{-}TTF)_2MHg(SCN)_4$ with M = K and NH_4 at Low Temperature—the Charge Ordering Fluctuation with Breaking of the Inversion Symmetry," *Physica B* **405**, S153–S156 (2010).
M. HIGA, R. KONDO, A. MURATA, S. KAGOSHIMA, H. NISHIKAWA and K. YAKUSHI, "Electronic States of Organic Quasi-Two Dimensional Conductor β''-$(DODHT)_2PF_6$: Charge Ordering and Superconductivity," *Physica B* **405**, S172–S175 (2010).
Y. YUE, K. YAMAMOTO, C. NAKANO, M. URUICHI, K. YAKUSHI, M. INOKUCHI, T. HIEJIMA and A. KAWAMOTO, "Order–Disorder Type of Charge-Ordering Phase Transition in Narrow-Bandwidth Compound, α'-$(BEDT\text{-}TTF)_2IBr_2$," *Physica B* **405**, S232–S236 (2010).
T. YAMAMOTO, Y. NAKAZAWA, R. KATO, K. YAKUSHI, H. AKUTSU, A. S. AKUTSU, H. YAMAMOTO, A. KAWAMOTO, S. S. TURNER and P. DAY, "Charge Fluctuation of the Superconducting Molecular Crystals," *Physica B* **405**, S237–S239 (2010).
K. YAMAMOTO, A. KOWALSKA, C. NAKANO and K. YAKUSHI, "Inhomogeneous Ferroelectric Polarization in α'-$(BEDT\text{-}TTF)_2IBr_2$ Revealed by Second-Harmonic Generation Microscopy," *Physica B* **405**, S363–S364 (2010).

K. FURUKAWA, T. HARA and T. NAKAMURA, "Anomalous Temperature Dependence of *g*-Tensor in Organic Conductor, $(TMTTF)_2X$ (X = Br, PF_6 and SbF_6)," *J. Phys. Soc. Jpn.* **78**, 104713 (6 pages) (2009).
F. IWASE, K. SUGIURA, K. FURUKAWA and T. NAKAMURA, "Electronic Properties of a TMTTF-Family Salt, $(TMTTF)_2TaF_6$: New Member Located on the Modified Generalized Phase-Diagram," *J. Phys. Soc. Jpn.* **78**, 104717 (7 pages) (2009).
H. OHTA, N. MATSUMI, S. OKUBO, M. FUJISAWA, T. SAKURAI, H. KIKUCHI, K. FURUKAWA and T. NAKAMURA, "Spin Gap Observation in Triangular Lattice Antiferromagnet $InMnO_3$ by High Field ESR," *J. Phys.: Conf. Series* **200**, 022041 (4 pages) (2010).
K. FURUKAWA, T. HARA and T. NAKAMURA, "Spin-Dynamics in Vicinity of Spin-Gap Phase Transition for Organic Conductor $(TMTTF)_2X$," *J. Phys. Soc. Jpn.* **79**, 043702 (4 pages) (2010).
K. FURUKAWA, T. NAKAMURA, Y. KOBAYASHI and T. OGURA, "Novel Type of Career Generated System: Magnetic Investigations of TTF-Based Self-Doped Hydrogen-Bonding Conductor," *J. Phys. Soc. Jpn.* **79**, 053701 (4 pages) (2010).
N. YONEYAMA, T. SASAKI, N. KOBAYASHI, K. FURUKAWA and T. NAKAMURA, "Magnetic Properties of X-Ray Irradiated Organic Mott Insulator κ-$(BEDT\text{-}TTF)_2Cu[N(CN)_2]Cl$," *J. Phys. Soc. Jpn.* **79**, 063706 (4 pages) (2010).
N. YONEYAMA, T. SASAKI, N. KOBAYASHI, K. FURUKAWA and T. NAKAMURA, "X-Ray Irradiation Effect on Magnetic Properties of Dimer-Mott Insulators: κ-$(BEDT\text{-}TTF)_2Cu[N(CN)_2]Cl$ and β'-$(BEDT\text{-}TTF)_2ICl_2$," *Physica B* **405**, S244–S246 (2010).
K. YOKOGAWA, H. YOSHINO, T. NAKAMURA, J. S. BROOKS and K. MURATA, "First Observation of Superconductivity by Uniaxial Strain in $(TMTTF)_2X$-Salt," *Physica B* **405**, S291–S294 (2010).
F. IWASE, K. SUGIURA, K. FURUKAWA and T. NAKAMURA, "The Ground States and Critical Behavior in the Quasi-One-Dimensional Complexes $(TMTTF)_2[(AsF_6)_x(SbF_6)_{1-x}]$," *Phys. Rev. B* **81**, 245126 (6 pages) (2010).

