

LIST OF PUBLICATIONS

Department of Theoretical Studies

- Y. MAEDA, G. M. A. RAHMAN, T. WAKAHARA, M. KAKO, M. OKAMURA, S. SATO, T. AKASAKA, K. KOBAYASHI and S. NAGASE**, "Synthesis and Characterization of Tetrakis-Silylated C₆₀ Isomers," *J. Org. Chem.* **68**, 6791–6794 (2003).
- T. WAKAHARA, Y. MAEDA, M. KAKO, T. AKASAKA, K. KOBAYASHI and S. NAGASE**, "Silylation of Fullerenes with Active Species in Photolysis of Polysilane," *J. Organomet. Chem.* **685**, 177–188 (2003).
- T. TAJIMA, K. HATANO, T. SASAKI, T. SASAMORI, N. TAKEDA, N. TOKITOH, N. TAKAGI and S. NAGASE**, "Syntheses and Structures of Silicon Analogues of Cyclopropabenzene," *J. Organomet. Chem.* **686**, 118–126 (2003).
- M. T. H. LIU, Y. -K. CHOE, M. KIMURA, K. KOBAYASHI, S. NAGASE, T. WAKAHARA, Y. NIINO, M. ISHITUKA and T. AKASAKA**, "The Effect of Substituents on the Thermal Decomposition of Diazirines: Experimental and Computational Studies," *J. Org. Chem.* **68**, 7471–7478 (2003).
- J. LU, S. NAGASE, L. PENG and S. ZHANG**, "Strongly Size-Dependent Electronic Properties in C₆₀-Encapsulated Zigzag Nanotubes and Lower Size Limit of Carbon Nanopeapods," *Phys. Rev. B* **68**, 121402 (4 pages) (2003).
- T. WAKAHARA, Y. MATSUNAGA, A. KATAYAMA, Y. MAEDA, M. KAKO, T. AKASAKA, M. OKAMURA, T. KATO, Y. -K. CHOE, K. KOBAYASHI, S. NAGASE, H. HUANG and M. ATA**, "A Comparison of the Photochemical Reactivity between N@C₆₀ and C₆₀: Photolysis with Disilirane," *Chem. Commun.* 2940–2941 (2003).
- Z. SLANINA, K. KOBAYASHI and S. NAGASE**, "Temperature Development in a Set of C₆₀H₃₆ Isomers," *Chem. Phys. Lett.* **382**, 211–215 (2003).
- Z. CHEN, A. HIRSCH, S. NAGASE, W. THIEL and P. v. R. SCHLEYER**, "Spherical Sila- and Germa-Homoaromaticity," *J. Am. Chem. Soc.* **125**, 15507–15511 (2003).
- B. CAO, T. WAKAHARA, Y. MAEDA, A. HAN, T. AKASAKA, T. KATO, K. KOBAYASHI and S. NAGASE**, "Lanthanum Endohedral Metallofulleropyrrolidines: Synthesis, Isolation, and EPR Characterization," *Chem. Eur. J.* **10**, 716–720 (2004).
- Z. CHEN, S. NAGASE, A. HIRSCH, R. C. HADDON, W. THIEL and P. v. R. SCHLEYER**, "Side-Wall Opening of Single-Walled Carbon Nanotubes (SWCNTs) by Chemical Modification: A Critical Theoretical Study," *Angew. Chem., Int. Ed.* **43**, 1552–1554 (2004).
- Z. SLANINA, K. KOBAYASHI and S. NAGASE**, "Ca@C₈₂ Isomers: Computed Temperature Dependence of Relative Concentrations," *J. Chem. Phys.* **120**, 3397–3400 (2004).
- Z. SLANINA, K. ISHIMURA, K. KOBAYASHI and S. NAGASE**, "C₇₂ Isomers: The IPR-Satisfying Cage is Disfavored by Both Energy and Entropy," *Chem. Phys. Lett.* **384**, 114–118 (2004).
- S. RE and S. NAGASE**, "How is the CH/π Interaction Important for Molecular Recognition?" *Chem. Commun.* 658–659 (2004).
- S. IWAMATU, T. UOZAKI, K. KOBAYASHI, S. RE, S. NAGASE and S. MURATA**, "A Bowl-Shaped Fullerene Encapsulates a Water into the Cage," *J. Am. Chem. Soc.* **126**, 2668–2669 (2004).
- Z. SLANINA, K. KOBAYASHI and S. NAGASE**, "Ca@C₇₄ Isomers: Relative Concentrations at Higher Temperatures," *Chem. Phys.* **301**, 153–157 (2004).
- Z. SLANINA, K. KOBAYASHI and S. NAGASE**, "Computed Temperature Development of the Relative Stabilities of La@C₈₂ Isomers," *Chem. Phys. Lett.* **388**, 74–78 (2004).
- T. WAKAHARA, J. KOBAYASHI, M. YAMADA, Y. MAEDA, T. TSUCHIYA, M. OKAMURA, T. AKASAKA, M. WAELCHLI, K. KOBAYASHI, S. NAGASE, T. KATO, M. KAKO, K. YAMAMOTO and K. M. KADISH**, "Characterization of Ce@C₈₂ and Its Anion," *J. Am. Chem. Soc.* **126**, 4883–4887 (2004).
- J. LU, S. NAGASE, S. ZHANG and L. PENG**, "Energetic, Geometric, and Electronic Evolutions of K-Doped Single-Wall Carbon Nanotube Ropes with K intercalation Concentration," *Phys. Rev. B* **69**, 205304 (4 pages) (2004).
- Y. MAEDA, Y. MATSUNAGA, T. WAKAHARA, S. TAKAHASHI, T. TSUCHIYA, M. O. ISHITSUKA, T. HASEGAWA, T. AKASAKA, M. T. H. LIU, K. KOKURA, E. HORN, K. YOZA, T. KATO, S. OKUBO, K. KOBAYASHI, S. NAGASE and K. YAMAMOTO**, "Isolation and Characterization of a Carbene Derivative of La@C₈₂," *J. Am. Chem. Soc.* **126**, 6858–6859 (2004).
- Y. ONO, Y. FUJII, S. NAGASE and T. ISHIDA**, "A Density Functional Theory Study Applied for Carbon Isotope Effects in the Non-Aqueous [Cu(CO)]⁺/CO System," *Chem. Phys. Lett.* **390**, 71–78 (2004).
- B. CAO, T. WAKAHARA, T. TSUCHIYA, M. KONDO, Y. MAEDA, G. M. A. RAHMAN, T. AKASAKA, K. KOBAYASHI, S. NAGASE and K. YAMAMOTO**, "Isolation, Characterization, and Theoretical Study of La₂@C₇₈," *J. Am. Chem. Soc.* **126**, 9164–9165 (2004).
- M. O. ISHITSUKA, Y. NIINO, T. WAKAHARA, T. AKASAKA, M. T. H. LIU, K. KOBAYASHI and S. NAGASE**, "A Verification of the Photolytic Decomposition Pathways of 3-Tert-Butyl-3-Chlorodiazirine Based on the Application of the C₆₀ Probe Technique," *Tetrahedron Lett.* **45**, 6321–6322 (2004).

- G. LA PENNA, A. MITSUTAKE, M. MASUYA and Y. OKAMOTO**, "Molecular Dynamics of C-Peptide of Ribonuclease A Studied by Replica-Exchange Monte Carlo Method and Diffusion Theory," *Chem. Phys. Lett.* **380**, 609–619 (2003).
- B. A. BERG, H. NOGUCHI and Y. OKAMOTO**, "Multioverlap Simulations for Transitions between Reference Configurations," *Phys. Rev. E* **68**, 036126 (11 pages) (2003).
- Y. SAKAE and Y. OKAMOTO**, "Optimization of Protein Force-Field Parameters with the Protein Data Bank," *Chem. Phys. Lett.* **382**, 626–636 (2003).
- H. OKUMURA and Y. OKAMOTO**, "Monte Carlo Simulations in Multibaric-Multithermal Ensemble," *Chem. Phys. Lett.* **383**, 391–396 (2004).
- H. KOKUBO and Y. OKAMOTO**, "Prediction of Transmembrane Helix Configurations by Replica-Exchange Simulations," *Chem. Phys. Lett.* **383**, 397–402 (2004).
- K. MURATA, Y. SUGITA and Y. OKAMOTO**, "Free Energy Calculations for DNA Base Stacking by Replica-Exchange Umbrella Sampling," *Chem. Phys. Lett.* **385**, 1–7 (2004).
- T. YODA, Y. SUGITA and Y. OKAMOTO**, "Comparisons of Force Fields for Proteins by Generalized-Ensemble Simulations," *Chem. Phys. Lett.* **386**, 460–467 (2004).
- C. MUGURUMA, Y. OKAMOTO and M. MIKAMI**, "New Approach to the First-Order Phase Transition of Lennard-Jones Fluids," *J. Chem. Phys.* **120**, 7557–7563 (2004).
- H. KOKUBO and Y. OKAMOTO**, "Prediction of Membrane Protein Structures by Replica-Exchange Monte Carlo Simulations: Case of Two Helices," *J. Chem. Phys.* **120**, 10837–10847 (2004).
- H. OKUMURA and Y. OKAMOTO**, "Molecular Dynamics Simulations in the Multibaric-Multithermal Ensemble," *Chem. Phys. Lett.* **391**, 248–253 (2004).
- A. MITSUTAKE and Y. OKAMOTO**, "Replica-Exchange Extensions of Simulated Tempering Method," *J. Chem. Phys.* **121**, 2491–2504 (2004).
- H. KOKUBO and Y. OKAMOTO**, "Self-Assembly of Transmembrane Helices of Bacteriorhodopsin by a Replica-Exchange Monte Carlo Simulation," *Chem. Phys. Lett.* **392**, 168–175 (2004).
- H. OKUMURA and Y. OKAMOTO**, "Monte Carlo Simulations in Generalized Isobaric-Isothermal Ensembles," *Phys. Rev. E* **70**, 026702 (14 pages) (2004).
- K. MURATA, Y. SUGITA and Y. OKAMOTO**, "Free Energy Calculations of the Stacked and Unstacked States for DNA Dimers by Replica-Exchange Umbrella Sampling," in *AIP Conf. Proc.* **708**: SLOW DYNAMICS IN COMPLEX SYSTEMS, M. Tokuyama and I. Oppenheim, Eds., American Institute of Physics; Melville, pp. 332–333 (2004).
- H. NAKAMURA**, "Analytic Solution to Wave Packet Dynamics in a Laser Field: the Case of Linear Chirp," *Chem. Phys.* **295**, 269–273 (2003).
- V. I. OSHEROV, V. G. USHAKOV and H. NAKAMURA**, "Semiclassical Theory of Nonadiabatic Transitions Between Asymptotically Degenerate States," *Russ. Chem. Phys.* **22**, 87–102 (2003).
- V. I. OSHEROV, V. G. USHAKOV and H. NAKAMURA**, "Analytical Treatment of S-P Type Collisional Resonant Excitation Transfer," *Russ. Chem. Phys.* **22**, 103–108 (2003).
- P. OLOYEDE, G. MIL'NIKOV and H. NAKAMURA**, "On The Determination of Caustics," *J. Theor. Comput. Chem.* **3**, 91–102 (2004).
- G. V. MIL'NIKOV, K. YAGI, T. TAKETSUGU, H. NAKAMURA and K. HIRAO**, "Simple and Accurate Method to Evaluate Tunneling Splitting in Polyatomic Molecules," *J. Chem. Phys.* **120**, 5036–45 (2004).
- A. KONDORSKIY and H. NAKAMURA**, "Semiclassical Theory of Electronically Nonadiabatic Chemical Dynamics: Incorporation of the Zhu-Nakamura Theory into the Frozen Gaussian Propagation Method," *J. Chem. Phys.* **120**, 8937–8954 (2004).
- K. NOBUSADA and T. YAMAKI**, "Electronic Properties of Palladium-Thiolate Complexes with Tiara-Like Structures," *J. Phys. Chem. A* **108**, 1813–1817 (2004).
- K. NOBUSADA**, "Electronic Structure and Photochemical Properties of a Monolayer-Protected Gold Cluster," *J. Phys. Chem. B* **108**, 11904–11908 (2004).
- T. IMAI and F. HIRATA**, "Partial Molar Volume and Compressibility of a Molecule with Internal Degrees of Freedom," *J. Chem. Phys.* **119**, 5623–5631 (2003).
- A. TANIMURA, A. KOVALENKO and F. HIRATA**, "Molecular Theory of an Electrochemical Double Layer in a Nanoporous Carbon Supercapacitor," *Chem. Phys. Lett.* **378**, 638–646 (2003).
- T. YAMAZAKI, H. SATO and F. HIRATA**, "A Quantum Solute-Solvent Interaction Using Spectral Representation Technique Applied to the Electronic Structure Theory in Solution," *J. Chem. Phys.* **119**, 6663–6670 (2003).
- A. KOVALENKO and F. HIRATA**, "Molecular Description of Electrolyte Solution in a Carbon Aerogel Electrode," *Cond. Matt. Phys.* **6**, 583–609 (2003).
- K. NISHIYAMA, T. YAMAGUCHI, F. HIRATA and T. OKADA**, "Polar Solvation Dynamics: A Combination of the Reference Interaction-Site Model and Mode-Coupling Theories," *Pure Appl. Chem.* **76**, 71–77 (2004).
- T. YAMAGUCHI, S. -H. CHONG and F. HIRATA**, "A Mode-Coupling Analysis of the Translational and Rotational Diffusion of Polar Liquids; Acetonitrile and Water," *J. Mol. Liquids* **112/3**, 117–124 (2004).

- Y. KOBORI, T. YAGO, K. AKIYAMA, S. TERO-KUBOTA, H. SATO, F. HIRATA and J. R. NORRIS, Jr.**, "Superexchange Electron Tunneling Mediated by Solvent Molecules: Pulsed Electron Paramagnetic Resonance Study on Electronic Coupling in Solvent-Separated Radical Ion," *J. Phys. Chem. B* **108**, 10226–10240 (2004).
- H. SATO, F. HIRATA and S. SAKAKI**, "Distortion of Electronic Structure in Solvated Molecules: Tautomeric Equilibrium of 2-Pyridone and 2-Hydroxypyridine in Water Studied by the RISM-SCF/MCSCF Method," *J. Phys. Chem. A* **108**, 2097–2102 (2004).
- H. SATO, Y. KOBORI, S. TERO-KUBOTA and F. HIRATA**, "Theoretical Study on Electronic and Solvent Reorganization Associated with a Charging Process of Organic Compounds. 2. A New Decomposition Procedure into Electrostatic and Non-Electrostatic Responses," *J. Phys. Chem. B* **108**, 11709–11715 (2004).
- T. IMAI, A. KOVALENKO and F. HIRATA**, "Solvation Thermodynamics of Protein Studied by the 3D-RISM Theory," *Chem. Phys. Lett.* **395**, 1–6 (2004).
- N. MIYASHITA, M. KUWABARA and K. YONEMITSU**, "Electronic and Lattice Dynamics in the Photo-induced Ionic-to-Neutral Phase Transition in a One-Dimensional Extended Peierls-Hubbard Model," *J. Phys. Soc. Jpn.* **72**, 2282–2290 (2003).
- J. KISHINE, T. LUTY and K. YONEMITSU**, "Ferroelectric Phase Transition, Ionicity Condensation, and Multicriticality in Charge-Transfer Organic Complexes," *Phys. Rev. B* **69**, 075115 (5 pages) (2004).
- Y. OTSUKA and K. YONEMITSU**, "Two-Step Photo-Induced Phase Transitions in a Two-Sublattice Model," *J. Phys. IV France* **114**, 637–639 (2004).
- T. LUTY and K. YONEMITSU**, "On Thermo- and Photo-Induced Symmetry-Broken Transformation in Spin-Crossover Complex; Cooperative Activation," *J. Phys. Soc. Jpn.* **73**, 1237–1243 (2004).
- Y. NAGAE, Y. OISHI, N. NARUSE and M. NAGAOKA**, "Hydrated Structure of Ammonia-Water Molecule Pair via Free Energy Gradient Method: Realization of Zero Gradient and Force Balance on Free Energy Surface," *J. Chem. Phys.* **119**, 7972–7978 (2003).
- M. NAGAOKA**, "Structure Optimization of Solute Molecules via Free Energy Gradient Method," *Bull. Korean Chem. Soc.* **24**, 805–808 (2004).
- I. YU and M. NAGAOKA**, "Slowdown of Water Diffusion around Protein in Aqueous Solution with Ectoine," *Chem. Phys. Lett.* **388**, 316–321 (2004).
- R. FUKUDA, M. HADA and H. NAKATSUJI**, "Quasirelativistic Theory for the Magnetic Shielding Constant. I. Formulation of Douglas-Kroll-Hess Transformation for the Magnetic Field and Its Application to Atomic Systems," *J. Chem. Phys.* **118**, 1015–1026 (2003).
- R. FUKUDA, M. HADA and H. NAKATSUJI**, "Quasirelativistic Theory for the Magnetic Shielding Constant. II. Gauge-Including Atomic Orbitals and Applications to Molecules," *J. Chem. Phys.* **118**, 1027–1035 (2003).
- M. HADA**, "Quantum-Chemical Calculations for Paramagnetic ^{13}C NMR Chemical Shifts of Iron-Bound Cyanide Ions of Iron Porphyrins in Ground and Low-Lying Excited States Containing Ferric $(d_{xy})^2(d_{xz,yz})^3$ and $(d_{xy})^1(d_{xz,yz})^4$ Configurations," *J. Am. Chem. Soc.* **126**, 486–487 (2004).
- H. TORII**, "Pressure Dependence of the Liquid Structure and the Raman Noncoincidence Effect of Liquid Methanol Revisited," *Pure Appl. Chem.* **76**, 247–254 (2004).
- H. TORII**, "Extent of Delocalization of Vibrational Modes in Liquids as a Result of Competition between Diagonal Disorder and Off-Diagonal Coupling," *J. Phys. Chem. A* **108**, 2103–2107 (2004).
- H. TORII**, "Atomic Quadrupolar Effect in the Methanol- CCl_4 and Water- CCl_4 Intermolecular Interactions," *Chem. Phys. Lett.* **393**, 153–158 (2004).
- H. TORII**, "Vibrational Interactions in the Amide I Subspace of the Oligomers and Hydration Clusters of *N*-Methylacetamide," *J. Phys. Chem. A* **108**, 7272–7280 (2004).
- T. NAKAJIMA, N. YONEKURA, Y. MATSUO, T. KOBAYASHI and Y. FUKUYAMA**, "Simultaneous Production of Spin-Polarized Ions/Electrons Based on Two-Photon Ionization of Laser-Ablated Metallic Atoms," *Appl. Phys. Lett.* **83**, 2103–2105 (2003).
- N. YONEKURA, T. NAKAJIMA, Y. MATSUO, T. KOBAYASHI and Y. FUKUYAMA**, "Electron-Spin Polarization of Photoions Produced through Photoionization from the Laser-Excited Triplet State of Sr," *J. Chem. Phys.* **120**, 1806 (2004).
- T. NAKAJIMA**, "Control of the Spin-Polarization of Photoelectrons/Photoions Using Short Laser Pulses," *Appl. Phys. Lett.* **84**, 3786–3788 (2004).
- N. MIYAMOTO, M. KAMEI, D. YOSHITOMI, T. KANAI, T. SEKIKAWA, T. NAKAJIMA and S. WATANABE**, "Observation of Two-Photon Above-Threshold Ionization of Rare Gases by XUV Harmonic Photons," *Phys. Rev. Lett.* **93**, 083903 (2004).