L. CHEN, Y. HONSHO, S. SEKI and D. JIANG, "Light-Harvesting Conjugated Microporous Polymers: Rapid and Highly Efficient Flow of Light Energy with a Porous Polyphenylene Framework as Antenna," *J. Am. Chem. Soc.* **132**, 6742–6748 (2010).
L. CHEN, Y. YANG and D. JIANG, "CMPs as Scaffolds for Constructing Porous Catalytic Frameworks: A Built-In Heterogeneous Catalyst with High Activity and Selectivity Based on Nanoporous Metalloporphyrin Polymers," *J. Am. Chem. Soc.* **132**, 9138–9143 (2010).

T. IIJIMA, T. YAMASE, M. TANSHO, T. SHIMIZU and K. NISHIMURA, "Solid-State ^{95}Mo NMR of Mixed-Valence Polyoxomolybdates (V, VI) with Localized or Delocalized d^1 Electrons," *Chem. Phys. Lett.* **487**, 232–236 (2010).
N. UEKAMA, T. AOKI, T. MARUOKA, S. KURISU, A. HATAKEYAMA, S. YAMAGUCHI, M. OKADA, H. YAGISAWA, K. NISHIMURA and S. TUZI, "Influence of Membrane Curvature on the Structure of the Membrane-Associated Pleckstrin Homology Domain of Phospholipase C-δ1," *Biochim. Biophys. Acta, Biomembr.* **1788**, 2575–2583 (2009).

M. HIRAMOTO and H. SHIOKAWA, "One Month Continuous Operation of Organic *p-i-n* Solar Cells Covered with a Zinc Oxide Protection Layer," *Appl. Phys. Express* **3**, 082301 (2 pages) (2010).
K. NISHIYAMA, T. HANAMOTO, H. SHIGEMATSU, K. KITADA, K. IKETAKI, T. KAJI and M. HIRAMOTO, "Morphology of Rare-Earth (Y, Sm) Nanostructures Synthesized by the Surfactant-Assenbled Method," *Chem. Lett.* **39**, 974–976 (2010).

S. L. WONG, H. HUANG, Y. L. HUANG, Y. Z. WANG, X. Y. GAO, T. SUZUKI, W. CHEN and A. T. S. WEE, "Effect of Fluorination on the Molecular Packing of Perfluoropentacene and Pentacene Ultrathin Films on Ag (111)," *J. Phys. Chem. C* **114**, 9356–9361 (2010).

T. NISHINO, R. NEGISHI, M. KAWAO, T. NAGATA, H. OZAWA and K. ISHIBASHI, "The Fabrication and Single Electron Transport of Au Nano-Particles Placed between Nb Nanogap Electrodes," *Nanotechnology* **21**, 225301 (6 pages) (2010).
H. UOYAMA, K. S. KIM, K. KUROKI, J.-Y. SHIN, T. NAGATA, T. OKUJIMA, H. YAMADA, N. ONO, D. KIM and H. UNO, "Highly Pure Synthesis, Spectral Assignments, and Two-Photon Properties of Cruciform Porphyrin Pentamers Fused with Benzene Units," *Chem. –Eur. J.* **16**, 4063–4074 (2010).

H. KON and T. NAGATA, "Syntheses of the Terpyridine-Bipyridine Linked Binary Ligands and Structural and Redox Properties of Their Cobalt Complexes," *Inorg. Chem.* **48**, 8593–8602 (2009).
T. NAGATA, Y. KIKUZAWA, T. NAGASAWA and S. I. ALLAKHVERDIEV, "Single-Molecular Quinone Pools: A Synthetic Model of Biochemical Energy Transducer," *Trans. Mater. Res. Soc. Jpn.* **34**, 505–508 (2009).

H. KITAHARA and H. SAKURAI, "Gold Nanocluster as a Catalyst for Intramolecular Addition of Primary Amines to Unactivated Alkenes under Aerobic Conditions," *Chem. Lett.* **39**, 46–48 (2010).
R. TSURUOKA, S. HIGASHIBAYASHI, T. ISHIKAWA, S. TOYOTA and H. SAKURAI, "Optical Resolution of Chiral Buckybowls by Chiral HPLC," *Chem. Lett.* **39**, 646–647 (2010).
S. HIGASHIBAYASHI, A. F. G. MASUD REZA and H. SAKURAI, "Stereoselective Cyclotrimerization of Enantiopure Iodonorbornenes Catalyzed by Pd Nanoclusters for C_3 or C_{3v} Symmetric *syn*-Tris(norborneno)benzenes," *J. Org. Chem.* **75**, 4626–4628 (2010).