Department of Molecular Structure

- T. NAGAHARA, K. IMURA and H. OKAMOTO**, "Spectral Inhomogeneities and Spatially Resolved Dynamics in Porphyrin J-Aggregate Studied in the Near-Field," *Chem. Phys. Lett.* **381**, 368–375 (2003).

K. IMURA, H. OHOYAMA and T. KASAI, “Structures and Its Dipole Moments of Half-Sandwich Type Metal-Benzene (1:1) Complexes Determined by 2-m Long Electrostatic Hexapole,” *Chem. Phys.* **301**, 183–187 (2004).

Y. ICHIYANAGI, H. KONDOH, T. YOKOYAMA, K. OKAMOTO, K. NAGAI and T. OHTA, “X-Ray Absorption Fine-Structure Study on the Ni(OH)₂ Monolayer Nanoclusters,” *Chem. Phys. Lett.* **379**, 345–350 (2003).

K. TONO, A. TERASAKI, T. OHTA and T. KONDOW, “Chemically Induced Ferromagnetic Spin Coupling: Electronic and Geometric Structures of Chromium-Oxide Cluster Anions, Cr₂O_n⁻ (n = 1–3), Studied by Photoelectron Spectroscopy,” *J. Chem. Phys.* **119**, 11221–11227 (2003).

K. AMEMIYA and T. OHTA, “Design of a Variable Included Angle Monk-Gillieson Monochromator with Varied Line Spacing Grating,” *J. Synchrotron Radiat.* **11**, 171–176 (2004).

Y. NAKAYAMA, H. KONDOH and T. OHTA, “Structure-Dependent Mixed Valence of Sm on Cu(111) Studied by XPS and STM,” *Surf. Sci.* **552**, 53–62 (2004).

K. AMEMIYA, S. KITAGAWA, D. MATSUMURA, H. ABE, T. YOKOYAMA and T. OHTA, “Direct Observation of Magnetic Depth Profiles of Thin Fe Films on Cu(100) and Ni/Cu(100) with the Depth-Resolved X-Ray Magnetic Circular Dichroism,” *Appl. Phys. Lett.* **84**, 936–939 (2004).

Y. L. HOU, S. GAO, T. OHTA and H. KONDOH, “Toward Three-Dimensional Spherical Self-Assembly via Ternary Surfactant Combination: The Case of Magnetite Nanoparticles,” *Eur. J. Inorg. Chem.* 1169–1173 (2004).

Y. L. HOU, S. GAO, T. OHTA and H. KONDOH, “Fabrication of Anisotropic Magnetic Nanostructures by Soft Chemical Approach,” *Trans. Mater. Res. Soc. Jpn.* **49**, 123–126 (2004).

P. ZHU, T. SHIMADA, H. KONDOH, I. NAKAI, M. NAGASAKA and T. OHTA, “Adsorption Structures of NO on Pt(111) Studied by the Near Edge X-Ray Absorption Fine Structure Spectroscopy,” *Surf. Sci.* **565**, 232–242 (2004).

A. NAMBU, J. -M. BUSSAT, M. WEST, B. C. SELL, M. WATANABE, A. W. KAY, N. MANNELLA, B. A. LUDEWIGT, M. PRESS, B. TURKO, G. MEDDELER, G. ZIZKA, H. SPIELER, H. VAN DER LIPPE, P. DENES, T. OHTA, Z. HUSSAIN and C. S. FADLEY, “An Ultrahigh Speed One-Dimensional Detector for Use in Synchrotron Radiation Spectroscopy: First Photoemission Results,” *J. Electron Spectrosc.* **137-140**, 691–697 (2004).

K. ONDA, K. TANABE, H. NOGUCHI, K. DOMEN and A. WADA, “Dynamic Processes of Olefins Adsorbed on Hydroxyl Groups of DM20 Zeolite Excited by Picosecond Infrared Pulses,” *J. Phys. Chem. B* **107**, 11391–11396 (2003).

R. MIZOGUCHI, S. S. KANO and A. WADA, “Optical Control of Excited States of α -Perylene Crystal Using Optimized Pulse Shaping Method,” *Chem. Phys. Lett.* **379**, 319–324 (2003).

J. KUBOTA, E. YODA, N. ISHIZAWA, A. WADA, K. DOMEN and S. S. KANO, “Site-Hopping of Adsorbed CO in c(4×2)-CO/Ni(111) by Laser-Induced Temperature Jump: Time-Resolved Sum-Frequency Generation Observation,” *J. Phys. Chem. B* **107**, 10329–10332 (2003).

J. KUBOTA, A. WADA, S. S. KANO and K. DOMEN, “Time-Resolved Study of D₂O Ice Crystal on CO/Pt(111) by Ultra-Short NIR Laser Pumping: Melting and Recrystallization without Desorption,” *Chem. Phys. Lett.* **377**, 217–222 (2003).

S. KATANO, S. DOBASHI, J. KUBOTA, K. ONDA, A. WADA, S. S. KANO and K. DOMEN, “Structural Change of CO Adsorbed on Pt(111) by Laser Heating: Time-Resolved Sum-Frequency Generation Study,” *Chem. Phys. Lett.* **377**, 601 (2003).

K. AMEMIYA, S. KITAGAWA, D. MATSUMURA, H. ABE, T. OHTA and T. YOKOYAMA, “Direct Observation of Magnetic Depth Profiles of Thin Fe Films on Cu(100) and Ni/Cu(100) with the Depth-Resolved X-Ray Magnetic Circular Dichroism,” *Appl. Phys. Lett.* **84**, 936–938 (2004).

K. OKAMOTO, J. MIYAWAKI, K. NAGAI, D. MATSUMURA, A. NOJIMA, T. YOKOYAMA, H. KONDOH and T. OHTA, “Structural Study on Highly Oxidized States of a Water Oxidation Complex [Ru^{III}(bpy)₂(H₂O)]₂(μ -O)⁴⁺ by Ruthenium K-Edge X-Ray Absorption Fine Structure Spectroscopy,” *Inorg. Chem.* **42**, 8682–8689 (2003).

Y. ICHIYANAGI, H. KONDOH, T. YOKOYAMA, K. OKAMOTO, K. NAGAI and T. OHTA, “X-Ray Absorption Fine-Structure Study on the Ni(OH)₂ Monolayer Nanoclusters,” *Chem. Phys. Lett.* **379**, 345–350 (2003).

N. NISHI, K. KOSUGI, K. HINO and T. YOKOYAMA, “Matrix Embedded Cobalt-Carbon Nano-Cluster Magnets: Behavior as Room Temperature Single Domain Magnets,” *Eur. Phys. J. D* **24**, 97–100 (2003).

A. NAKAMOTO, Y. ONO, N. KOJIMA, D. MATSUMURA and T. YOKOYAMA, “Spin Crossover Complex Film, [Fe^{II}(H-trz)₃]-Nafion, with a Spin Transition around Room Temperature,” *Chem. Lett.* **32**, 476–476 (2003).

A. NAKAMOTO, Y. ONO, N. KOJIMA, D. MATSUMURA, T. YOKOYAMA, X. J. LIU and Y. MORITOMO, “Spin Transition and Its Photo-Induced Effect in Spin Crossover Complex Film Based on [Fe(H)(trz)₃],” *Synth. Met.* **137**, 1219–1220 (2003).

A. NAKAMOTO, Y. ONO, N. KOJIMA, D. MATSUMURA and T. YOKOYAMA, “Spin Crossover Complex Film, [Fe^{II}(H-trz)₃]-Nafion, with a Spin Transition around Room Temperature,” *Chem. Lett.* **32**, 336–337 (2003).

N. NISHI, K. KOSUGI, K. HINO, T. YOKOYAMA and E. OKUNISHI, “Formation and Magnetic Characteristics of Cobalt-Carbon Nanocluster Magnets Embedded in Amorphous Carbon Matrices,” *Chem. Phys. Lett.* **369**, 198–203 (2003).

- A. ITO, H. INO, Y. MATSUI, Y. HIRAO, K. TANAKA, K. KANEMOTO and T. KATO**, "A Bindschedler's Green-Based Arylamine: Its Polycations with High-Spin Multiplicity," *J. Phys. Chem. A* **108**, 5715–5720 (2004).
- T. WAKAHARA, J. KOBAYASHI, M. YAMADA, Y. MAEDA, T. TSUCHIYA, M. OKAMURA, T. AKASAKA, M. WAELCHLI, K. KOBAYASHI, S. NAGASE, T. KATO, M. KAKO, K. YAMAMOTO and M. K. KARL**, "Characterization of Ce@C₈₂ and Its Anion," *J. Am. Chem. Soc.* **126**, 4883–87 (2004).
- Y. MAEDA, Y. MATSUNAGA, T. WAKAHARA, S. TAKAHASHI, T. TSUCHIYA, M. O. ISHITUKA, T. HASEGAWA, T. AKASAKA, M. T. H. LIU, K. KOKURA, E. HORN, K. YOZA, T. KATO, S. OKUBO, K. KOBAYASHI, S. NAGASE and K. YAMAMOTO**, "Isolation and Characterization of Carbene Derivative of La@C₈₂," *J. Am. Chem. Soc.* **126**, 6858–59 (2004).
- B. CAO, T. WAKAHARA, Y. MAEDA, A. HAN, T. AKASAKA, T. KATO, K. KOBAYASHI and S. NAGASE**, "Lanthanum Endohedral Metallofulleropyrrolidines: Synthesis, Isolation, and EPR Characterization," *Chem. Eur. J.* **10**, 716–720 (2004).
- T. WAKAHARA, Y. MATSUNAGA, A. KATAYAMA, Y. MAEDA, M. KAKO, T. AKASAKA, M. OKAMURA, T. KATO, Y. -K. CHOE, K. KOBAYASHI, S. NAGASE, H. HUANGE and M. ATAE**, "A Comparison of the Photochemical Reactivity of N@C₆₀ and C₆₀: Photolysis with Disilirane," *Chem. Commun.* 2940–41 (2003).
- K. KANEMOTO, T. KATO, Y. ASO and T. OTSUBO**, "ESR Studies on Polarons in Long Oligothiophenes," *Phys. Rev. B* **68**, 092302 (2003).
- K. FURUKAWA, S. OKUBO, H. KATO, H. SHINOHARA and T. KATO**, "High-Field/High-Frequency ESR Study of Gd@C₈₂-I," *J. Phys. Chem. A* **107**, 10933–37 (2003).

Department of Electronic Structure

- Y. INOKUCHI and N. NISHI**, "Infrared Photodissociation Spectroscopy of Protonated Formic Acid and Acetic Acid Clusters," *J. Phys. Chem. A* **107**, 11319–11323 (2003).
- K. YOSHIDA, T. YAMAGUCHI, T. ADACHI, T. OTOMO, D. MATSUO, T. TAKAMUKU and N. NISHI**, "Structure and Dynamics of Hexafluoroisopropanol-Water Mixtures by X-Ray Diffraction, Small-Angle Neutron Scattering, NMR Spectroscopy, and Mass Spectroscopy," *J. Chem. Phys.* **119**, 6132–6142 (2003).
- C. OKABE, T. NAKABAYASHI, N. NISHI, T. FUKAMINATO, T. KAWAI, M. IRIE and H. SEKIYA**, "Picosecond Time-Resolved Stokes and Anti-Stokes Raman Studies on the Photochromic Reaction of Diarylethene Derivatives," *J. Phys. Chem. A* **107**, 5384–5390 (2003).
- K. KOSUGI, M. J. BUSHIRI and N. NISHI**, "Formation of Air Stable Carbon-Skinned Iron Nanocrystals from FeC₂," *Appl. Phys. Lett.* **84**, 1753–1755 (2004).
- Y. INOKUCHI, K. OHSHIMO, F. MISAIZU and N. NISHI**, "Structures of [Mg(H₂O)_{1,2}]⁺ and [Al(H₂O)₂]⁺ Ions Studied by Infrared Photodissociation Spectroscopy: Evidence of [HO–Al–H]⁺ Ion Core Structure in [Al(H₂O)₂]⁺," *Chem. Phys. Lett.* **390**, 140–144 (2004).
- Y. INOKUCHI, K. OHSHIMO, F. MISAIZU and N. NISHI**, "Infrared Photodissociation Spectroscopy of [Mg·(H₂O)_{1–4}]⁺ and [Mg·(H₂O)_{1–4}·Ar]⁺," *J. Phys. Chem. A* **108**, 5034–5040 (2004).
- M. SHINOZAKI, M. SAKAI, S. YAMAGUCHI, T. FUJIOKA and M. FUJII**, "S₁–S₀ Electronic Spectrum of Jet-Cooled *m*-Aminophenol," *Phys. Chem. Chem. Phys.* **5**, 5044–5050 (2003).
- K. DAIGOKU, S. ISHIUCHI, M. SAKAI, M. FUJII and K. HASHIMOTO**, "Photochemistry of Phenol–(NH₃)_n Clusters: Solvent Effect on a Radical Cleavage of an OH Bond in an Electronically Excited State and Intracuster Reactions in the Product NH₄(NH₃)_{n–1} (*n* < 5)," *J. Chem. Phys.* **119**, 5149–5157 (2003).
- Y. IKETAKI, T. WATANABE, S. ISHIUCHI, M. SAKAI, T. OMATSU, K. YAMAMOTO and M. FUJII**, "Predicted Spatial Resolution of Super-Resolving Fluorescence Microscopy Using Two-Color Fluorescence Dip Spectroscopy," *Appl. Spectrosc.* **57**, 1312–1316 (2003).
- T. WATANABE, Y. IKETAKI, T. OMATSU, K. YAMAMOTO, M. SAKAI and M. FUJII**, "Two-Point-Separation in Super-Resolution Fluorescence Microscope Based on Up-Conversion Fluorescence Depletion Technique," *Opt. Express* **11**, 3271–3276 (2003).
- Y. IKETAKI, T. WATANABE, M. SAKAI, S. ISHIUCHI, T. OMATSU, K. YAMAMOTO and M. FUJII**, "Super-Resolution Fluorescence Microscopy in Nano-Meter Scale Region Using Two-Color Laser Beams," *J. Surf. Sci. Soc. Jpn.* **24**, 392–399 (2003).
- S. ISHIUCHI, K. DAIGOKU, K. HASHIMOTO and M. FUJII**, "Four-Color Hole Burning Spectra of Phenol/Ammonia 1:3 and 1:4 Clusters," *J. Chem. Phys.* **120**, 3215–3220 (2004).
- T. WATANABE, Y. IGASAKI, N. FUKUCHI, M. SAKAI, S. ISHIUCHI, M. SAKAI, T. OMATSU, K. YAMAMOTO and Y. IKETAKI**, "Formation of Doughnut Laser Beam for Super-Resolving Microscopy Using a Phase Spatial Light Modulator," *Opt. Eng.* **43**, 1136–1143 (2004).
- K. OHMORI, Y. SATO, E. E. NIKITIN and S. A. RICE**, "High Precision Molecular Wave-Packet Interferometry with Hg-Ar Dimers," *Phys. Rev. Lett.* **91**, 243003 (4 pages) (2003).