K. ONO, O. TOKURA and M. TOMURA, "(3*Z*,3'*Z*)-3,3'-(Ethane-1,2-diylidene)diisobenzofuran-1(3*H*)-one," *Acta Crystallogr., Sect. E: Struct. Rep. Online* **65**, o2118–o2118 (2009).
K. ONO, J. HASHIZUME, H. YAMAGUCHI, M. TOMURA, J. NISHIDA and Y. YAMASHITA, "Synthesis, Crystal Structure, and Electron-Accepting Property of BF_2 Complex of a Dihydroxydione with a Perfluorotetracene Skeleton," *Org. Lett.* **11**, 4326–4329 (2009).
M. TOMURA and Y. YAMASHITA, "Unsymmetrical Tetrathiafulvalene with a Fused 1,2,5-Thiadiazole Ring and Methylthio Groups," *Molecules* **14**, 4266–4274 (2009).
M. TOMURA and Y. YAMASHITA, "A Two-Dimensional Ladder-Type Network in the 2:1 Co-Crystal of 1,2,5-Thiadiazole-3,4-dicarboxylic Acid and 4,4'-Bipyridine," *Struct. Chem.* **21**, 107–111 (2010).
K. ONO, T. YAMAGUCHI and M. TOMURA, "Structure and Photovoltaic Properties of (*E*)-2-Cyano-3-[4-(diphenylamino)phenyl]acrylic Acid Substituted by *tert*-Butyl Groups," *Chem. Lett.* **39**, 864–866 (2010).

K. FURUKAWA, K. OHASHI, T. IMAMURA, J. SASAKI, K. JUDAI, N. NISHI and H. SEKIYA, "Methanol Solvation of the Ag^+ Ion Probed with Infrared Photodissociation Spectroscopy of $Ag^+(CH_3OH)_n$ (n = 1–5)," *Chem. Phys. Lett.* **495**, 8–13 (2010).
Y. NAGAI, K. SAITA, K. SAKOTA, S. NANBU, M. SEKINE, M. NAKATA and H. SEKIYA, "Electronic Spectra of Two Long-Lived Photoproducts: Double-Proton Transfer in 7-Hydroxyquinoline Dimer in a 2-Methyltetrahydrofuran Glass Matrix," *J. Phys. Chem.* **114**, 5041–5048 (2010).
M. SEKINE, Y. NAGAI, H. SEKIYA and M. NAKATA, "Electronic Absorption Spectra of Photoreaction Intermediates of 7-Hydroxyquinoline Monomer in a Low-Temperature Argon Matrix and Time-Dependent Density-Functional-Theory Calculations," *Chem. Phys. Lett.* **490**, 46–49 (2010).
Y. KAGEURA, K. SAKOTA and H. SEKIYA, "Charge Transfer Interaction of Intermolecular Hydrogen Bonds in 7-Azaindole$(MeOH)_n$ (n = 1, 2) with IR-Dip Spectroscopy and Natural Bond Orbital Analysis," *J. Phys. Chem. A* **113**, 6880–6885 (2009).
K. SAKOTA, Y. SHIMAZAKI and H. SEKIYA, "Formation of a Dual Hydrogen Bond in the N–H···C=O Moiety in the Indole-(*N*-methylacetamide)$_1$ Cluster Revealed by IR-Dip Spectroscopy with Natural Bond Orbital Analysis," *J. Phys. Chem. A* **114**, 5041–5048 (2009).
K. SAKOTA, N. KOMURE, W. ISHIKAWA and H. SEKIYA, "Spectroscopic Study on the Structural Isomers of 7-Azaindole$(ethanol)_n$ (n = 1–3) and Multiple-Proton Transfer Reactions in the Gas Phase," *J. Chem. Phys.* **130**, 224307 (7 pages) (2009).
K. SAKOTA and H. SEKIYA, "Probe of the NH Bond Strength in La and Lb States of 7-Azaindole with IR-Dip Spectroscopy: Insights into the Electronic-State Dependence of the Multiple Proton/Hydrogen Transfers in Hydrogen-Bonded Clusters," *J. Phys. Chem. A* **113**, 2663–2665 (2009).
K. SAITA, M. NAKAZONO, K. ZAITSU, S. NANBU and H. SEKIYA, "Theoretical Study of Photophysical Properties of Bisindolylmaleimide Derivatives," *J. Phys. Chem. A* **113**, 8213–8220 (2009).
M. SEKINE, Y. NAGAI, H. SEKIYA and M. NAKATA, "Photoinduced Hydrogen-Atom Eliminations of 6-Hydroxyquinoline and 7-Hydroxyquinoline Studied by Low-Temperature Matrix-Isolation Infrared Spectroscopy and Density-Functional-Theory Calculations," *J. Phys. Chem. A* **113**, 8286–8298 (2009).