- M. YUDASAKA, K. AJIMA, K. SUENAGA, T. ICHIHASHI, A. HASHIMOTO and S. IJIMA**, "Nano-Extraction and Nano-Condensation for C₆₀ Incorporation into Single-Wall Carbon Nanotubes in Liquid Phases," *Chem. Phys. Lett.* **380**, 42–46 (2003).
- F. NIHEY, H. HONGO, Y. OCHIAI, M. YUDASAKA and S. IJIMA**, "Carbon-Nanotubes Field-Effect Transistors with Very High Intrinsic Transconductance," *Jpn. J. Appl. Phys.* **42**, L1288–L1291 (2003).
- H. HONGO, F. NIHEY, T. ICHIHASHI, Y. OCHIAI, M. YUDASAKA and S. IJIMA**, "Support Materials Based on Converted Aluminum Films for Chemical Vapor Deposition Growth of Single-Wall Carbon Nanotubes," *Chem. Phys. Lett.* **380**, 158–164 (2003).
- K. TAKAI, M. OGA, H. SATO, T. ENOKI, Y. OHKI, A. TAOMOTO, K. SUENAGA and S. IJIMA**, "Structure and Electronic Properties of a Nongraphitic Disordered Carbon System and Its Heat-Treatment Effects," *Phys. Rev. B* **67**, 214202 (11 pages) (2003).
- K. KIMURA, N. IKEDA, Y. MARUYAMA, T. OKAZAKI, H. SHINOHARA, S. BANDOW and S. IJIMA**, "Evidence for Substantial Interaction between Gd Ion and SWNT in (Gd@C₈₂)@SWNT Peapods Revealed by STM Studies," *Chem. Phys. Lett.* **379**, 340–344 (2003).
- K. SUENAGA, R. TANIGUCHI, T. SHIMADA, T. OKAZAKI, H. SHINOHARA and S. IJIMA**, "Evidence for the Intermolecular Motion of Gd Atoms in a Gd₂@C₉₂ Nanopeapod," *Nano Lett.* **3**, 1395–1398 (2003).
- J. ZHU, M. YUDASAKA and S. IJIMA**, "A Catalytic Chemical Vapor Deposition Synthesis of Double-Walled Carbon Nanotubes over Metal Catalysts Supported on a Mesoporous Material," *Chem. Phys. Lett.* **380**, 496–502 (2003).
- M. YUDASAKA, T. ICHIHASHI, D. KASUYA, H. KATAURA and S. IJIMA**, "Structure Changes of Single-Wall Carbon Nanotubes and Single-Wall Carbon Nanohorns Cued by Heat Treatment," *Carbon* **41**, 1273–1280 (2003).
- E. BEKYAROVA, K. KANEKO, M. YUDASAKA, D. KASUYA, S. IJIMA, A. HUIDOBRO and F. RODRIGUEZ-REINOSO**, "Controlled Opening of Single-Wall Carbon Nanohorns by Heat Treatment in Carbon Dioxide," *J. Phys. Chem. B* **107**, 4479–4484 (2003).
- F. KOKAI, K. TAKAHASHI, D. KASUYA, A. NAKAYAMA, Y. KOGA, M. YUDASAKA and S. IJIMA**, "Laser Vaporization Synthesis of Polyhedral Graphite," *Appl. Phys. A* **77**, 69–71 (2003).
- S. CHE, K. LUND, T. TATSUMI, S. IJIMA, S. -H. JOO, R. RYOO and O. TERASAKI**, "Direct Observation of 3D Mesoporous Structure by Scanning Electron Microscopy (SEM): SBA-15 Silica and CMK-5 Carbon," *Angew. Chem.* **42**, 2182–2185 (2003).
- S. BANDOW, T. HIRAOKA, T. YUMURA, K. HIRAHARA, H. SHINOHARA and S. IJIMA**, "Raman Scattering Study on Fullerene Derived Intermediates Formed within Single-Wall Carbon Nanotube: From Peapod to Double-Wall Carbon Nanotube," *Chem. Phys. Lett.* **384**, 320–325 (2004).
- M. ZHANG, M. YUDASAKA and S. IJIMA**, "Diameter Enlargement of Single-Wall Carbon Nanotubes by Oxidation," *J. Phys. Chem. B* **108**, 149–153 (2004).
- Y. J. ZHANG, H. AGO, M. YUMURA, S. OHSHIMA, K. UCHIDA, T. KOMATSU and S. IJIMA**, "Study of the Growth of Boron Nanowires Synthesized by Laser Ablation," *Chem. Phys. Lett.* **385**, 177–183 (2004).
- K. AJIMA, M. YUDASAKA, K. SUENAGA, D. KASUYA, T. AZAMI and S. IJIMA**, "Material Storage Mechanism in Porous Nanocarbon," *Adv. Mater.* **16**, 397–401 (2004).
- T. YUMURA, K. HIRAHARA, S. BANDOW, K. YOSHIZAWA and S. IJIMA**, "A Theoretical Study on the Geometrical Features on Finite-Length Carbon Nanotubes Capped with Fullerenes Hemisphere," *Chem. Phys. Lett.* **386**, 38–43 (2004).
- T. YAMAGUCHI, S. BANDOW and S. IJIMA**, "Synthesis of Carbon Nanohorn Particles by Simple Pulsed Arc Discharge Ignited between Pre-Heated Carbon Rods," *Chem. Phys. Lett.* **389**, 181–185 (2004).
- T. OHBA, T. OMORI, H. KANO, M. YUDASAKA, S. IJIMA and K. KANEKO**, "Interstitial Nanopore Change of Single Wall Carbon Nanohorn Assemblies with High Temperature Treatment," *Chem. Phys. Lett.* **389**, 332–336 (2004).
- M. YUDASAKA, Y. KASUYA, F. JING, M. ZHANG and S. IJIMA**, "Fe-Sapphire and C-Fe-Sapphire Interactions and Their Effect on the Growth of Single-Walled Carbon Nanotubes by Chemical Vapor Deposition," *J. Nanosci. Nanotechnol.* **4**, 1–5 (2004).
- A. GLOTER, K. SUENAGA, H. KATAURA, R. FUJII, T. KODAMA, H. NISHIKAWA, I. IKEMOTO, K. KIKUCHI, S. SUZUKI, Y. ACHIBA and S. IJIMA**, "Structural Evolutions of Carbon Nano-Peapods under Electron Microscopic Observation," *Chem. Phys. Lett.* **390**, 462–466 (2004).
- A. NAKAYAMA, S. IJIMA, Y. KOGA, K. SHIMIZU, K. HIRAHARA and F. KOKAI**, "Compression of Polyhedral Graphite up to 43 GPa and X-Ray Diffraction Study on Elasticity and Stability of the Graphite Phase," *Appl. Phys. Lett.* **84**, 5112–5114 (2004).
- Y. HATTORI, H. KANO, F. OKINO, H. TOUHARA, D. KASUYA, M. YUDASAKA, S. IJIMA and K. KANEKO**, "Direct Thermal Fluorination of Single Wall Carbon Nanohorns," *J. Phys. Chem. B* **108**, 9614–9618 (2004).
- A. HASHIMOTO, H. YORIMITSU, K. AJIMA, K. SUENAGA, H. ISOBE, J. MIYAWAKI, M. YUDASAKA, S. IJIMA and E. NAKAMURA**, "Selective Deposition of a Gadolinium (III) Cluster in a Hole Opening of Single-Wall Carbon Nanohorn," *Proc. Natl. Acad. Sci.* **101**, 8527–8530 (2004).
- J. MIYAWAKI, M. YUDASAKA and S. IJIMA**, "Solvent Effects on Hole-Edge Structure for Single-Wall Carbon Nanotubes and Single-Wall Carbon Nanohorns," *J. Phys. Chem.* **108**, 10732–10735 (2004).

T. YUMURA, S. BANDOW, K. YOSHIZAWA and S. IJIMA, "The Role of Fullerene Hemisphere in Determining the Geometrical Features of Finite-Length Carbon Nanotubes," *J. Phys. Chem. B* **108**, 11426–11434 (2004).
R. YUGE, T. ICHIHASHI, Y. SHIMAKAWA, Y. KUBO, M. YUDASAKA and S. IJIMA, "Preferential Deposition of Pt Nanoparticles Inside Single-Wall Carbon Nanohorns," *Adv. Mater.* **16**, 1420–1423 (2004).
A. HASHIMOTO, K. SUENAGA, A. GLOTER, K. URITA and S. IJIMA, "Direct Evidence for Atomic Defects in Graphene Layers," *Nature* **430**, 870–873 (2004).

Y. MATSUSHITA, T. SUZUKI, T. ICHIMURA and T. HIKIDA, "The Cavity Size Effect on the Fluorescence Properties of 4'-Dimethylaminoacetophenone Complexed with Cyclodextrins," *Chem. Phys.* **286**, 399–407 (2003).
S. WATANABE, T. SUZUKI and T. ICHIMURA, "Calorimetric Standards for Photothermal Methods at the 248 nm Excitation," *Chem. Phys. Lett.* **374**, 41–44 (2003).
H. KOJIMA, K. MIYAKE, K. SAKEDA, T. SUZUKI, T. ICHIMURA, N. TANAKA, D. NEGISHI, M. TKAYANAGI and I. HANASAKI, "Methyl Torsional Potentials of Rotational Isomers of *m*-Methylanisole Studied by Spectral Hole-Burning Spectroscopy," *J. Mol. Struct.* **655**, 185–190 (2003).

K. MISAWA, I. MATSUDA, N. T. HASHIMOTO and R. LANG, "Single Molecular Phase-to-Amplitude Converter Using Femtosecond Wave Packet Engineering," *Technical Digest of Conference on Lasers and Electro-Optics 2004* (OSA), IWA (2004).

K. WATANABE, N. TAKAGI and Y. MATSUMOTO, "Direct Time-Domain Observation of Ultrafast Dephasing in Adsorbate-Substrate Vibration under the Influence of a Hot Electron Bath: Cs Adsorbed on Pt(111)," *Phys. Rev. Lett.* **92**, 057401 (4pages) (2004).
T. SAWADA, Z. LIU, N. TAKAGI, K. WATANABE and Y. MATSUMOTO, "Reactivity of Molecular Oxygen: Conversion of Methanol to Formate at Low Temperatures on Pt(111)," *Chem. Phys. Lett.* **392**, 334–339 (2004).

Department of Molecular Assemblies

I. SHIROTANI, J. HAYASHI, K. HIRANO, H. KAWAMURA, M. INOKUCHI, K. YAKUSHI and H. INOKUCHI, "Shear Stress Effects on Electronic Spectra on the One-Dimensional Bis(diphenylglyoximate) metal(II) Complexes, $M(\text{dpg})_2$ [$M = \text{Ni}$ and Pt] under High Pressure," *Proc. Jpn. Acad.* **79**, Ser B, 267–273 (2003).
K. SUZUKI, K. YAMAMOTO and K. YAKUSHI, "Charge-Ordering Transition in Two Crystal Modifications of θ -(BEDT-TTF) $_2$ TlZn(SCN) $_4$ Studied by Vibrational Spectroscopy," *Phys. Rev. B* **69**, 085114 (11 pages) (2004).
R. SWIETLIK, K. YAKUSHI, K. YAMAMOTO, T. KAWAMOTO and T. MORI, "Infrared and Raman Studies of TTM-TTP and TSM-TTP Charge-Transfer Salts," *J. Mol. Struct.* **704**, 89–93 (2004).
O. DROZDOVA, K. YAKUSHI, K. YAMAMOTO, A. OTA, H. YAMOCHI, G. SAITO, H. TASHIRO and D. B. TANNER, "Optical Characterization of $2k_F$ Bond-Charge-Density Wave in Quasi-One-Dimensional 3/4-Filled (EDO-TTF) $_2$ X ($X = \text{PF}_6$, and AsF_6)," *Phys. Rev. B* **70**, 075107 (8 pages) (2004).
T. YAMAMOTO, K. YAKUSHI, Y. SHIMIZU and G. SAITO, "Infrared and Raman Study of the Phase Transition of θ -(ET) $_2$ Cu $_2$ (CN)[N(CN) $_2$] $_2$," *J. Phys. Soc. Jpn.* **73**, 2326–2332 (2004).
K. YAKUSHI, K. YAMAMOTO, R. SWIETLIK, R. WOJCIECHOWSKI, K. SUZUKI, T. KAWAMOTO, T. MORI, Y. MISAKI and K. TANAKA, "Spectroscopic Studies of Charge-Ordering System in Organic Conductors," *Macromol. Symp.* **212**, 159–168 (2004).
R. SWIETLIK, L. OUAHAB, J. GUILLEVIC and K. YAKUSHI, "Infrared and Raman Studies of the Charge Ordering in the Organic Semiconductor κ -[(Et) $_4$ N](ET) $_4$ Co(CN) $_6$ ·3H $_2$ O," *Macromol. Symp.* **212**, 219–224 (2004).
P. TOMAN, S. NESPUREK and K. YAKUSHI, "Quantum Chemical Study of Oxidation Processes in Metal-Phthalocyanines," *Macromol. Symp.* **212**, 327–334 (2004).
R. SWIETLIK, K. YAKUSHI, K. YAMAMOTO, T. KAWAMOTO and T. MORI, "Phase Transition in the Organic Conductor (TTM-TTP) $_3$ Studied by Infrared and Raman Spectroscopies," *J. Phys. IV France* **114**, 87–90 (2004).
K. YAKUSHI, M. URUICHI, H. M. YAMAMOTO and R. KATO, "Dynamical Fluctuation of the Site-Charge Density in Metallic β '-(BEDT-TTF)(TCNQ)," *J. Phys. IV France* **114**, 149–151 (2004).
K. YAMAMOTO and K. YAKUSHI, "Electron-Molecular Vibration Coupling Effect on the Raman Spectrum of Organic Charge-Transfer Salts," *J. Phys. IV France* **114**, 153–155 (2004).
K. SUZUKI, K. YAMAMOTO and K. YAKUSHI, "Charge-Ordering in θ -(BEDT-TTF) $_2$ MM'(SCN) $_4$ [$M = \text{Cs}$, Rb , Tl , $M' = \text{Zn}$, Co]," *J. Phys. IV France* **114**, 379–381 (2004).
R. WOJCIECHOWSKI, A. KOWALSKA, J. ULANSKI, M. MAS-TORRENT, E. LAUKHINA, C. ROVIRA, V. TKACHEVA, K. YAMAMOTO and K. YAKUSHI, "Raman Studies of the Charge Ordering and Semiconductor-Metal Phase Transition in Polymorphic Forms of (BEDT-TTF) $_2$ Br $_{1.3}$ I $_{1.1}$ Cl $_{0.6}$," *J. Phys. IV France* **114**, 393–395 (2004).
T. YAMAMOTO, M. URUICHI, K. YAKUSHI, J. YAMAURA, H. TAJIMA and A. KAWAMOTO, "Charge Disproportionate State of BEDT-TTF β '-Salts," *J. Phys. IV France* **114**, 397–399 (2004).

H. YAMOCI, T. HANEDA, A. TRACZ, J. ULANSKI, O. DROZDOVA, K. YAKUSHI and G. SAITO, “Humidity Sensitive Conductivity of (BEDO-TTF)₂Br(H₂O)₃ as a Bulk Property,” *J. Phys. IV France* **114**, 591–593 (2004).

T. NAKAMURA and K. MAEDA, “Competition Electronic States of (TMTTF)₂MF₆: ESR Investigations,” *J. Phys. IV France* **114**, 123–124 (2004).

T. TAKAHASHI, R. CHIBA, K. HIRAKI, H. M. YAMAMOTO and T. NAKAMURA, “Dynamical Charge Disproportionation in Metallic State in θ -(BEDT-TTF)₂RbZn(SCN)₄,” *J. Phys. IV France* **114**, 269–272 (2004).

S. MOROTO, K. HIRAKI, Y. TAKANO, T. TAKAHASHI, H. M. YAMAMOTO and T. NAKAMURA, “Charge Disproportionation in the Metallic States of α -(BEDT-TTF)₂I₃,” *J. Phys. IV France* **114**, 399–340 (2004).

M. A. TANATAR, T. ISHIGURO, H. TANAKA and H. KOBAYASHI, “Thermal Conductivity of λ -(BETS)₂GaCl₄,” *Synth. Met.* **133**, 215–217 (2003).

H. FUJIWARA, E. FUJIWARA and H. KOBAYASHI, “Synthesis, Structures and Properties of New Organic Donors Connecting to TEMPO Radical through a Pyrrolidine Ring,” *Synth. Met.* **133-134**, 359–360 (2003).

J. S. BROOKS, L. BALICAS, K. A. STORR, H. KOBAYASHI, H. TANAKA, A. KOBAYASHI and M. TOKUMOTO, “Novel Features of the Newly Discovered Field-Induced Superconducting Phase of λ -(BETS)₂FeCl₄,” *Synth. Met.* **133**, 485–488 (2003).

M. A. TANATAR, M. SUZUKI, T. ISHIGURO, H. FUJIWARA and H. KOBAYASHI, “Thermal Conductivity of Antiferromagnetic Organic Superconductor κ -(BETS)₂FeBr₄ in the Low-Field and Field-Induced Superconducting States,” *Physica C* **388**, 613–614 (2003).

W. SUZUKI, E. FUJIWARA, A. KOBAYASHI, Y. FUJISHIRO, M. TANAKA, M. SAKATA, Y. OKANO and H. KOBAYASHI, “Structure of a Single-Component Palladium Complex with Extended TTF-Type Dithiolate Ligands, Bis(tetrathiafulvalenedithiolato)palladium Determined by Powder X-Ray Diffraction,” *Chem. Lett.* 1106–1107 (2003).

A. KOBAYASHI, M. SASA, W. SUZUKI, E. FUJIWARA and H. KOBAYASHI, “Infrared Electronic Absorption in a Single-Component Molecular Metal,” *J. Am. Chem. Soc.* **126**, 426–427 (2004).

E. FUJIWARA, A. KOBAYASHI, H. FUJIWARA and H. KOBAYASHI, “Syntheses, Structures, and Physical Properties of Nickel Bis(dithiolene) Complexes Containing Tetrathiafulvalene (TTF) Units,” *Inorg. Chem.* **43**, 1122–1129 (2004).

Z. WANG, B. ZHANG, H. FUJIWARA, H. KOBAYASHI and M. KUROMOO, “Mn₃(HCOO)₆: A 3D Porous Magnet of Diamond Framework with Nodes of Mn-Centered MnMn₄ Tetrahedron and Guest-Modulated Ordering Temperature,” *Chem. Commun.* 416–417 (2004).

J. S. BROOKS, S. UJI, E. S. CHOI, H. KOBAYASHI, A. KOBAYASHI, H. TANAKA and M. TOKUMOTO, “Investigation of the Field-Induced Phases in λ -(BETS)₂Fe_xGa_{1-x}Cl₄,” *J. Phys. IV France* **114**, 175–181 (2004).

L. BALICAS, V. BARZYKIN, K. STORR, J. S. BROOKS, M. TOKUMOTO, S. UJI, H. TANAKA, H. KOBAYASHI and A. KOBAYASHI, “The Effect of Pressure on the Phase Diagram of the Magnetic Field-Induced Superconducting State of λ -(BETS)₂FeCl₄,” *J. Phys. IV France* **114**, 199–203 (2004).

M. TOKUMOTO, S. ISHIBASHI, D. GRAF, E. S. CHOI, J. S. BROOKS, T. KONOIKE, H. FUJIWARA, B. ZHANG, H. KOBAYASHI, M. NISHIMURA, S. YASUZUKA, K. ENOMOTO and S. UJI, “Strong Evidence of Field-Induced Superconductivity and Shubnikov-de Haas Oscillation in κ -(BETS)₂FeBr₄,” *J. Phys. IV France* **114**, 223–226 (2004).

N. DRICHIKO, B. PETROV, V. N. SEMIKIN, R. M. VLASONA, O. A. BOGDANOVA, E. I. ZHILYAEVA, R. N. LYUBOVSKAYA, I. OLEJNICZAK, H. KOBAYASHI and A. KOBAYASHI, “A Comparative Mid-Infrared Study of Superconductor BETS₄Hg_{2.84}Br₈ and Metal BETS₄Hg₃Cl₈,” *J. Phys. IV France* **114**, 305–307 (2004).

Y. J. JO, H. KANG, T. TANAKA, M. TOKUMOTO, A. KOBAYASHI, H. KOBAYASHI, S. UJI and W. KANG, “*H-T* Phase Diagram of λ -(BETS)₂FeCl₄ under High Pressure,” *J. Phys. IV France* **114**, 323–325 (2004).

S. UJI, S. YASUZUKA, H. TANAKA, M. TOKUMOTO, B. ZHANG, H. KOBAYASHI, E. S. CHOI, D. GRAF and J. S. BROOKS, “Phase Diagram of Magnetic-Field-Induced Superconductor in λ -(BETS)₂Fe_xCl_{4-x}Br_x,” *J. Phys. IV France* **114**, 391–392 (2004).

A. KOBAYASHI, E. FUJIWARA, W. SUZUKI, M. SASA, Y. FUJISHIRO, E. NISHIBORI, M. TANAKA, M. SAKATA, Y. OKANO, H. FUJIWARA and H. KOBAYASHI, “Recent Progress in Development of Single-Component Molecular Metals,” *J. Phys. IV France* **114**, 419–424 (2004).

H. J. LEE, H. B. CUI, H. FUJIWARA, H. KOBAYASHI, E. FUJIWARA and E. FUJIWARA, “Development of New Magnetic Organic Conductors Based on Donor Molecules with Stable Organic Radical Part,” *J. Phys. IV France* **114**, 533–535 (2004).

T. OTSUKA, H. CUI, H. FUJIWARA, H. KOBAYASHI, E. FUJIWARA and A. KOBAYASHI, “The Pressure Effect on the Antiferromagnetic and Superconducting Transition of κ -(BETS)₂FeBr₄,” *J. Mater. Chem.* **14**, 1682–1685 (2004).

Y. OKANO, T. ADACHI, B. NARYMBETOV, H. KOBAYASHI, B. ZHOU and A. KOBAYASHI, “Crystal Structure of [(C₂H₅)₂(CH₃)₂N][Pd(dmit)₂]₂ at High Pressure,” *Chem. Lett.* 938–939 (2004).

Z. WANG, B. ZHANG, T. OTSUKA, K. INOUE, H. KOBAYASHI and M. KURMOO, "Anionic NaCl-type Frameworks of $[\text{Mn}^{\text{II}}(\text{HCOO})_3^-]$, Templated by Alkylammonium, Exhibit Weak Ferromagnetism," *Dalton Trans.* 2209–2216 (2004).

J. NISHIJO, A. MIYAZAKI and T. ENOKI, "Weak-Ferromagnetism in Molecular Magnets Based on Transition Metal Complexes of Crown Thioether," *Polyhedron* **22**, 1755–1758 (2003).

F. SETIFI, L. OUAHAB, S. GOLHEN, A. MIYAZAKI, T. ENOKI and J. YAMADA, "New Bulk Weak Ferromagnet in Ferrimagnetic Chains of Molecular Material Based on DTDH-TTP and Paramagnetic Thiocyanato Complex Anion: $(\text{DTDH-TTP})[\text{Cr}(\text{isoq})_2(\text{NCS})_4]$," *C. R. Chim.* **6**, 309–3168 (2003).

A. MIYAZAKI, T. KATO, H. YAMAZAKI, T. ENOKI, E. OGURA, Y. KUWATANI, M. IYODA and J. YAMAURA, "Anomalous Metallic State of One-Dimensional Molecular Conductor $(\text{EDO-TTFBr}_2)_3\text{I}_3$," *Phys. Rev. B* **68**, 085108 (6 pages) (2003).

Y. YOKOTA, R. YUGE, A. MIYAZAKI, T. ENOKI and M. HARA, "Property of Self-Assembled Monolayers of Long-Alkyl-Chain-Substituted TTF Derivative," *Mol. Cryst. Liq. Cryst.* **407**, 121/[517]–127/[523] (2003).

M. INAKUMA, A. TANIHARA, H. KATO, H. SHINOHARA and T. ENOKI, "Magnetic Anisotropy of Cerium Endohedral Metallofullerene," *J. Phys. Chem. B* **107**, 6965–6973 (2003).

M. PIMENTA, A. JORIO, M. S. DANTAS, C. FANTINI, M. DE SOUZA, L. G. Cançado, Ge. G. SAMSONIDZE, G. DRESSELHAUS, M. S. DRESSELHAUS, A. GRÜNEIS, R. SAITO, A. G. SOUZA FILHO, Y. KOBAYASHI, K. TAKAI, K. FUKUI and T. ENOKI, "Resonance Raman Scattering in Carbon Nanotubes and Nanographites," Molecular Nanostructures: Proceedings XVII International Winterschool on Electronic Properties of Novel Materials, H. Kuzmany, J. Fink, M. Mehring and S Roth., Eds., *AIP Conf. Proc.* **685**, page 219–224 (2003).

W. TU, K. TAKAI, K. FUKUI, A. MIYAZAKI and T. ENOKI, "Interface Effect on the Electronic Structure of Alkanethiol-Coated Platinum Nanoparticles," *J. Phys. Chem. B* **107**, 10134–10140 (2003).

K. HARIGAYA, Y. KOBAYASHI, N. KAWATSU, K. TAKAI, H. SATO, J. RAVIER, T. ENOKI and M. ENDO, "Tuning Magnetism and Novel Electronic Wave Interference Patterns in Nanographite Materials," *Physica E* **22**, 708–711 (2004).

M. SUZUKI, I. SUZUKI, T. MONYANGO and T. ENOKI, "Magnetic Phase Diagram of Three-Dimensional Diluted Ising Antiferromagnet $\text{Ni}_{0.8}\text{Mg}_{0.2}(\text{OH})_2$," *J. Phys. Soc. Jpn.* **73**, 206–215 (2004).

Y. KOBAYASHI, K. TAKAI, K. FUKUI, T. ENOKI, K. HARIGAYA, Y. KABURAGI and Y. HISHIYAMA, "STM Observation of Electronic Wave Interference Effect in Finite-Sized Graphite with Distortion-Network Structures," *Phys. Rev. B* **69**, 035418 (7 pages) (2004).

Y. KOBAYASHI, K. TAKAI, K. FUKUI, T. ENOKI, K. HARIGAYA, Y. KABURAGI and Y. HISHIYAMA, "STM Observation of the Quantum Interference Effect in Finite-Sized Graphite," *J. Phys. Chem. Solids* **65**, 199–203 (2004).

K. HARIGAYA, A. YAMASHIRO, Y. SHIOMI, K. WAKABAYASHI, Y. KOBAYASHI, N. KAWATSU, H. SATO, J. RAVIER, T. ENOKI and M. ENDO, "Theoretical Study on Novel Electronic Properties in Nanographite Materials," *J. Phys. Chem. Solids* **65**, 123–126 (2004).

J. NISHIJO, A. MIYAZAKI and T. ENOKI, "Structure and Physical Properties of Molecular Magnets Based on Transition Metal Complexes of Crown Thioether," *Bull. Chem. Soc. Jpn.* **77**, 715–727 (2004).

K. TAKAI, M. OGA, T. ENOKI and A. TAOMOTO, "Effect of Heat-Treatment on Magnetic Properties of Non-Graphitic Disordered Carbon," *Diamnod Rel. Mater.* **13**, 1469–1473 (2004).

T. ENOKI, Y. YOKOTA, R. YUGE, W. TU, A. MIYAZAKI, K. TAKAI and K. FUKUI, "Development of TTF-Based Self-Assembled Monolayer Systems and Their Electronic Properties," *J. Phys. IV France* **114**, 667–671 (2004).

A. MIYAZAKI, M. AIMATSU, H. YAMAZAKI, T. ENOKI, K. UGAWA, E. OGURA, Y. KUWATANI and M. IYODA, "Crystal Structure and Physical Properties of $(\text{EDO-TTFBr}_2)_2\text{FeX}_4$ (X = Cl, Br)," *J. Phys. IV France* **114**, 545–547 (2004).

J. NISHIJO, A. MIYAZAKI, T. ENOKI, R. WATANABE, Y. KUWATANI and M. IYODA, "Strong π -d Interaction Based on Brominated TTF-type Donor EDT-TTFBr₂," *J. Phys. IV France* **114**, 561–563 (2004).

L. G. CAN ADO, M. A. PIMENTA, B. R. A. NEVES, G. MEDEIROS-RIBEIRO, T. ENOKI, Y. KOBAYASHI, K. TAKAI, K. FUKUI, M. S. DRESSELHAUS, R. SAITO and A. JORIO, "Anisotropy of the Raman Spectra of Nanographite Ribbons," *Phys. Rev. Lett.* **93**, 047403 (4 pages) (2004).

T. NAITO, T. INABE, T. AKUTAGAWA, T. HASEGAWA and T. NAKAMURA, "ET₃(MnCl₃)₂(EtOH)₂: a New Organic Conductor with a Perovskite Structure," *Synth. Met.* **133-134**, 445–447 (2003).

T. INABE, T. ASARI, H. HASEGAWA, M. MATSUDA, E. H. GACHO, N. MATSUMURA, S. TAKEDA, K. TAKEDA and T. NAITO, "Phthalocyanine-Based Multi-Dimensional Conductors," *Synth. Met.* **133-134**, 515–518 (2003).

N. HANASAKI, M. MATSUDA, H. TAJIMA, T. NAITO and T. INABE, "One-Dimensional π -d Electron System in $\text{TPP}[\text{Fe}(\text{Pc})(\text{CN})_2]_2$, $[\text{PXX}][\text{Fe}(\text{Pc})(\text{CN})_2]$, and $(\text{PTMA})_x[\text{Fe}(\text{Pc})(\text{CN})_2]_y(\text{CH}_3\text{CN})$: Electron Spin Resonance and Negative Magnetoresistance," *Synth. Met.* **133-134**, 519–521 (2003).

M. MATSUDA, N. HANASAKI, H. TAJIMA, T. NAITO and T. INABE, "Magnetic and Optical Properties of One-Dimensional π -d System with Axially Substituted Iron(III) Phthalocyanine," *Synth. Met.* **133-134**, 547–548 (2003).

- M. MATSUDA, N. HANASAKI, H. TAJIMA, F. SAKAI, T. NAITO and T. INABE**, "Magnetic Properties of d - π Conducting System, $\text{TPP}[\text{Fe}^{\text{III}}_x\text{Co}^{\text{III}}_{1-x}(\text{Pc})(\text{CN})_2]_2$," *Synth. Met.* **135-136**, 635–636 (2003).
- T. NAITO, T. INABE, T. AKUTAGAWA, T. HASEGAWA, T. NAKAMURA, Y. HOSOKOSHI and K. INOUE**, "Physical Properties of $(\text{ET})_3(\text{MnCl}_4)(\text{TCE})$ and the Related Salts," *Synth. Met.* **135-136**, 613–614 (2003).
- N. HANASAKI, M. MATSUDA, H. TAJIMA, T. NAITO and T. INABE**, "Torque Study of $\text{TPP}[\text{Fe}(\text{Pc})(\text{CN})_2]_2$ (TPP = Tetraphenyl Phosphonium and Pc = Phthalocyanine)," *Synth. Met.* **137**, 1227–1228 (2003).
- N. KOBAYASHI, T. NAITO and T. INABE**, "Hydrogen-Bond Networks of Mellitate Anions ($[\text{C}_6(\text{COO})_6\text{H}_{6-n}]^{n-}$) in Salts with Pyridine Derivatives," *Bull. Chem. Soc. Jpn.* **76**, 1351–1362 (2003).
- M. MATSUDA, T. ASARI, T. NAITO, T. INABE, N. HANASAKI, and H. TAJIMA**, "Structural and Physical Properties of Low-Dimensional Molecular Conductors, $[\text{PXX}][\text{Fe}^{\text{III}}(\text{Pc})(\text{CN})_2]$ and $[\text{PXX}][\text{Co}^{\text{III}}(\text{Pc})(\text{CN})_2]$ (PXX = *peri*-xanthenoxanthene, Pc = phthalocyaninato)," *Bull. Chem. Soc. Jpn.* **76**, 1935–1940 (2003).
- T. NAITO and T. INABE**, "Molecular Hexagonal Perovskite: a New Type of Organic-Inorganic Hybrid Conductor," *J. Solid State Chem.* **176**, 243–249 (2003).
- A. E. KOVALEV, S. HILL, K. KAWANO, M. TAMURA, T. NAITO and H. KOBAYASHI**, "Angle-Resolved Mapping of the Fermi Velocity in a Quasi-Two-Dimensional Organic Conductor," *Phys. Rev. Lett.* **91**, 216402 (2003).
- N. HANASAKI, M. MATSUDA, H. TAJIMA, T. NAITO and T. INABE**, "Contribution of Degenerate Molecular Orbitals to Molecular Orbital Angular Momentum in Molecular Magnet $\text{Fe}(\text{Pc})(\text{CN})_2$," *J. Phys. Soc. Jpn.* **72**, 3226–3230 (2003).
- T. ASARI, T. NAITO, T. INABE, M. MATSUDA and H. TAJIMA**, "Novel Phthalocyanine Conductor Containing Two-Dimensional Pc Stacks, $[\text{PXX}]_2[\text{Co}(\text{Pc})(\text{CN})_2]$ (PXX = *peri*-Xanthenoxanthene, $\text{Co}(\text{Pc})(\text{CN})_2$ = Dicyano(phthalocyaninato)cobalt(III))," *Chem. Lett.* **33**, 128–129 (2004).
- M. MATSUDA, N. HANASAKI, H. TAJIMA, T. NAITO and T. INABE**, "Anisotropic Giant Magnetoresistance Originating from the π - d Interaction in a Molecule," *J. Phys. Chem. Solids* **65**, 749–752 (2004).
- T. NAITO and T. INABE**, "Molecular Conductors Containing Photoreactive Species," *J. Phys. IV France* **114**, 553–555 (2004).
- M. MATSUDA, N. HANASAKI, S. IKEDA, H. TAJIMA, T. NAITO and T. INABE**, "Molecular Unit Based on Metal Phthalocyanine; Designed for Molecular Electronics," *J. Phys. IV France* **114**, 541–543 (2004).
- T. INABE, N. KOBAYASHI and T. NAITO**, "Crystal Design of Cation-Radical Salts Based on the Supramolecular Self-Organizing Arrangement of Mellitate Anions," *J. Phys. IV France* **114**, 449–453 (2004).
- N. KOBAYASHI, T. NAITO and T. INABE**, "Network Formation of Mellitate Anions ($[\text{C}_6(\text{COO})_6\text{H}_{6-n}]^{n-}$) in the Salts with Piperidinium Derivatives and *o*-Phenylenediammonium," *CrystEngComm* **6**, 189–196 (2004).