Life and Coordination-Complex Molecular Science

H. SAWAI, H. SUGIMOTO, Y. ASANO, Y. KATO, Y. SHIRO and S. AONO, "X-Ray Crystal Structure of Michaelis Complex of Aldoxime Dehydratase," *J. Biol. Chem.* **284**, 32089–32096 (2009).
H. NAKAJIMA, N. TAKATANI, K. YOSHIMITSU, M. ITOH, S. AONO, Y. TAKAHASHI and Y. WATANABE, "The Role of the Fe–S Cluster in the Sensory Domain of Nitrogenase Transcriptional Activator VnfA from *Azotobacter vinelandii*," *FEBS J.* **277**, 817–832 (2010).
H. SAWAI, S. YOSHIOKA, T. UCHIDA, M. HYODO, Y. HAYAKAWA, K. ISHIMORI and S. AONO, "Molecular Oxygen Regulates the Enzymatic Activity of a Heme-Containing Diguanylate Cyclase (HemDGC) for the Synthesis of Cyclic Di-GMP," *Biochim. Biophys. Acta, Proteins Proteomics* **1804**, 166–172 (2010).

T. KANZAKI, S. USHIOKU, A. NAKAGAWA, T. OKA, K. TAKAHASHI, T. NAKAMURA, K. KUWAJIMA, A. YAMAGISHI and M. YOHDA, "Adaptation of a Hyperthermophilic Group II Chaperonin to Relatively Moderate Temperatures," *Protein Eng., Des. Sel.* **23**, 393–402 (2010).
T. NAKAMURA, K. MAKABE, K. TOMOYORI, K. MAKI, A. MUKAIYAMA and K. KUWAJIMA, "Different Folding Pathways Taken by Highly Homologous Proteins, Goat α-Lactalbumin and Canine Milk Lysozyme," *J. Mol. Biol.* **396**, 1361–1378 (2010).

LIST OF PUBLICATIONS

A. OCHI, K. MAKABE, K. KUWAJIMA and H. HORI, "Flexible Recognition of the tRNA G18 Methylation Target Site by TrmH Methyltransferase through First Binding and Induced Fit Processes," *J. Biol. Chem.* **285**, 9018–9029 (2010).

T. KOHNO, Y. NAKANO, N. KITOH, H. YAGI, K. KATO, A. BABA and M. HATTORI, "C-Terminal Region-Dependent Change of Antibody-Binding to the Eighth Reelin Repeat Reflects the Signaling Activity of Reelin," *J. Neurosci. Res.* **87**, 3043–3053 (2009).

H. DAN, Y. KAMIYA, K. TOTANI, D. KAMIYA, N. KAWASAKI, D. YAMAGUCHI, I. MATSUO, N. MATSUMONO, Y. ITO, K. KATO and K. YAMAMOTO, "Sugar-Binding Activity of the MRH Domain in ER α-Glucosidase II β Subunit Is Important for Efficient Glucose Trimming," *Glycobiology* **19**, 1127–1135 (2009).

M. UTSUMI, Y. YAMAGUCHI, H. SASAKAWA, N. YAMAMOTO, K. YANAGISAWA and K. KATO, "Up-and-Down Topological Mode of Amyloid β-Peptide Lying on Hydrophilic/Hydrophobic Interface of Ganglioside Clusters," *Glycoconjugate J.* **26**, 999–1006 (2009).

M. SUGIYAMA, E. KURIMOTO, Y. MORIMOTO, H. SAHASHI, E. SAKATA, K. HAMADA, K. ITOH, K. MORI, T. FUKUNAGA, Y. MINAMI and K. KATO, "Assembly State of Proteasome Activator 28 in an Aqueous Solution as Studied by Small-Angle Neutron Scattering," *J. Phys. Soc. Jpn.* **78**, 124802 (2009).

E. SAKATA, T. SATOH, S. YAMAMOTO, Y. YAMAGUCHI, M. YAGI-UTSUMI, E. KURIMOTO, K. TANAKA, S. WAKATSUKI and K. KATO, "Crystal Structure of UbcH5b~ubiquitin Intermediate: Insight into the Formation of the Self-Assembled E2~Ub Conjugates," *Structure* **18**, 138–147 (2010).

Y. YAMAGUCHI, M. MASUDA, H. SASAKAWA, T. NONAKA, S. HANASHIMA, S.-I. HISANAGA, K. KATO and M. HASEGAWA, "Characterization of Inhibitor-Bound α-Synuclein Dimer: Role of α-Synuclein N-Terminal Region in Dimerization and Inhibitor Binding," *J. Mol. Biol.* **395**, 445–456 (2010).

H. YAGI, M. YAMAMOTO, S.-Y. YU, N. TAKAHASHI, K.-H. KHOO, Y. C. LEE and K. KATO, "*N*-Glycosylation Profiling of Turtle Egg Yolk: Expression of Galabiose Structure," *Carbohydr. Res.* **345**, 442–448 (2010).

O. SERVE, Y. KAMIYA, A. MAENO, M. NAKANO, C. MURAKAMI, H. SASAKAWA, Y. YAMAGUCHI, T. HARADA, E. KURIMOTO, M. YAGI-UTSUMI, T. IGUCHI, K. INABA, J. KIKUCHI, O. ASAMI, T. KAJINO, T. OKA, M. NAKASAKO and K. KATO, "Redox-Dependent Domain Rearrangement of Protein Disulfide Isomerase Coupled with Exposure of Its Substrate-Binding Hydrophobic Surface," *J. Mol. Biol.* **396**, 361–374 (2010).

M. YAGI-UTSUMI, T. KAMEDA, Y. YAMAGUCHI and K. KATO, "NMR Characterization of the Interactions between Lyso-GM1 Aqueous Micelles and Amyloid β," *FEBS Lett.* **584**, 831–836 (2010).

T. DOJIMA, T. NISHINA, T. KATO, T. UNO, H. YAGI, K. KATO, H. UEDA and E. Y. PARK, "Improved Secretion of Molecular Chaperone-Assisted Human IgG in Silkworm, and No Alterations in Their *N*-Linked Glycan Structures," *Biotechnol. Prog.* **26**, 232–238 (2010).

M. NISHIO, Y. KAMIYA, T. MIZUSHIMA, S. WAKATSUKI, H. SASAKAWA, K. YAMAMOTO, S. UCHIYAMA, M. NODA, A. R. MCKAY, K. FUKUI, H.-P. HAURI and K. KATO, "Structural Basis for the Cooperative Interplay between the Two Causative Gene Products of Combined Factor V and Factor VIII Deficiency," *Proc. Natl. Acad. Sci. U.S.A.* **107**, 4034–4039 (2010).

N. TAKEMAE, R. RUTTANAPUMMA, S. PARCHARIYANON, S. YONEYAMA, T. HAYASHI, H. HIRAMATSU, N. SRIWILAIJAROEN, Y. UCHIDA, S. KONDO, H. YAGI, K. KATO, Y. SUZUKI and T. SAITO, "Alterations in Receptor-Binding Properties of Swine Influenza Viruses of the H1 Subtype After Isolation in Embryonated Chicken Eggs," *J. Gen. Virol.* **91**, 938–948 (2010).

Y. YAMAGUCHI, S. HANASHIMA, H. YAGI, Y. TAKAHASHI, H. SASAKAWA, E. KURIMOTO, T. IGUCHI, S. KON, T. UEDA and K. KATO, "NMR Characterization of Intramolecular Interaction of Osteopontin, an Intrinsically Disordered Protein with Cryptic Integrin-Binding Motifs," *Biochem. Biophys. Res. Commun.* **393**, 487–491 (2010).

S. SATO, O. MOROHARA, D. FUJITA, Y. YAMAGUCHI, K. KATO and M. FUJITA, "Parallel-Stacked Aromatic Hosts for Orienting Small Molecules in a Magnetic Field: Induced Residual Dipolar Coupling by Encapsulation," *J. Am. Chem. Soc.* **132**, 3670–3671 (2010).

Y. WADA, A. DELL, S. M. HASLAM, B. TISSOT, K. CANIS, P. AZADI, M. BÄCKSTRÖM, C. E. COSTELLO, G. C. HANSSON, Y. HIKI, M. ISHIHARA, H. ITO, K. KAKEHI, N. KARLSSON, C. E. HAYES, K. KATO, N. KAWASAKI, K.-H. KHOO, K. KOBAYASHI, D. KOLARICH, A. KONDO, C. LEBRILLA, M. NAKANO, H. NARIMATSU, J. NOVAK, M. V. NOVOTNY, E. OHNO, N. H. PACKER, E. PALAIMA, M. B. RENFROW, M. TAJIRI, K. A. THOMSSON, H. YAGI, S.-Y. YU and N. TANIGUCHI, "Comparison of Methods for Profiling *O*-Glycosylation: Human Proteome Organization Human Disease Glycomics/Proteome Initiative Multi-Institutional Study of IgA1," *Mol. Cell. Proteomics* **9**, 719–727 (2010).