Department of Applied Molecular Science

- N. ASAKUMA, T. FUKUI, M. TOKI, K. AWAZU and H. IMAI**, "Photoinduced Hydroxylation at ZnO Surface," *Thin Solid Films* **445**, 284–287 (2003).
- K. AWAZU**, "Ablation and Compaction of Amorphous SiO_2 Irradiated with ArF Excimer Laser," *J. Non-Cryst. Solids* **337**, 241–253 (2004).
- R. DAVYDOV, T. MATSUI, H. FUJII, M. IKEDA-SAITO and B. M. HOFFMAN**, "Kinetic Isotope Effects on the Rate-Limiting Step of Heme Oxygenase Catalysis Indicate Concerted Proton Transfer/Heme Hydroxylation," *J. Am. Chem. Soc.* **125**, 16208–16209 (2003).
- A. -L. BULTEAU, M. IKEDA-SAITO and L. I. SZWEDA**, "Modulation of Mitochondrial Aconitase Activity in Response to Changes in Redox Status," *Biochemistry* **42**, 14846–14855 (2003).
- S. HIROTSU, G. C. CHU, M. UNNO, D. -S. LEE, T. YOSHIDA, T. S. -Y. PARK, Y. SHIRO and M. IKEDA-SAITO**, "The Crystal Structures of the Ferric and Ferrous Forms of the Heme Complex of HmuO, a Heme Oxygenase of *Corynebacterium diphtheriae*," *J. Biol. Chem.* **279**, 11937–11947 (2004).
- M. UNNO, M. MATSUI, G. C. CHU, M. COUTURE, T. YOSHIDA, D. L. ROUSSEAU, J. S. OLSON and M. IKEDA-SAITO**, "Crystal Structure of the Dioxygen-Bound Heme Oxygenase from *Corynebacterium diphtheriae*: Implications for Heme Oxygenase Function," *J. Biol. Chem.* **279**, 21055–21061 (2004).
- H. SUZUKI, H. TASHIO, S. HIRA, J. SUN, C. YAMAZAKI, Y. ZENKA, M. IKEDA-SAITO, M. YOSHIDA and K. IGARASHI**, "Heme Regulates Gene Expression by Triggering Crml-Dependent Nuclear Export of Bach1," *EMBO J.* **23**, 2544–2553 (2004).
- A. -L. BULTEAU, H. A. O'NEILL, M. C. KENNEDY, M. IKEDA-SAITO, G. ISAYA and L. I. SZWEDA**, "Fratxin: An Iron Chaperone Protein Required for Mitochondrial Aconitase Reactivation and Prevention of [4Fe–4S] Cluster Disassembly," *Science* **305**, 242–245 (2004).

Department of Vacuum UV Photoscience

- T. HATSUI, E. SHIGEMASA and N. KOSUGI**, "Design of a Transmission Grating Spectrometer and an Undulator Beamline for Soft X-Ray Emission Studies," *AIP Conf. Proc.* **705**, 921–924 (2004).
- N. KOSUGI**, "Spin-Orbit and Exchange Interactions in Molecular Inner Shell Spectroscopy," *J. Electron Spectrosc. Relat. Phenom.* **137-140**, 335–343 (2004).
- S. MASUDA, T. HATSUI and N. KOSUGI**, "Spin-Forbidden Shake-Up States of OCS Molecule Studied by Resonant Photoelectron Spectroscopy," *J. Electron Spectrosc. Relat. Phenom.* **137-140**, 351–355 (2004).
- T. HATSUI T, M. NAGASONO and N. KOSUGI**, "Ar 2p Excited States of Argon in Non-Polar Media," *J. Electron Spectrosc. Relat. Phenom.* **137-140**, 435–439 (2004).
- T. HATSUI and N. KOSUGI**, "Metal-to-Ligand Charge Transfer in Polarized Metal L-Edge X-Ray Absorption of Ni and Cu Complexes," *J. Electron Spectrosc. Relat. Phenom.* **136**, 67–75 (2004).
- T. HATSUI, T. YAMAMOTO, H. TAJIMA and N. KOSUGI**, "Cu L₂, L₃-Edge X-Ray Absorption Spectra of (2,5-Dimethyl-*N,N'*-Dicyanoquinonediimine)₂Li_{1-x}Cu_x Alloys," *Chem. Phys.* **298**, 189–193 (2004).
- H. S. KATO, M. FURUKAWA, M. KAWAI, M. TANIGUCHI, T. KAWAI, T. HATSUI and N. KOSUGI**, "Electronic Structure of Bases in DNA Duplexes Characterized by Resonant Photoemission Spectroscopy Near the Fermi Level," *Phys. Rev. Lett.* **93**, 086403 (4 pages) (2004).
- A. HISHIKAWA, H. HASEGAWA and K. YAMANOUCHI**, "Nuclear Dynamics on the Light-Dressed Potential Energy Surface of CS₂ by Coincidence Momentum Imaging," *Chem. Phys. Lett.* **388**, 1–6 (2004).
- A. HISHIKAWA, H. HASEGAWA and K. YAMANOUCHI**, "Hydrogen Migration in Acetonitrile in Intense Laser Fields Studied by Coincidence Momentum Imaging," *Phys. Scr.* **T108**, 108–111 (2004).
- Y. NONOGAKI, M. KATOH, E. SHIGEMASA, K. MATSUSHITA, M. SUZUI and T. URISU**, "Design and Performance of Undulator Beamline (BL7U) For In-Situ Observation of Synchrotron Radiation Stimulated Etching by STM," *AIP Conf. Proc.* **705**, 368–371 (2004).
- R. TERO, M. TAKIZAWA, Y. -J. LI, M. YAMAZAKI and T. URISU**, "Lipid Membrane Formation by Vesicle Fusion on Silicon Dioxide Surfaces Modified with Alkyl Self-Assembled-Monolayer Islands," *Langmuir* **20**, 7526–7531 (2004).
- Z. -H. WANG, T. URISU, S. NANBU, J. MAKI, G. RANGA RAO, M. AOYAGI, H. WATANABE and K. OOI**, "Three Pairs of Doublet Bands Assigned to SiH₂ Scissoring Modes Observed in H₂O-induced Oxidation of Si(100) Surfaces," *Phys. Rev. B* **69**, 045309 (5 pages) (2004).
- Y. -J. LI, R. TERO, T. NAGASAWA, T. NAGATA, Y. HARUYAMA and T. URISU**, "Structure and Deposition Mechanism of 10-Undecenoic Acid Self-Assembled Layers on H-Si(111) Surfaces Studied by AFM and FT-IR," *Jpn. J. Appl. Phys.* **43**, 4591–4594 (2004).
- M. TAKIZAWA, Y. -H. KIM and T. URISU**, "Deposition Of DPPC Monolayers by the Langmuir-Blodgett Method on SiO₂ Surfaces Covered by Octadecyltrichlorosilane Self-Assembled Monolayer Islands," *Chem. Phys. Lett.* **385**, 220–224 (2004).
- S. FUJIKI, Y. KUBOZONO, T. HOSOKAWA, T. KANBARA, A. FUJIWARA, Y. NONOGAKI and T. URISU**, "Scanning Tunneling Microscopy of Dy@C₈₂ and Dy@C₆₀ adsorbed on Si (111)-(7×7) Surfaces," *Phys. Rev. B* **69**, 045415 (5 pages) (2004).
- MD. M. RAHMAN, R. TERO and T. URISU**, "Shrinking of Spin-on-Glass Films Induced by Synchrotron Radiation and Its Application to the Three-Dimensional Microfabrications," *Jpn. J. Appl. Phys.* **43**, 3941–3944 (2004).
- Y. -H. KIM, R. TERO, M. TAKIZAWA and T. URISU**, "Characterization of Dipalmitoylphosphatidylcholine/Cholesterol Langmuir-Blodgett Monolayers Investigated by AFM and FT-IR," *Jpn. J. Appl. Phys.* **43**, 3860–3864 (2004).
- K. FUKUI, S. TAKAKUSAGI, R. TERO, M. AIZAWA, Y. NAMAI and Y. IWASAWA**, "Dynamic Aspects and Associated Structures of TiO₂(110) and CeO₂(111) Surfaces Relevant to Oxide Catalyses," *Phys. Chem. Chem. Phys.* **5**, 5349–5359 (2003).
- H. WATANABE, S. NANBU, Z. -H. WANG, J. MAKI, T. URISU, M. AOYAGI and K. OOI**, "Theoretical Analysis of the Oxygen Insertion Process in the Oxidation Reactions of H₂O+H/Si(100) and 2H+H₂O/Si(100): a Molecular Orbital Calculation and an Analysis of Tunneling Reaction," *Chem. Phys. Lett.* **383**, 523–527 (2004).
- T. KANBARA, K. SHIBATA, S. FUJIKI, Y. KUBOZONO, S. KASHINO, T. URISU, M. SAKAI, A. FUJIWARA, R. KUMASHIRO and K. TANIGAKI**, "N-Channel Field Effect Transistors with Fullerene Thin Films and their Application to a Logic Gate Circuit," *Chem. Phys. Lett.* **379**, 223–229 (2003).
- M. ONO and K. MITSUKE**, "Kinetic Energy Distribution and Anisotropy of Fragment Ions from SF₆ by Photoexcitation of a Sulfur 2p-Electron," *Chem. Phys. Lett.* **379**, 248–254 (2003).
- J. KOU, T. MORI, S. V. K. KUMAR, Y. HARUYAMA, Y. KUBOZONO and K. MITSUKE**, "Double Photoionization of C₆₀ and C₇₀ in the Valence Region," *J. Chem. Phys.* **120**, 6005–6009 (2004).
- Y. HIKOSAKA and K. MITSUKE**, "Autoionization and Neutral Dissociation of Superexcited HI Studied by Two-Dimensional Photoelectron Spectroscopy," *J. Chem. Phys.* **121**, 792–799 (2004).

Department of Computational Molecular Science

S. MIURA and J. TANAKA, "Path Integral Hybrid Monte Carlo Algorithm for Correlated Bose Fluids," *J. Chem. Phys.* **120**, 2160–2168 (2004).

A. MORITA, M. SUGIYAMA, H. KAMEDA, S. KODA and D. R. HANSON, "Mass Accommodation Coefficient of Water: Molecular Dynamics Simulation and Revised Analysis of Droplet Train/Flow Reactor Experiment," *J. Phys. Chem. B* **108**, 9111–9120 (2004).

A. MORITA, Y. KANAYA and J. S. FRANCISCO, "Uptake of the HO₂ Radical by Water: Molecular Dynamics Calculations and Their Implications to Atmospheric Modeling," *J. Geophys. Res.* **109**, D09201, 10.1029/2003JD004240 (2004).

D. R. HANSON, M. SUGIYAMA and A. MORITA, "Revised Kinetics in the Droplet Train Apparatus Due to a Wall Loss," *J. Phys. Chem. A* **108**, 3739–3744 (2004).

I. TOKUE, K. YAMASAKI and S. NANBU, "He (2³S) Penning Ionization of H₂S I. Theoretical Franck-Condon Factors for the H₂S (X¹A₁, v' = 0) → H₂S⁺ (X²B₁, A²A₁) Ionization and the H₂S⁺ (A–X) Transition," *J. Chem. Phys.* **119**, 5874–5881 (2003).

I. TOKUE, K. YAMASAKI and S. NANBU, "He (2³S) Penning Ionization of H₂S II. Formation of the SH⁺(A³Π) and H₂S⁺ (A²A₁) Ions," *J. Chem. Phys.* **119**, 5882–5888 (2003).

Z. -H. WANG, T. URISU, S. NANBU, J. MAKI, M. AOYAGI, H. WATANABE and K. OOI, "Three Pairs of Doublet Bands Assigned to Scissors Modes of SiH₂ on Si(100) Surfaces Observed in Several H₂O-Induced Oxidation systems," *Phys. Rev. B* **69**, 045309 (5 pages) (2004).

H. WATANABE, S. NANBU, J. MAKI, Z. -H. WANG, T. URISU, M. AOYAGI and K. OOI, "Theoretical Analysis of the Oxygen Insertion Process in the Reaction of H₂O with H-Terminated Si(100) Surface," *Chem. Phys. Lett.* **383**, 523–527 (2004).

J. -I. CHOE, S. H. LEE, D. -S. OH, S. -K. CHANG and S. NANBU, "Ab Initio Study of Complexation Behavior of p-Tert-Butylcalix[5]arene Derivative toward Alkyl Ammonium Cations," *Bull. Korean Chem. Soc.* **25**, 190–194, (2004).

Coordination Chemistry Laboratories

M. UMEMIYA, K. GOTO, S. TAKAISHI, H. MIYASAKA, K. SUGIURA, M. YAMASHITA, H. NISHIKAWA, K. KIKUCHI, I. IKEMOTO, Y. YOKOCHI, H. ITO and S. KURODA, "New Organic Conductor (DMET)₂CuCl₂: Synthesis, Structure and Physical Properties," *J. Phys. IV France* **114**, 589–590 (2004).

H. MIYASAKA, K. NAKATA, K. SUGIURA, M. YAMASHITA and R. CLÉRAC, "A Three-Dimensional Ferrimagnet Composed of Mixed-Valence Mn₄ Clusters Linked by an {Mn[N(CN)₂]₆}⁴⁻ Unit," *Angew. Chem., Int. Ed.* **43**, 707–711 (2004).

H. MIYASAKA, R. CLÉRAC, W. WERNSDORFER, L. LECREN, C. BONHOMME, K. SUGIURA and M. YAMASHITA, "A Dimeric Manganese(III) Tertadentate Schiff Base Complexes as a Single-Molecular Magnet," *Angew. Chem., Int. Ed.* **43**, 2801–2805 (2004).

H. MATSUZAKI, K. IWANO, T. AIZAWA, M. ONO, H. KISHIDA, M. YAMASHITA and H. OKAMOTO, "Tuning the Electronic Structure from Charge-Transfer Insulator to Mott-Hubbard and Peierls Insulators in One-Dimensional Halogen-Bridged Mixed-Metal Compounds," *Phys. Rev. B* **70**, 035204 (6 pages) (2004).

A. KATO, K. SUGIURA, H. MIYASAKA, H. TANAKA, T. KAWAJI, M. SUGIMOTO and M. YAMASHITA, "A Square Cyclic Porphyrin Dodecamer: Synthesis and Single-Molecule Characterization," *Chem. Lett.* **33**, 578–579 (2004).

S. TAKAISHI, H. MIYASAKA, K. SUGIURA, M. YAMASHITA, H. MATSUZAKI, H. KISHIDA, H. OKAMOTO, H. TANAKA, K. MARUMOTO, H. ITO, S. KURODA and T. TAKAMI, "Visualization of Local Valence Structure in Quasi-One-Dimensional Halogen-Bridged Complexes [Ni_{1-x}Pd_x(chxn)₂Br]Br₂ by STM," *Angew. Chem., Int. Ed.* **43**, 3171–3175 (2004).

S. TAKEMOTO, S. OSHIO, T. KOBAYASHI, H. MATSUZAKA, M. HOSHI, H. OKIMURA, M. YAMASHITA, H. MIYASAKA, T. ISHII and M. YAMASHITA, "A Dinuclear Ruthenium(II) Chelating Amido Complex: Synthesis, Characterization, and Coupling Reaction with Carbon Monoxide," *Organometallics* **23**, 3587–3589 (2004).

T. OSHIKI, K. TANAKA, J. YAMADA, T. ISHIYAMA, Y. KATAOKA, K. MASHIMA, K. TANI and K. TAKAI, "Synthesis, Structural Characterization, and Reactions of Tantalum-Alkyne Complexes TaCl₃(R¹C≡CR²)L₂ (L₂ = DME, Bipy, and TMEDA; L = Py)," *Organometallics* **22**, 464–472 (2003).