J. HOSEKI, H. SASAKAWA, Y. YAMAGUCHI, M. MAEDA, H. KUBOTA, K. KATO and K. NAGATA, "Solution Structure and Dynamics of Mouse ARMET," *FEBS Lett.* **584**, 1536–1542 (2010).

C. A. SANDOVAL, F. BIE, A. MATSUOKA, Y. YAMAGUCHI, H. NAKA, Y. LI, K. KATO, N. UTSUMI, K. TSUTSUMI, T. OHKUMA, K. MURATA and R. NOYORI, "Chiral η^6-Arene/*N*-Tosylethylenediamine–Ruthenium(II) Complexes: Solution Behavior and Catalytic Activity for Asymmetric Hydrogenation," *Chem. –Asian J.* **5**, 806–816 (2010).

N. HOSOKAWA, L. O. TREMBLAY, B. SLENO, Y. KAMIYA, I. WADA, K. NAGATA, K. KATO and A. HERSCOVICS, "EDEM1 Accelerates the Trimming of α1,2-Linked Mannose on the C Branch of *N*-Glycans," *Glycobiology* **20**, 567–575 (2010).

S. KIM, Y. SAEKI, K. FUKUNAGA, A. SUZUKI, K. TAKAGI, T. YAMANE, K. TANAKA, T. MIZUSHIMA and K. KATO, "Crystal Structure of Yeast Rpn14, a Chaperone of the 19 S Regulatory Particle of the Proteasome," *J. Biol. Chem.* **285**, 15159–15166 (2010).

H. YAGI, M. YANAGISAWA, K. KATO and R. K. YU, "Lysosome-Associated Membrane Protein 1 Is a Major SSEA-1-Carrier Protein in Mouse Neural Stem Cells," *Glycobiology* **20**, 976–981 (2010).

K. MASUDA, Y. YAMAGUCHI, N. TAKAHASHI, R. JEFFERIS and K. KATO, "Mutational Deglycosylation of the Fc Portion of Immunoglobulin G Causes *O*-Sulfation of Tyrosine Adjacently Preceding the Originally Glycosylated Site," *FEBS Lett.* **584**, 3474–3479 (2010).

M. NAKASAKO, A. MAENO, E. KURIMOTO, T. HARADA, Y. YAMAGUCHI, T. OKA, Y. TAKAYAMA, A. IWATA and K. KATO, "Redox-Dependent Domain Rearrangement of Protein Disulfide Isomerase from a Thermophilic Fungus," *Biochemistry* **49**, 6953–6962 (2010).

T. KURAHASHI, M. HADA and H. FUJII, "Critical Role of External Axial Ligands in Chirality Amplification of *trans*-Cyclohexane-1,2-diamine in Salen Complexes," *J. Am. Chem. Soc.* **131**, 12394–12405 (2009).
T. KURAHASHI, A. KIKUCHI, Y. SHIRO, M. HADA and H. FUJII, "Unique Property and Reactivity of High-Valent Manganese-Oxo versus Manganese-Hydroxo in the Salen Platform," *Inorg. Chem.* **49**, 6664–6672 (2010).
H. ISHIMARU, H. FUJII and T. OGURA, "Resonance Raman Study of a High-Valent Fe=O Porphyrin Complex as a Model for Peroxidase Compound II," *Chem. Lett.* **39**, 332–333 (2010).
S. NOZAWA, T. SATO, M. CHOLLET, K. ICHIYANAGI, A. TOMITA, H. FUJII, S. ADACHI and S. KOSHIHARA, "Direct Probing of Spin State Dynamics Coupled with Electronic and Structural Modifications by Picosecond Time-Resolved XAFS," *J. Am. Chem. Soc.* **132**, 61–63 (2010).
D. NONAKA, H. WARIISHI, K. G. WELINDER and H. FUJII, "Paramagnetic ^{13}C and ^{15}N NMR Analyses of the Push- and Pull-Effects in Cytochrome *c* Peroxidase and *Coprinus cinereus* Peroxidase Variants: Functional Roles of Highly-Conserved Amino Acids around Heme," *Biochemistry* **49**, 49–57 (2010).

T.-C. HE, C.-S. WANG, T. URISU, T. NAGAHIRO, R. TERO and R. XIA, "The PDMS-Based Microfluidic Channel Fabricated by Synchrotron Radiation Stimulated Etching," *Opt. Express* **18**, 9733–9738 (2010).
Y.-L. MAO, Z.-G. SHANG, Y. IMAI, T. HOSHINO, R. TERO, M. TANAKA, N. YAMAMOTO, K. YANAGISAWA and T. URISU, "Surface-Induced Phase Separation of a Sphingomyelin/Cholesterol/Ganglioside GM1-Planar Bilayer on Mica Surfaces and Microdomain Molecular Conformation that Accelerate Aβ Oligomerization," *Biochim. Biophys. Acta, Biomembr.* **1798**, 1090–1099 (2010).
T.-Y. CHIANG, T. MAKIMURA, T.-C. HE, S. TORII, T. YOSHIDA, R. TERO. C.-S. WANG and T. URISU, "Synchrotron-Radiation-Stimulated Etching of Polydimethylsiloxane (PDMS) Using XeF_2 as a Reaction Gas," *J. Synchrotron Radiat.* **17**, 69–74 (2010).

D. SUZUKI, Y. FURUTANI, K. INOUE, T. KIKUKAWA, M. SAKAI, M. FUJII, H. KANDORI, M. HOMMA and Y. SUDO, "Effects of Chloride Ion Binding on the Photochemical Properties of *Salinibacter* Sensory Rhodopsin I," *J. Mol. Biol.* **392**, 48–62 (2009).
A. KAWANABE, Y. FURUTANI, K.-H. JUNG and H. KANDORI, "Engineering an Inward Proton Transport from a Bacterial Sensor Rhodopsin," *J. Am. Chem. Soc.* **131**, 16439–16444 (2009).
Y. SUDO, A. OKADA, D. SUZUKI, K. INOUE, H. IRIEDA, M. SAKAI, M. FUJII, Y. FURUTANI, H. KANDORI and M. HOMMA, "Characterization of Signaling Complex Composed of Sensory Rhodopsin I and Its Cognate Transducer Protein from the Eubacterium *Salinibacter Rubber*," *Biochemistry* **48**, 10136–10145 (2009).
Y. SUDO, Y. KITADE, Y. FURUTANI, M. KOJIMA, S. KOJIMA, M. HOMMA and H. KANDORI, "Interaction between Na^+ Ion and Carboxylates of the PomA-PomB Stator Unit Studied by ATR-FTIR Spectroscopy," *Biochemistry* **48**, 11699–11705 (2009).
K. KATAYAMA, Y. FURUTANI, H. IMAI and H. KANDORI, "An FTIR Study of Monkey Green- and Red-Sensitive Visual Pigments," *Angew. Chem., Int. Ed.* **49**, 891–894 (2010).
K. HASHIMOTO, A. R. CHOI, Y. FURUTANI, K.-H. JUNG and H. KANDORI, "Low-Temperature FTIR Study of Gloeobacter Rhodopsin: Presence of Strongly Hydrogen-Bonded Water and Long-Range Structural Protein Perturbation upon Retinal Photoisomerization," *Biochemistry* **49**, 3343–3350 (2010).
V. A. LORENZ-FONFRIA, Y. FURUTANI, T. OTA, K. IDO and H. KANDORI, "Protein Fluctuations as the Possible Origin of the Thermal Activation of Rod Photoreceptors in the Dark," *J. Am. Chem. Soc.* **132**, 5693–5703 (2010).
K. KATAYAMA, Y. FURUTANI and H. KANDORI, "An FTIR Study of the Photoreaction of Bovine Rhodopsin in the Presence of Hydroxylamine," *J. Phys. Chem. B* **114**, 9039–9046 (2010).
S. NEYA, M. SUZUKI, T. HOSHINO, H. ODE, K. IMAI, T. KOMATSU, A. IKEZAKI, M. NAKAMURA, Y. FURUTANI and H. KANDORI, "Molecular Insight into Intrinsic Heme Distortion in Ligand Binding in Hemoprotein," *Biochemistry* **49**, 5642–5650 (2010).