K. MASHIMA, D. SHIMIZU, T. YAMAGATA and K. TANI, "Unique Ring-Methyl Deprotonation of η⁴-1,2-Dimethyl-3,4-di(*tert*-butyl)cyclobutadiene Complexes of Palladium(II) Bearing Phosphine Ligand," *Inorg. Chim. Acta (Special Issue dedicated to Professor M. A. Bennett)* **352**, 105–109 (2003).

R. Y. C. SHIN, M. A. BENNETT, L. Y. GOH, W. CHEN, D. V. R. HOCKLESS, W. K. LEONG, K. MASHIMA and A. C. WILLIS, "Arene-Ruthenium Complexes of an Acyclic Thiolate-Thioether and Tridentate Thioether Derivatives Resulting from Ring-Closure Reactions," *Inorg. Chem.* **42**, 96–106 (2003).

H. TSURUGI, T. YAMAGATA, K. TANI and K. MASHIMA, "Unusual Enhancement of Ethylene Polymerization Activity of Benzyl Zirconium Complexes by Benzoylation of the Imino Moiety of 2-(*N*-Aryliminomethyl)pyrrolyl Ligand," *Chem. Lett.* **32**, 756–757 (2003).

K. MASHIMA, H. YONEKURA, T. YAMAGATA and K. TANI, "Synthesis, Characterization, and Reactions of a Half-Metallocene Benzylidene Complex of Tantalum Bearing 2,3-Dimethyl-1,3-Butadiene and Pentamethylcyclopentadienyl Ligands," *Organometallics* **22**, 3766–3772 (2003).

Y. MATSUO, H. TSURUGI, T. YAMAGATA, K. TANI and K. MASHIMA, "Synthesis and Structural Characterization of 2,5-Bis(*N*-aryliminomethyl)pyrrolyl Complexes of Aluminum," *Bull. Chem. Soc. Jpn.* **76**, 1965–1968 (2003).

H. TSURUGI, T. YAMAGATA and K. MASHIMA, "Intramolecular Benzoylation of an Imino Group of Tridentate 2,5-Bis(*N*-aryliminomethyl)pyrrolyl Ligands Bound to Zirconium and Hafnium Gives Amido-Pyrrolyl Complexes That Catalyze Ethylene Polymerization," *Organometallics* **23**, 2797–2805 (2004).

T. ASAUMI, N. CHATANI, T. MATSUO, F. KAKIUCHI and S. MURAI, "Ruthenium-Catalyzed C–H/CO/Olefin Coupling Reaction of *N*-Arylpyrazoles. Extraordinary Reactivity of *N*-Arylpyrazoles toward Carbonylation at C–H Bonds," *J. Org. Chem.* **68**, 7538–7540 (2003).

F. KAKIUCHI, M. MATSUMOTO, K. TSUCHIYA, K. IGI, T. HAYAMIZU, N. CHATANI and S. MURAI, "The Ruthenium-Catalyzed Silylation of Aromatic C–H Bonds with Triethylsilane," *J. Organomet. Chem.* **686**, 133–144 (2003).

K. YOKOTA, H. TATAMIDANI, Y. FUKUMOTO and N. CHATANI, "A Chelation-Assisted Hydroesterification of Alkenes Catalyzed by Rhodium Complex," *Org. Lett.* **5**, 4329–4331 (2003).

F. KAKIUCHI, M. USUI, S. UENO, N. CHATANI and S. MURAI, "The Ruthenium-Catalyzed Functionalization of Aryl Carbon–Oxygen Bonds in Aromatic Ethers with Organoboron Compounds," *J. Am. Chem. Soc.* **126**, 2706–2707 (2004).

T. ASAUMI, T. MATSUO, T. FUKUYAMA, Y. IE, F. KAKIUCHI and N. CHATANI, "Ruthenium- and Rhodium-Catalyzed Direct Carbonylation of the *Ortho* C–H Bonds in the Benzene Ring of *N*-Arylpyrazoles," *J. Org. Chem.* **69**, 4433–4440 (2004).

H. TATAMIDANI, K. YOKOTA, F. KAKIUCHI and N. CHATANI, "Catalytic Cross-Coupling Reaction of Esters with Organoboron Compounds and Decarbonylative Reduction of Esters with HCOONH₄: A New Route to Acyl Transition Metal Complexes through the Cleavage of Acyl–Oxygen Bonds in Esters," *J. Org. Chem.* **69**, 5615–5621 (2004).

D. OYAMA, T. KOBAYASHI, K. SHIREN and K. TANAKA, "Regulation of Electron Donating Ability to Metal Center: Isolation and Characterization of Ruthenium Carbonyl Complexes with *N,N*- and/or *N,O*-Donor Polypyridyl Ligands," *J. Organomet. Chem.* **665**, 107–113 (2003).

H. SUGIMOTO, K. SHIREN, H. TSUKUBE and K. TANAKA, "Mono-Dithiolene Molybdenum(IV) Complexes of *cis*-1,2-Dicyano-1,2-Ethylenedithiolate (mnt²⁻): New Models for Molybdenum Enzymes," *Eur. J. Inorg. Chem.* **14**, 2633–2638 (2003).

K. KOBAYASHI, H. OHTSU, T. WADA and K. TANAKA, "Characterization of a Stable Ruthenium Complex with an Oxyl Radical," *J. Am. Chem. Soc.* **125**, 6729–39 (2003).

T. KOIZUMI, T. TOMON and K. TANAKA, "Synthesis, Structures and Fluxional Behavior of Ruthenium(II) Complexes Bearing a Bidentate 1,8-Naphthyridine Ligand," *Bull. Chem. Soc. Jpn.* **76**, 1969–1975 (2003).

T. KOIZUMI, K. TSUTSUI and K. TANAKA, "Selective Formation of Inter- and Intramolecular A–D–A π - π Stacking: Solid-State Structures of Bis(pyridiniopropyl)benzenes," *Eur. J. Org. Chem.* **23**, 4528–4532 (2003).

H. OHTSU and K. TANAKA, "Equilibrium of Low- and High-Spin States of Ni(II) Complexes Controlled by the Donor Ability of the Bidentate Ligands," *Inorg. Chem.* **43**, 3024–30 (2004).

T. FUJIHARA, T. WADA and K. TANAKA, "Acid-Base Equilibria of Various Oxidation States of Aqua-Ruthenium Complexes with 1,10-Phenanthroline-5,6-Dione in Aqueous Media," *Dalton Trans.* 645–52 (2004).

T. FUJIHARA, T. WADA and K. TANAKA, "Syntheses and Electrochemical Properties of Ruthenium(II) Complexes with 4,4'-Bipyrimidine and 4,4'-Bipyrimidinium Ligands," *Inorg. Chim. Acta* **357**, 1205–1212 (2004).

T. WADA, T. FUJIHARA, T. MIZUNO, D. OYAMA and K. TANAKA, "Strong Interaction between Carbonyl and Dioxolene Ligands Caused by Charge Distribution of Ruthenium-Dioxolene Frameworks of Mono- and Dicarbonylruthenium Complexes," *Bull. Chem. Soc. Jpn.* **77**, 741–749 (2004).

T. KOIZUMI and K. TANAKA, "Synthesis and Crystal Structures of Mono- and Dinuclear Silver(I) Complexes Bearing 1,8-Naphthyridine Ligand," *Inorg. Chim. Acta* **357**, 3666–3672 (2004).

H. SUGIMOTO, K. SATO, T. TAKEI and K. TANAKA, "Unprecedented Sequential Deprotonation of Ruthenium-Aqua Framework Affording Ruthenium-Oxo-Dithiolene Complex," *Chem. Lett.* 1082–1083 (2004).

H. KAWAGUCHI and T. MATSUO, "Aryl–Oxygen Bond Cleavage by a Trihydride-Bridging Ditantalum Complex," *J. Am. Chem. Soc.* **125**, 14254–14255 (2003).

T. MATSUO and H. KAWAGUCHI, "Triple Hydrogen Bridged Ditungsten(III) and Dizirconium(IV) Aryloxide Complexes," *Organometallics* **22**, 5379–5381 (2003).

M. YUKI, T. MATSUO and H. KAWAGUCHI, "Formation of an Iron(II) Carbene Thiolato Complex *via* Insertion of Carbon Monoxide into Si–C Bond," *Angew. Chem., Int. Ed.* **43**, 1404–1407 (2004).

T. KOMURO, T. MATSUO, H. KAWAGUCHI and K. TATSUMI, "Synthesis and Structural Characterization of Silanethiolato Complexes Having *tert*-Butyldimethylsilyl and Trimethylsilyl Groups," *Dalton Trans.* 1618–1625 (2004).

T. MATSUO and H. KAWAGUCHI, "Tridentate Aryloxide Ligands: New Supporting Ligands in Coordination Chemistry of Early Transition Metals," *Chem. Lett.* **33**, 640–645 (2004).

S. TAKEMOTO, T. KOBAYASHI and H. MATSUZAKA, "Reactivity of Amido Ligands on a Dinuclear Ru(II) Center: Formation of Imido Complexes and C–N Coupling Reaction with Alkyne," *J. Am. Chem. Soc.* **126**, 10802–10803 (2004).

S. TAKEMOTO, S. OSHIO, T. KOBAYASHI, H. MATSUZAKA, M. HOSHI, H. OKIMURA, M. YAMASHITA, H. MIYASAKA, T. ISHII and M. YASHITA, "A Dinuclear Ru(II) Chelating Amido Complex: Synthesis, Characterization, and Coupling Reaction with Carbon Monoxide," *Organometallics* **23**, 3587–3589 (2004).

K. UENO, T. WATANABE and H. OGINO, "Synthesis, Structure, and Reactivity of Cationic Base-Stabilized Gallyleneiron Complexes," *Appl. Organomet. Chem.* **17**, 403–408 (2003).

K. UENO, T. WATANABE, H. TOBITA and H. OGINO, "Synthesis and Structure of the First Dinuclear Complex Bridged by a Substituent-Free Gallium Atom," *Organometallics* **22**, 4375–4377 (2003).

H. TOBITA, A. MATSUDA, H. HASHIMOTO, K. UENO and H. OGINO, "Direct Evidence for Extremely Facile 1,2- and 1,3-Group-Migrations on an FeSi₂ System," *Angew. Chem., Int. Ed.* **43**, 221–224 (2004).

B. A. S. MOHAMED, M. KIKUCHI, H. HASHIMOTO, K. UENO, H. TOBITA and H. OGINO, "Synthesis and Characterization of Triplet Germylene-Bridged Diiron Complexes and Singlet Stannylene-Bridged Diiron Complexes," *Chem. Lett.* **33**, 112–113 (2004).

Laser Research Center for Molecular Science

H. TAKAHASHI, A. QUEMA, M. GOTO, S. ONO and N. SARUKURA, "Terahertz Radiation Mechanism from Femtosecond-Laser-Irradiated InAs (100) Surface," *Jpn. J. Appl. Phys.* **42**, L1259–L1261 (2003).

H. TAKAHASHI, M. P. HASSELBECK, A. QUEMA, M. GOTO, S. ONO and N. SARUKURA, "Broadband Terahertz Radiation Emitter Using Femtosecond-Laser-Irradiated *n*-Type InAs under Magnetic Field," *Jpn. J. Appl. Phys.* **43**, L221–L223 (2004).

M. GOTO, A. QUEMA, H. TAKAHASHI, S. ONO and N. SARUKURA, "Teflon Photonic Crystal Fiber as Terahertz Waveguide," *Jpn. J. Appl. Phys.* **43**, L317–L319 (2004).

J. B. SHIM, A. YOSHIKAWA, T. FUKUDA, J. PEJCHAL, M. NIKL, N. SARUKURA and D. H. YOON, "Growth and Charge Transfer Luminescence of Yb³⁺-Doped YAlO₃ Single Crystals," *J. Appl. Phys.* **95**, 3063–3068 (2004).

H. TAKAHASHI, M. SAKAI, A. QUEMA, S. ONO, N. SARUKURA, G. NISHIJIMA and K. WATANABE, "Terahertz Radiation from InAs with Various Surface Orientations under Magnetic Field Irradiated with Femtosecond Optical Pulses at Different Wavelengths," *J. Appl. Phys.* **95**, 4545–4550 (2004).

M. YAMAGA, S. YABASHI, Y. MASUI, M. HONDA, H. TAKAHASHI, M. SAKAI, N. SARUKURA, J. -P. R. WELLS and G. D. JONES, "Optical, Infrared and EPR Spectroscopy of CaF₂:Ce³⁺ Crystals Co-Doped with Li⁺ or Na⁺," *J. Lumin.* **108**, 307–311 (2004).

H. TAKAHASHI, M. P. HASSELBECK, A. QUEMA, M. GOTO, S. ONO and N. SARUKURA, "Effect of Ultrafast Optical Pulses with Different Pulse Duration on the Terahertz Radiation Spectrum of *n*-Type InAs," *Jpn. J. Appl. Phys.* **43**, L746–L748 (2004).

H. TAKAHASHI, A. QUEMA, M. GOTO, S. ONO, N. SARUKURA, G. NISHIJIMA and K. WATANABE, "Physical Origin of Magnetically Induced Periodic Structure Observed in Terahertz Radiation Spectrum Emitted from InAs," *Jpn. J. Appl. Phys.* **43**, L1017–L1019 (2004).

R. E. OUENZERFI, S. ONO, A. QUEMA, M. GOTO, N. SARUKURA, T. NISHIMATSU, N. TERAOKUBO, H. MIZUSEKI, Y. KAWAZOE, A. YOSHIKAWA and T. FUKUDA, "Design Proposal of Light Emitting Diode in Vacuum Ultraviolet Based on Perovskite-Like Fluoride Crystals," *Jpn. J. Appl. Phys.* **43**, L1140–L1143 (2004).

K. MIZUUCHI, A. MORIKAWA, T. SUGITA, K. YAMAMOTO, N. PAVEL, I. SHOJI and T. TAIRA, "High-Power Continuous Wave Green Generation by Single-Pass Frequency Doubling of a Nd:GdVO₄ Laser in a Periodically Poled MgO:LiNbO₃ Operating at Room Temperature," *Jpn. J. Appl. Phys.* **42**, L1296–L1298 (2003).

V. LUPEI, N. PAVEL and T. TAIRA, "Basic Enhancement of the Overall Optical Efficiency of Intracavity Frequency-Doubling Devices for the One-Micron Continuous-Wave Nd:Y₃Al₅O₁₂ Laser Emission," *Appl. Phys. Lett.* **83**, 3653–3655 (2003).

- M. IWAI, T. YOSHINO, S. YAMAGUCHI, M. IMAEDA, N. PAVEL, I. SHOJI and T. TAIRA**, "High-Power Blue Generation from a Periodically Poled MgO:LiNbO₃ Ridge-Type Waveguide by Frequency Doubling of a Diode End-Pumped Nd:Y₃Al₅O₁₂ Laser," *Appl. Phys. Lett.* **83**, 3659–3661 (2003).
- T. DASCALU, N. PAVEL and T. TAIRA**, "90 W Continuous-Wave Diode Edge-Pumped Microchip Composite Yb:Y₃Al₅O₁₂ Laser," *Appl. Phys. Lett.* **83**, 4086–4088 (2003).
- V. LUPEL, N. PAVE, Y. SATO and T. TAIRA**, "Highly Efficient 1063-nm Continuous-Wave Laser Emission in Nd:GdVO₄," *Opt. Lett.* **28**, 2366–2368 (2003).
- W. K. JANG, T. TAIRA, Y. SATO and Y. M. YU**, "Laser Emission under ⁴F_{5/2} and ⁴F_{3/2} Pumping in Nd:LSB Micro-Laser," *Jpn. J. Appl. Phys.* **43**, L70–72 (2004).
- S. ASHIHARA, T. SHIMURA, K. KURODA, N. E. YU, S. KURIMURA, K. KITAMURA, M. CHA and T. TAIRA**, "Optical Pulse Compression using Cascaded Quadratic Nonlinearities in Periodically Poled Lithium Niobate," *Appl. Phys. Lett.* **84**, 1055–1057 (2004).
- Y. SATO and T. TAIRA**, "Saturation Factors of Pump Absorption in Solid-State Lasers," *IEEE J. Quantum Electron.* **40**, 270–280. (2004).
- N. PAVEL, I. SHOJI, T. TAIRA, K. MIZUUCHI, A. MORIKAWA, T. SUGITA and K. YAMAMOTO**, "Room-Temperature, Continuous-Wave 1-W Green Power by Single-Pass Frequency Doubling in a Bulk Periodically Poled MgO:LiNbO₃ Crystal," *Opt. Lett.* **29**, 830–832 (2004).
- R. KAWAI, Y. MIYASAKA, K. OTSUKA, J. Y. KO, I. SHOJI and T. TAIRA**, "Oscillation Spectra and Dynamic Effects in a Highly-Doped Microchip Nd:YAG Ceramic Laser," *Optics Express* **12**, 2293–2301 (2004).
- Y. SATO, J. SAIKAWA, I. SHOJI, T. TAIRA and A. IKESUE**, "Spectroscopic Properties and Laser Operation of Nd:Y₃ScAl₄O₁₂ Polycrystalline Gain Media, Solid-Solution of Nd:Y₃Al₅O₁₂ and Nd: Y₃Sc₂Al₃O₁₂ Ceramics," *J. Ceram. Soc. Jpn.* **112**, 313–316 (2004).
- N. PAVEL, I. SHOJI and T. TAIRA**, "Continuous-Wave High-Power Nd:YAG-KNbO₃ Laser at 473 nm," *Opt. Laser Tech.* **36**, 581–585 (2004).
- I. SHOJI, T. TAIRA, A. IKESUE and K. YOSHIDA**, "Reduction of the Thermal Load by Laser Oscillation in Highly Nd³⁺-Doped Ceramic YAG," *OSA TOPS on Advanced Solid-State Photonics* **94**, 415–420 (2004).

Research Center for Molecular-scale Nanoscience List of Publications

- K. ARAKI, H. ENDO, G. MASUDA and T. OGAWA**, "Bridging Nanogap Electrodes by *In Situ* Electropolymerization of a Bis-Terthiophenylphenanthroline Ruthenium Complex," *Chem. Eur. J.* **10**, 3331–3340 (2004).
- K. ARAKI, H. ENDO, H. TANAKA and T. OGAWA**, "Simultaneous Multi Curve Fitting Analysis of Temperature Dependent *I-V* Curves from Polythiophene Bridged Nanogap Devices," *Jpn. J. Appl. Phys.* **43**, L634–L636 (2004).
- H. TANAKA, M. E. ANDERSON, M. W. HORN and P. S. WEISS**, "Position-Selected Molecular Ruler," *Jpn. J. Appl. Phys.* **43**, L950–L953 (2004).
- M. E. ANDERSON, L. P. TAN, H. TANAKA, M. MIHOK, H. LEE, M. W. HORN and P. S. WEISS**, "Advances in Nanolithography Using Molecular Rulers," *J. Vac. Sci. Technol., Sect. B* **21**, 3116–3119 (2003).
- Y. INOUE, S. TOKITO, K. ITO and T. SUZUKI**, "Organic Thin-Film Transistors Based on Anthracene Oligomers," *J. Appl. Phys.* **95**, 5795–5799 (2004).
- Y. SAKAMOTO, T. SUZUKI, M. KOBAYASHI, Y. GAO, Y. FUKAI, Y. INOUE, F. SATO and S. TOKITO**, "Perfluoropentacene: High-Performance *p-n* Junctions and Complementary Circuits with Pentacene," *J. Am. Chem. Soc.* **126**, 8138–8140 (2004).
- M. ARA, A. SASAHARA, H. OHNISHI and H. TADA**, "Non-Contact Atomic Force Microscopy Using Silicon Cantilevers Covered with Organic Monolayers *via* Silicon–Carbon Covalent Bonds," *Nanotechnology* **15**, S65–S68 (2004).
- R. YAMADA, M. ARA and H. TADA**, "Temperature Dependence of the Structure of Alkyl Monolayers on Si(111) Surface *via* Si–C Bond by ATR-FT-IR Spectroscopy," *Chem. Lett.* **33**, 492–493 (2004).
- T. SAKANOUÉ, E. FUJIWARA, R. YAMADA and H. TADA**, "Visible Light Emission from Polymer-Based Field-Effect Transistors," *Appl. Phys. Lett.* **84**, 3037–3039 (2004).
- M. TAKADA and H. TADA**, "Low Temperature Scanning Tunneling Microscopy of Phthalocyanine Multilayers on Au(111) Surfaces," *Chem. Phys. Lett.* **392**, 265–269 (2004).
- J. NISHIDA, NARASO, S. MURAI, E. FUJIWARA, H. TADA, M. TOMURA and Y. YAMASHITA**, "Preparation, Characterization and FET Properties of Novel Dicyanopyrazinoquinoxaline Derivatives," *Org. Lett.* **6**, 2007–2010 (2004).
- MCR. DELGADO, V. HERNANDEZ, JTL NAVARRETE, S. TANAKA and Y. YAMASHITA**, "Combined Spectroscopic and Theoretical Study of Narrow Band Gap Heterocyclic Co-Oligomers Containing Alternating Aromatic Donor and *o*-Quinoid Acceptor Units," *J. Phys. Chem. B* **108**, 2516–2526 (2004).

T. KUMAGAI, M. TOMURA, J. NISHIDA and Y. YAMASHITA, "Preparation, Structures and Properties of Novel 1,3-Dithiol-2-Ylidene Derivatives Containing Bis(ethynylpyridine) Units," *Tetrahedron Lett.* **44**, 6845–6848 (2003).

M. TOMURA and Y. YAMASHITA, "(1,3-Dithiol-2-ylidene)propanedinitrile," *Acta Crystallogr., Sect. E* **59**, o1941–o1943 (2003).

M. TOMURA and Y. YAMASHITA, "Crystal Structure of 4,7-Dibromo-2,1,3-Benzothiadiazole, $C_6H_2Br_2N_2S$," *Z. Kristallogr. NCS* **218**, 555–556 (2003).

M. TOMURA and Y. YAMASHITA, "4,5-Diiodo[1,2,5]thiadiazolotetrathiafulvalene," *Acta Crystallogr., Sect. E* **60**, o63–o65 (2004).

M. AKHTARUZZAMAN, M. TOMURA, J. NISHIDA and Y. YAMASHITA, "Synthesis and Characterization of Novel Dipyritylbenzothiadiazole and Bisbenzothiadiazole Derivatives," *J. Org. Chem.* **69**, 2953–2958 (2004).

K. TAKENAKA and Y. UOZUMI, "Development of Chiral Pincer Palladium Complexes Bearing a Pyrroloimidazolone Unit. Catalytic Use for Asymmetric Michael Addition," *Org. Lett.* **6**, 1833–1835 (2004).

T. HAYASHI, K. YAMASAKI, M. MIURA and Y. UOZUMI, "Deuterium-Labeling Studies Establishing Stereochemistry at the Oxypalladation Step in Wacker-Type Oxidative Cyclization of an *o*-Allylphenol," *J. Am. Chem. Soc.* **126**, 3036–3037 (2004).

Y. UOZUMI, H. TANAKA and K. SHIBATOMI, "Asymmetric Allylic Amination in Water Catalyzed by an Amphiphilic Resin-Supported Chiral Palladium Complex," *Org. Lett.* **6**, 281–283 (2004).

Y. UOZUMI and R. NAKAO, "Catalytic Oxidation of Alcohols in Water under Atmospheric Oxygen by Use of an Amphiphilic Resin-Dispersion of a NanoPalladium Catalyst," *Angew. Chem.* **115**, 204–207 (2003).

Y. KIKUZAWA and T. NAGATA, "Synthesis and Properties of New, Spatially Relaxed Dendrons Containing Internal Carboxyl Groups," *Bull. Chem. Soc. Jpn.* **75**, 993–1000 (2004).

D. INO, K. WATANABE, N. TAKAGI and Y. MATSUMOTO, "Ultrafast Excited State Dynamics in 3,4,9,10-Perylene Tetracarboxylic Dianhydride (PTCDA) Thin Films," *Chem. Phys. Lett.* **383**, 261–265 (2003).

Y. MATSUMOTO, O. NAKAGOE, K. WATANABE and N. TAKAGI, "Dynamic Formation of Reaction Sites at Nano-Structured One-Dimensional Surface Compounds," *Proc. SPIE* **5223**, 232–240 (2003).

K. WATANABE, N. TAKAGI and Y. MATSUMOTO, "Direct Time-Domain Observation of Ultrafast Dephasing in Adsorbate-Substrate Vibration under the Influence of a Hot Electron Bath: Cs adatoms on Pt(111)," *Phys. Rev. Lett.* **92**, 57401 (4 pages) (2004).

T. SAWADA, Z. LIU, N. TAKAGI, K. WATANABE and Y. MATSUMOTO, "Reactivity of Molecular Oxygen: Conversion of Methanol to Formate at Low Temperatures on Pt(111)," *Chem. Phys. Lett.* **92**, 334–339 (2004).

T. TSUKUDA and T. NAGATA, "Gas Phase Reactions of Hydrated CO_2^- Anion Radical with CH_3I ," *J. Phys. Chem. A* **107**, 8476–8483 (2003).

Y. NEGISHI and T. TSUKUDA, "Visible Photoluminescence from Nearly Monodispersed Au_{12} Clusters Protected by meso-2,3-Dimercaptosuccinic Acid," *Chem. Phys. Lett.* **383**, 161–165 (2004).

H. TANAKA, K. TAKEUCHI, Y. NEGISHI and T. TSUKUDA, "Highly Oxygenated Fullerene Anions $C_{60}O_n^-$ Formed by Corona Discharge Ionization in the Gas Phase," *Chem. Phys. Lett.* **384**, 283–287 (2004).

H. MURAYAMA, T. NARUSHIMA, Y. NEGISHI and T. TSUKUDA, "Structures and Stabilities of Alkanethiolate Monolayers on Palladium Clusters as Studied by Gel Permeation Chromatography," *J. Phys. Chem. B* **108**, 3496–3503 (2004).

Y. NEGISHI, Y. TAKASUGI, S. SATO, H. YAO, K. KIMURA and T. TSUKUDA, "Magic-Numbered Au_n Clusters Protected by Glutathione Monolayers ($n = 18, 21, 25, 28, 32, 39$): Isolation and Spectroscopic Characterization," *J. Am. Chem. Soc.* **126**, 6518–6519 (2004).

O. YOGI, T. KAWAKAMI and A. MIZUNO, "On-Demand Mixing Droplet Spotter for Preparing Picoliter Droplets on Surfaces," *Anal. Chem.* **76**, 2991–2996 (2004).

Z. Z. SU, J. SAWADA, K. TAKASHIMA, S. KATSURA and A. MIZUNO, "Basic Study for Gas Cleaning Using Discharge and Electrophoresis," *Catal. Today* **89**, 103–107 (2004).

Y. MATSUI, M. INABA, K. TAKASHIMA, S. KATSURA and A. MIZUNO, "Combination of Plasma and Pt Catalyst for Diesel Cleaning at Low Temperature," *J. Inst. Electrostatics* (in Japanese) **28**, 35–40 (2004).

T. LWIN, B. SUNG, K. TAKASHIMA, S. KATSURA and A. MIZUNO, "Charging Characteristic of Polypropylene (PP) Filter Using High Pressure DC Corona," *J. Inst. Electrostatics* (in Japanese) **28**, 41–46 (2004).

G. LI, K. TAKASHIMA, S. KATSURA and A. MIZUNO, "Electrostatic Assembly of Particle Chains from Fine Particles Suspended in Gas Phase," *J. Inst. Electrostatics* (in Japanese) **28**, 133–137 (2004).

M. SUZUKI, T. SATO, H. MATSUHASHI and A. MIZUNO, "Development of Ion Conveying Type Ionization System—Generation of Large Charged Particles by Ultrasonic/Electrostatic Atomization—," *J. Inst. Electrostatics* (in Japanese) **28**, 47–52 (2004).

G. LI, K. TAKASHIMA, S. KATSURA and A. MIZUNO, "Controlled Formation and Deposition of Chain Aggregates from Fine Al_2O_3 Particles," *Jpn. J. Appl. Phys.* **43**, 722–725 (2004).

- M. TAKAHASHI, Y. KHAJURIA and Y. UDAGAWA**, “(e,2e) Ionization-Excitation of H₂,” *Phys. Rev. A* **68**, 042710 (7 pages) (2003).
- Y. KHAJURIA, M. TAKAHASHI and Y. UDAGAWA**, “Electron Momentum Spectroscopy of N₂O,” *J. Electron Spectrosc. Relat. Phenom.* **133**, 113–121 (2003).
- L. Q. CHEN, Y. KHAJURIA, X. J. CHEN and K. Z. XU**, “Triple Differential Cross-Section of Ne(2s²) in Coplanar to Perpendicular Plane Geometry,” *Eur. Phys. J. D* **26**, 141–146 (2003).
- K. HOSAKA, J. ADACHI, M. TAKAHASHI and A. YAGISHITA**, “N 1s Photoionization Cross Sections of the NO Molecules in the Shape Resonance Region,” *J. Phys. B: At., Mol. Opt. Phys.* **36**, 4617–4629 (2003).
- J. ADACHI, K. HOSAKA, S. FURUYA, K. SOEJIMA, M. TAKAHASHI, A. YAGISHITA, S. K. SEMENOV and N. A. CHEREPKOV**, “Shape-Resonance-Enhanced Vibrational Effects in the Angular Distributions of C 1s Photoelectrons from Fixed-in-Space CO Molecules,” *Phys. Rev. Lett.* **91**, 163001 (4pages) (2003).
- A. De FANIS, M. OURA, N. SAITO, M. MACHIDA, M. NAGOSHI, A. KNAPP, J. NICKLES, A. CZASCH, R. DÖRNER, Y. TAMENORI, H. CHIBA, M. TAKAHASHI, J. H. D. ELAND and K. UEDA**, “Photoelectron-Photoion-Photoion Coincidence in Ar Dimers,” *J. Phys. B: At., Mol. Opt. Phys.* **37**, L1–L8 (2004).
- N. WATANABE, Y. KAMATA, K. YAMAUCHI, Y. UDAGAWA and T. MÜLLER**, “Coulomb Hole in N₂, CO and O₂ Deduced from X-Ray Scattering Cross Sections,” *Mol. Phys.* **102**, 649–657 (2004).
- K. HOSAKA, J. ADACHI, M. TAKAHASHI, A. YAGISHITA, P. LIN and R. R. LUCCHESI**, “Multiplet-Specific N 1s Photoelectron Angular Distributions from the Fixed-in-Space NO Molecules,” *J. Phys. B: At., Mol. Opt. Phys.* **37**, L49–L55 (2004).
- R. W. VAN BOEYEN, N. WATANABE, J. P. DOERING, J. H. MOORE and M. COPLAN**, “Practical Means for the Study of Electron Correlation in Atoms,” *Phys. Rev. Lett.* **92**, 223202 (4 pages) (2004).
- A. C. R. PIPINO, J. P. M. HOEFNAGELS and N. WATANABE**, “Absolute Surface Coverage Measurement Using a Vibrational Overtone,” *J. Chem. Phys.* **120**, 2879–2888 (2004).
- J. ADACHI, K. HOSAKA, S. FURUYA, K. SOEJIMA, M. TAKAHASHI, A. YAGISHITA, S. K. SEMENOV and N. A. CHEREPKOV**, “Angular Distributions of Vibrationally Resolved C 1s Photoelectrons from Fixed-in-Space CO Molecules: Vibrational Effect in the Shape-Resonant C 1s Photoionization of CO,” *J. Electron Spectrosc. Relat. Phenom.* **137-40**, 243–248 (2004).
- M. TAKAHASHI and Y. UDAGAWA**, “A High Sensitivity Electron Momentum Spectrometer with Two-Dimensional Detectors and Electron Momentum Distributions of Several Simple Molecules,” *J. Electron Spectrosc. Relat. Phenom.* **137-40**, 387–391 (2004).
- S. KERA, Y. YABUCHI, H. YAMANE, H. SETOYAMA, K. K. OKUDAIRA, A. KAHN and N. UENO**, “Impact of an Interface Dipole Layer on Molecular Level Alignment at an Organic-Conductor Interface Studied by UPS,” *Phys. Rev. B* **70**, 085304 (6 pages) (2004).
- H. YAMANE, H. HONDA, H. FUKAGAWA, M. OHYAMA, Y. HINUMA, S. KERA, K. K. OKUDAIRA and N. UENO**, “HOMO-Band Fine Structure of OTi- and Pb-Phthalocyanine Ultrathin Films: Effects of the Electric Dipole Layer,” *J. Electron Spectrosc. Relat. Phenom.* **137-140**, 223–227 (2004).
- K. K. OKUDAIRA, H. SETOYAMA, H. YAGI, K. MASE, S. KERA, A. KAHN and N. UENO**, “Study of Excited States of Fluorinated Copper Phthalocyanine by Inner Shell Excitation,” *J. Electron Spectrosc. Relat. Phenom.* **137-140**, 137–140 (2004).
- D. YOSHIMURA, H. ISHII, T. MIYAMAE, Y. OUCHI, K. K. OKUDAIRA, N. UENO and K. SEKI**, “Simulation Study of Angle-Resolved Photoemission Spectra and Intramolecular Energy-Band Dispersion of a PTFE Oligomer Film,” *J. Chem. Phys.* **120**, 10753–10762 (2004).
- K. CHIE, M. FUJIWARA, Y. FUJIWARA and Y. TANIMOTO**, “Magnetic Separation of Metal Ions,” *J. Phys. Chem. B* **107**, 14374–14377 (2003).
- YU. A. OSSIPYAN, R. B. MORGUNOV, A. A. BASKAKOV, S. Z. SHMURAK and Y. TANIMOTO**, “New Luminescent Bands Induced by Plastic Deformation of NaCl:Eu Phosphors,” *Phys. Status. Solidi A* **201**, 148–156 (2004).
- I. UECHI, A. KATSUKI, L. DUNIN-BARKOVSKY and Y. TANIMOTO**, “3D-Morphological Chirality Induction in Zinc Silicate Membrane Tube Using a High Magnetic Field,” *J. Phys. Chem. B* **108**, 2527–2530 (2004).
- A. KATSUKI, I. UECHI and Y. TANIMOTO**, “Effects of a High Magnetic Field on the Growth of 3-Dimensional Silver Dendrites,” *Bull. Chem. Soc. Jpn.* **77**, 275–279 (2004).
- M. FUJIWARA, K. CHIE, J. SAWAI, D. SHIMIZU and Y. TANIMOTO**, “On the Movement of Paramagnetic Ions in an Inhomogeneous Magnetic Field,” *J. Phys. Chem. B* **108**, 3531–3534 (2004).
- R. B. MORGUNOV, A. A. BASKAKOV, L. R. DUNIN-BARKOVSKIY, S. S. KHASANOV, R. P. SHIBAEVA, T. G. PROKHOROVA, E. B. YAGUBSKIY, T. KATO and Y. TANIMOTO**, “Localization of Conduction-Band Electrons in β⁻-(BEDT-TTF)₄NH₄[Cr(C₂O₄)₃]-DMF Single Crystals,” *J. Phys. IV France* **114**, 335–337 (2004).
- H. YONEMURA, H. NOBUKUNI, S. MORIBE, S. YAMADA, Y. FUJIWARA and Y. TANIMOTO**, “Magnetic Field Effects on the Decay Rates of Triplet Biradical Photogenerated from Intramolecular Electron-Transfer in a Zinc-Tetraphenylporphyrin-Fullerene Linked Compound,” *Chem. Phys. Lett.* **385**, 417–422 (2004).