T. OSAKO and Y. UOZUMI, "Aquacatalytic Aerobic Oxidation of Benzylic Alcohols with a Self-Supported Bipyridyl-Palladium Complex," *Chem. Lett.* **38**, 902–903 (2009).
Y. M. A. YAMADA, T. WATANABE, K. TORII and Y. UOZUMI, "Catalytic Membrane-Installed Microchannel Reactors for One-Second Allylic Arylation," *Chem. Commun.* 5594–5596 (2009).
T. OSAKO and Y. UOZUMI, "A Self-Supported Palladium-Bipyridyl Catalyst for the Suzuki-Miyaura Couplig in Water," *Heterocycles* **80**, 505–514 (2010).
T. SUZUKA, Y. OKADA, K. OOSHIRO and Y. UOZUMI, "Copper-Free Sonogashira Coupling in Water with an Amphiphilic Resin-Supoorted Palladium Complex," *Tetrahedron* **66**, 1064–1069 (2010).
Y. HIRAI and Y. UOZUMI, "Clean Synthesis of Triarylamines: Buchwald-Hartwig Reaction in Water with Amphiphilic Resin-Supported Palladium Complexes," *Chem. Commun.* **46**, 1103–1105 (2010).
C. K. JIN, Y. M. A. YAMADA and Y. UOZUMI, "Chemoselective Oxidation of Sulfides Promoted by a Tightly Convoluted Polypyridinium Phoshotungstate Catalyst with H_2O_2," *Bull. Korean Chem. Soc.* **31**, 547–548 (2010).
Y. HIRAI and Y. UOZUMI, "Heterogeneous Aromatic Amination of Aryl Halides with Arylamines in Water with PS-PEG Resin-Supported Palladium Complexes," *Chem. –Asian J.* **5**, 1788–1795 (2010).

M.-K. TSAI, J. ROCHFORD, D. POLYANSKY, T. WADA, K. TANAKA, E. FUJITA and J. MUCKERMAN, "Chracterization of Redox Sites of $[Ru(OH_2)(Q)(tpy)]^{2+}$ (Q = 3,5-Di-*tert*-butyl-1,2-benzoquinone, tpy = 2,2':6',2"-terpyridine) and Related Species through Experiment and Theoretical Studies," *Inorg. Chem.* **48**, 4372–4383 (2009).
T. FUKUSHIMA, E. FUJITA, J. T. MUCKERMAN, D. E. POLYANSKY, T. WADA and K. TANAKA, "Photochemical Stereospecific Hydrogenation of a Ru Complex with an NAD^+/NADH-Type Ligand," *Inorg. Chem.* **48**, 11510–11512 (2009).
S. FUKUI, N. SUZUKI, T. WADA, K. TANAKA and H. NAGAO, "Formation and Structure of an (Iminium Ion)Ruthenium Complex and Reaction of the Iminium Ion Moiety with Alcohols," *Organometallics* **29**, 1534–1536 (2010).

LIST OF PUBLICATIONS

T. KOSHIYAMA, N. KAWABA, T. HIKAGE, M. SHIRAI, Y. MIURA, C.-Y. HUANG, K. TANAKA, Y. WATANABE and T. UENO, "Modification of Porous Protein Crystals in Development of Bio-Hybrid Materials," *Bioconjugate Chem.* **21**, 264–269 (2010).

T. UENO, S. ABE, T. KOSHIYAMA, T. OHKI, T. HIKAGE and Y. WATANABE, "Metal Ion Accumulation Induced by Hydrogen Bonds on Protein Surfaces: Mechanistic Insights into the Initiation Steps of Biomineralization Obtained using Porous Lysozyme Crystals Containing Rh(III) Ions," *Chem. –Eur. J.* **16**, 2730–2740 (2010).

T. UENO, "An Engineered Metalloprotein as a Functional and Structural Bioinorganic Model System," *Angew. Chem., Int. Ed.* **49**, 3868–3869 (2010).

S. ABE, T. HIKAGE, Y. WATANABE, S. KITAGAWA and T. UENO, "Mechanism of Accumulation and Incorporation of Organometallic Pd Complexes into the Protein Nanocage of apo-Ferritin," *Inorg. Chem.* **49**, 6967–6973 (2010).

D. OYAMA, A. ASUMA, T. HAMADA and T. TAKASE, "Novel [Ru(polypyridine)$(CO)_2Cl_2$] and [Ru(polypyridine)$_2$$(CO)Cl]^+$-Type Complexes: Characterizing the Effects of Introducing Azopyridyl Ligands by Electrochemical, Spectroscopic and Crystallographic Measurements," *Inorg. Chim. Acta* **362**, 2581–2588 (2009).

D. OYAMA, M. KIDO, A. ORITA and T. TAKASE, "(2,2'-Bipyridine-κ^2*N*,*N*')chlorido[4'-(2,5-dimethoxyphenyl)-2,2':6',2"-terpyridine-κ^3*N*,*N*',*N*"]ruthenium(II) Hexafluoridophosphate Acetonitrile Monosolvate," *Acta Crystallogr., Sect. E: Struct. Rep. Online* **65**, m1117–m1118 (2009).

D. OYAMA, M. KIDO, A. ORITA and T. TAKASE, "Synthesis, Structure, Redox Property and Ligand Replacement Reaction of Ruthenium(II) Complexes Containing a Terpyridyl Ligand with a Redox Active Moiety," *Polyhedron* **29**, 1337–1343 (2010).