J. AIHARA and T. ISHIDA, "Aromatic Character of Annelated Dimethyldihydropyrenes," *J. Phys. Org. Chem.* **17**, 393–398 (2004).

M. HIRAMA, T. ISHIDA and J. AIHARA, "Possible Molecular Hydrogen Formation Mediated by the Inner and Outer Carbon Atoms of Typical PAH Cations," *Chem. Phys.* **305**, 307–316 (2004).

T. OBA and H. TAMIAKI, "Back and Face: Non-Planarity and Chirality of Planar Molecule," *Kagaku* **58**, 12–18 (2003).

UVSOR Facility

M. HOSAKA, M. KATOH, A. MOCHIHASHI, J. YAMAZAKI, K. HAYASHI and Y. TAKASHIMA, "Upgrade of the UVSOR Storage Ring FEL," *Nucl. Instrum. Methods Phys. Res., Sect. A* **528**, 291–295 (2004).

Y. HIKOSAKA, T. AOTO, R. I. HALL, K. ITO, R. HIRAYAMA, N. YAMAMOTO and E. MIYOSHI, "Inner-Valence States of O_2^+ and Dissociation Dynamics Studied by Threshold Photoelectron Spectroscopy and a Configuration Interaction Calculation," *J. Chem. Phys.* **119**, 7693–7700 (2003).

Y. HIKOSAKA, P. LABLANQUIE, M. AHMAD, R. I. HALL, J. G. LAMBOURNE, F. PENENT and J. H. D. ELAND, "Competition between Autoionization and Dissociation in the $[O_2^+(B^2\Sigma_g^-)]nl$ and $[O_2^+(c^4\Sigma_u^-)]nl$ Rydberg States Investigated by Photon Induced Dissociation to Neutral Fragments," *J. Phys. B* **36**, 4311–4326 (2003).

Y. HIKOSAKA and J. H. D. ELAND, "Photoionization into the Dissociation Continuum of $H_2^+(X^2\Sigma_g^+)$ Studied by Velocity Imaging Photoionization Coincidence Spectroscopy," *J. Electron Spectrosc. Relat. Phenom.* **133**, 77–86 (2003).

Y. HIKOSAKA, P. LABLANQUIE, M. AHMAD, F. PENENT, J. H. D. ELAND and R. I. HALL, "The Formation of Fluorescent and Metastable Fragments by Photoexcitation of Some Diatomic Molecules in the Vacuum Ultraviolet Region," *J. Phys. B* **37**, 283–293 (2003).

Y. HIKOSAKA and J. H. D. ELAND, "Dissociative Double Photoionisation of CO below the CO^{++} Threshold," *Chem. Phys.* **299**, 147–154 (2004).

T. AOTO, Y. HIKOSAKA, R. I. HALL, K. ITO, J. FERNÁNDEZ and F. MARTÍN, "Dissociative Photoionization of H_2 at High Photon Energies: Uncovering New Series of Doubly Excited States," *Chem. Phys. Lett.* **389**, 145–149 (2004).

Y. HIKOSAKA, P. LABLANQUIE, F. PENENT, J. G. LAMBOURNE, R. I. HALL, T. AOTO and K. ITO, "Sub-Natural Linewidth Auger Electron Spectroscopy of the 2s Hole Decay in H_2S ," *J. Electron Spectrosc. Relat. Phenom.* **137-140**, 287–291 (2004).

Y. HIKOSAKA, T. AOTO, E. SHIGEMASA and K. ITO, "Autoionization Selectivity of Ne^+ Rydberg States Converging to $Ne^{2+}(^1S^e)$," *J. Phys. B* **37**, 2823–2828 (2004).

S. KIMURA, M. OKUNO, H. KITAZAWA, F. ISHIYAMA and O. SAKAI, "Change of Electronic Structure Induced by Magnetic Transitions in CeBi," *J. Phys. Soc. Jpn.* **73**, 2041–2044 (2004).

Y. IKEMOTO, T. MORIWAKI, T. HIRONO, S. KIMURA, K. SHINODA, M. MATSUNAMI, N. NAGAI, T. NANBA, K. KOBAYASHI and H. KIMURA, "Infrared Microspectroscopy Station at BL43IR of SPring-8," *Infrared Phys. Tech.* **45**, 369–373 (2004).

S. KIMURA, E. NAKAMURA, J. YAMAZAKI, M. KATOH, T. NISHI, H. OKAMURA, M. MATSUNAMI, L. CHEN and T. NANBA, "New Infrared and Terahertz Beamline BL6B at UVSOR," *AIP Conf. Proc.* **705**, 416–419 (2004).

S. KIMURA, T. NISHI, J. SICHELSCHMIDT, V. VOEVODIN, J. FERSTL, C. GEIBEL and F. STEGLICH, "Optical Conductivity of a Non-Fermi-Liquid Material $YbRh_2Si_2$," *J. Magn. Magn. Mater.* **272-276**, 36–37 (2004).

H. OKAMURA, T. MICHIZAWA, M. MATSUNAMI, T. NANBA, S. KIMURA, T. EBIHARA, F. IGA and T. TAKABATAKE, "Optical Study on c-f Hybridization States in Mixed-Valent Yb Compounds: Metallic $YbAl_3$ vs Semiconducting YbB_{12} ," *J. Magn. Magn. Mater.* **272-276**, e51–e52 (2004).

Okazaki Institute for Integrative Bioscience

K. SHIMABUKURO, R. YASUDA, E. MUNAYUKI, K. Y. HARA, K. KINOSITA, Jr. and M. YOSHIDA, "Catalysis and Rotation of F_1 Motor: Cleavage of ATP at the Catalytic Site Occurs in 1 ms before 40° Substep Rotation," *Proc. Natl. Acad. Sci. U.S.A.* **100**, 14731–14736 (2003).

H. ITOH, A. TAKAHASHI, K. ADACHI, H. NOJI, R. YASUDA, M. YOSHIDA and K. KINOSITA, Jr., "Mechanically Driven ATP Synthesis by F_1 -ATPase," *Nature* **427**, 465–468 (2004).

T. NISHIZAKA, K. OIWA, H. NOJI, S. KIMURA, E. MUNAYUKI, M. YOSHIDA and K. KINOSITA, Jr., "Chemomechanical Coupling in F_1 -ATPase Revealed by Simultaneous Observation of Nucleotide Kinetics and Rotation," *Nat. Struct. Mol. Biol.* **11**, 142–148 (2004).

M. Y. ALI, K. HOMMA, A. H. IWANE, K. ADACHI, H. ITOH, K. KINOSITA, Jr., T. YANAGIDA and M. IKEBE, "Unconstrained Steps of Myosin VI Appear Longest among Known Molecular Motors," *Biophys. J.* **86**, 3804–3810 (2004).

S. AKIYAMA, T. FUJISAWA, K. ISHIMORI, I. MORISHIMA and S. AONO, "Activation Mechanisms of Transcriptional Regulator CooA Revealed by Small-Angle X-Ray Scattering," *J. Mol. Biol.* **341**, 651–668 (2004).

R. DAVYDOV, T. MATSUI, H. FUJII, M. IKEDA-SAITO and B. M. HOFFMAN, "Kinetic Isotope Effects on the Rate-Limiting Step of Heme Oxygenase Catalysis Indicate Concerted Proton Transfer/Heme Hydroxylation," *J. Am. Chem. Soc.* **125**, 16208–16209 (2003).

R. DAVYDOV, J. SATTERLEE, H. FUJII, A. SAUER-MASARWA, D. H. BUSCH and B. M. HOFFMAN, "A Superoxo-Ferrous State in a Reduced Oxy-Ferrous Hemoprotein and Model Compounds," *J. Am. Chem. Soc.* **125**, 16340–16346 (2003).

H. FUJII, X. ZHANG and T. YOSHIDA, "Essential Amino Acid Residues Controlling the Unique Regioselectivity of Heme Oxygenase in *Pseudomonas aeruginosa*," *J. Am. Chem. Soc.* **126**, 4466–4467 (2004).

T. FUJII, A. NAITO, S. YAMAGUCHI, A. WADA, Y. FUNAHASHI, K. JITSUKAWA, S. NAGATOMO, T. KITAGAWA and H. MASUDA, "Construction of a Square-Planar Hydroperoxo-Copper(II) Complex Inducing a Higher Catalytic Reactivity," *Chem. Commun.* 2700–2701 (2003).

S. YAMAGUCHI, S. NAGATOMO, T. KITAGAWA, Y. FUNAHASHI, T. OZAWA, K. JITSUKAWA and H. MASUDA, "Copper Hydroperoxo Species Activated by Hydrogen-Bonding Interaction with Its Distal Oxygen," *Inorg. Chem.* **42**, 6968–6970 (2003).

S. YAMAGUCHI, A. WADA, Y. FUNAHASHI, S. NAGATOMO, T. KITAGAWA, K. JITSUKAWA and H. MASUDA, "Thermal Stability and Absorption Spectroscopic Behavior of (μ -Peroxo)dicopper Complexes Regulated with Intramolecular Hydrogen Bonding Interactions," *Eur. J. Inorg. Chem.* **2003**, 4378–4386 (2003).

M. MIZUNO, H. HAYASHI, S. FUJINAMI, H. FURUTACHI, S. NAGATOMO, S. OTAKE, K. UOZUMI, M. SUZUKI and T. KITAGAWA, "Ligand Effect on Reversible Conversion Between Copper(I) and Bis(μ -oxo)dicopper(III) Complex with a Sterically Hindered Tetradentate Tripodal Ligand and Monooxygenase Activity of Bis(μ -oxo)dicopper(III) Complex," *Inorg. Chem.* **42**, 8534–8544 (2003).

J. IGARASHI, A. SATO, T. KITAGAWA, I. SAGAMI and T. SHIMIZU, "CO Binding Study of Mouse Heme-Regulated eIF-2 α Kinase: Kinetics and Resonance Raman Spectra," *Biochim. Biophys. Acta* **1650**, 99–104 (2003).

K. KOMIYAMA, H. FURUTACHI, S. NAGATOMO, A. HASHIMOTO, H. HAYASHI, S. FUJINAMI, M. SUZUKI and T. KITAGAWA, "Dioxygen Reactivity of Copper(I) Complexes with Tetradentate Tripodal Ligands Having Aliphatic Nitrogen Donors: Synthesis, Structures, and Properties of Peroxo and Superoxo Complexes," *Bull. Chem. Soc. Jpn.* **77**, 59–72 (2004).

Y. JIN, M. NAGAI, Y. NAGAI, S. NAGATOMO and T. KITAGAWA, "Heme Structures of Five Variants of Hemoglobin M Probed by Resonance Raman Spectroscopy," *Biochemistry* **43**, 8517–8527 (2004).

H. HIRAMATSU, Y. GOTO, H. NAIKI and T. KITAGAWA, "Core Structure of Amyloid Fibril Proposed from IR-microscope Linear Dichroism," *J. Am. Chem. Soc.* **126**, 3008–3009 (2004).

T. OGURA and T. KITAGAWA, "Resonance Raman Characterization of the P Intermediate in the Reaction of Bovine Cytochrome *c* Oxidase," *Biochim. Biophys. Acta* **1655**, 290–297 (2004).

J. IGARASHI, A. SATO, T. KITAGAWA, T. YOSHIMURA, S. YAMAUCHI, I. SAGAMI and T. SHIMIZU, "Activation of Heme-Regulated Eukaryotic Initiation Factor 2 α Kinase (HRI) Activation by Nitric Oxide Is Induced by the Formation of a Five-Coordinate NO-Heme Complex: Optical Absorption, Electron Spin Resonance and Resonance Raman Spectral Studies," *J. Biol. Chem.* **279**, 15752–15762 (2004).

B. PAL, Z. LI, T. OHTA, S. TAKENAKA, S. TSUYAMA and T. KITAGAWA, "Resonance Raman Study on Synergistic Activation of Soluble Guanylate Cyclase by Imidazole, YC-1 and GTP," *J. Inorg. Biochem.* **98**, 824–832 (2004).

S. TERAMAE, T. OSAKO, S. NAGATOMO, T. KITAGAWA, S. FUKUZUMI and S. ITOH, "Dinuclear Copper-Dioxygen Intermediates Supported by Polyamine Ligands," *J. Inorg. Biochem.* **98**, 746–757 (2004).

T. EGAWA, N. SUZUKI, T. DOKOH, T. HIGUCHI, H. SHIMADA, T. KITAGAWA and Y. ISHIMURA, "Vibronic Coupling Between Soret and Higher Energy Excited States in Iron(II) Porphyrins: Raman Excitation Profiles of A_{2g} modes in the Soret Region," *J. Phys. Chem. A* **108**, 568–577 (2004).

Y. MATSUDA, T. UCHIDA, H. HORI, T. KITAGAWA and H. ARATA, "Structural Characterization of a Binuclear Center of a Cu-Containing NO Reductase Homologue from *Roseobacter Denitrificans*: EPR and Resonance Raman Studies," *Biochim. Biophys. Acta* **1656**, 37–45 (2004).

M. TAKI, H. HATTORI, T. OSAKO, S. NAGATOMO, M. SHIRO, T. KITAGAWA and S. ITOH, "Model Complexes of the Active Site of Galactose Oxidase. Effects of the Metal Ion Binding Sites," *Inorg. Chim. Acta* **357**, 3369–3381 (2004).

K. OINUMA, T. OHTA, K. KONISHI, Y. HASHIMOTO, H. HIGASHIBTA, T. KITAGAWA and M. KOBAYASHI, "Heme Environment in Aldoxime Dehydratase Involved in Carbon–Nitrogen Triple Bond Synthesis," *FEBS Lett.* **568**, 44–48 (2004).

E. PINAKOULAKI, T. OHTA, T. SOULIMANE, T. KITAGAWA and C. VAROTSIS, "Simultaneous Resonance Raman Detection of the Heme a_3 -Fe-CO and Cu_B -CO Species in CO-bound ba_3 -Cytochrome *c* Oxidase from *Thermus thermophilus*," *J. Biol. Chem.* **279**, 22791–22794 (2004).

T. OHTA, E. PINAKOULAKI, T. SOULIMANE, T. KITAGAWA and C. VAROTSIS, "Detection of a Photostable Five-Coordinate Heme a_3 -Fe-CO Species and Functional Implications of His384/ α 10 in CO-Bound ba_3 -Cytochrome *c* Oxidase from *Thermus thermophilus*," *J. Phys. Chem. B* **108**, 5389–5491 (2004).

T. EGAWA, T. HISHIKI, Y. ICHIKAWA, Y. KANAMORI, H. SHIMADA, S. TAKAHASHI, T. KITAGAWA and Y. ISHIMURA, "Refolding Processes of Cytochrome P450_{cam} from Ferric and Ferrous Acid Forms to the Native Conformation," *J. Biol. Chem.* **279**, 32008–32017 (2004).

A. YAMADA, T. YAMATO, T. KAKITANI and S. YAMAMOTO, "Torsion Potential Works in Rhodopsin," *Photochem. Photobiol.* **79**, 476–486 (2004).

A. YAMADA, T. ISHIKURA and T. YAMATO, "Role of Protein in the Primary Step of the Photoreaction of Yellow Protein," *Proteins: Struct., Funct., Genet.* **55**, 1063–1069 (2004).

A. YAMADA, T. ISHIKURA and T. YAMATO, "Direct Measure of Functional Importance Visualized Atom-by-Atom for Photoactive Yellow Protein: Application to Photoisomerization Reaction," *Proteins: Struct. Funct., Genet.* **55**, 1070–1077 (2004).