

# LIST OF PUBLICATIONS

## Department of Theoretical Studies

- K. KOBAYASHI, Y. SANO and S. NAGASE**, "Theoretical Study of Endohedral Metallofullerenes:  $\text{Sc}_{3-n}\text{La}_n\text{N}@C_{80}$  ( $n = 0-3$ )," *J. Comput. Chem.* **22**, 1353 (2001).
- M. ICHINOHE, Y. ARAI, A. SEKIGHUCHI, N. TAKAGI and S. NAGASE**, "A New Approach to the Synthesis of Unsymmetrical Disilenes and Germanasilene: Unusual  $^{29}\text{Si}$  NMR Chemical Shifts and Regiospecific Methanol Addition," *Organometallics* **20**, 4141 (2001).
- N. TAKAGI and S. NAGASE**, "A Silicon-Silicon Triple Bond Surrounded by Bulky Terphenyl Groups," *Chem. Lett.* 966 (2001).
- A. HAN, T. WAKAHARA, Y. MAEDA, Y. NIINO, T. AKASAKA, K. YAMAMOTO, M. KAKO, Y. NAKADAIRA, K. KOBAYASHI and S. NAGASE**, "Photochemical Cycloaddition of  $\text{C}_{78}$  with Disilirane," *Chem. Lett.* 974 (2001).
- M. KIMURA and S. NAGASE**, "The Quest of Stable Silanones. Substituent Effects," *Chem. Lett.* 1098 (2001).
- N. TAKAGI and S. NAGASE**, "Substituent Effects on Germanium-Germanium and Tin-Tin Triple Bonds," *Organometallics* **20**, 5498 (2001).
- K. GOTO, Y. HINO, Y. TAKAHASHI, T. KAWASHIMA, G. YAMAMOTO, N. TAKAGI and S. NAGASE**, "Synthesis, Structure, and Reactions of the First Stable Aromatic S-Nitrosothiol Bearing a Novel Dendrimer-Type Steric Protection Group," *Chem. Lett.* 1204 (2001).
- A. SEKIGUCHI, Y. ISHIDA, N. FUKAYA, M. ICHINOHE, N. TAKAGI and S. NAGASE**, "The First Halogen-Substituted Cyclotrigermenes: A Unique Halogen Walk over the Three-Membered Ring Skeleton and Facial Stereoselectivity in the Diels-Alder Reaction," *J. Am. Chem. Soc.* **124**, 1158 (2002).
- T. SASAMORI, N. TAKEDA, M. FUJIO, M. KIMURA, S. NAGASE and N. TOKITOH**, "Synthesis and Structure of the First Stable Phosphabismuthene," *Angew. Chem. Int. Ed.* **41**, 139 (2002).
- J. KOBAYASHI, K. GOTO, T. KAWASHIMA, M. W. SCHMIDT and S. NAGASE**, "Synthesis, Structure, and Bonding Properties of 5-Carbaphosphatranes: A New Class of Main Group Atrane," *J. Am. Chem. Soc.* **124**, 3703 (2002).
- T. SASAMORI, Y. ARAI, N. TAKEDA, R. OKAZAKI, Y. FURUKAWA, M. KIMURA, S. NAGASE and N. TOKITOH**, "Syntheses, Structures and Properties of Kinetically Stabilized Distibenes and Dibismuthenes, Novel Doubly Bonded Systems between Heavier Group 15 Elements," *Bull. Chem. Soc. Jpn.* **75**, 661 (2002).
- T. WAKAHARA, A. HAN, Y. NIINO, Y. MAEDA, T. AKASAKA, T. SUZUKI, K. YAMAMOTO, M. KAKO, Y. NAKADAIRA, K. KOBAYASHI and S. NAGASE**, "Silylation of Higher Fullerenes," *J. Mater. Chem.* **12**, 2061 (2002).
- T. WAKAHARA, S. OKUBO, M. KONDO, Y. MAEDA, T. AKASAKA, M. WAELCHLI, M. KAKO, K. KOBAYASHI, S. NAGASE, T. KATO, K. YAMAMOTO, X. GAO, E. V. CAEMELBECKE and K. M. KADISH**, "Ionization and Structural Determination of the Major Isomer of  $\text{Pr}@C_{82}$ ," *Chem. Phys. Lett.* **360**, 235 (2002).
- T. WAKAHARA, Y. NIINO, T. KATO, Y. MAEDA, T. AKASAKA, M. T. H. LIU, K. KOBAYASHI and S. NAGASE**, "A Non-Spectroscopic Method to Determine the Photolytic Decomposition Pathways of 3-Chloro-3-Alkyldiazirine; Carbene, Diazo and Rearrangement in Excited State," *J. Am. Chem. Soc.* **124**, 9465 (2002).
- K. -Y. AKIBA, S. MATSUKAWA, T. ADACHI, Y. YAMAMOTO, S. Y. RE and S. NAGASE**, "Effect of  $\sigma^*_{\text{P-O}}$  Orbital on Structure, Stereomutation, and Reactivity of C-Apical O-Equatorial Spirophosphoranes," *Phosphorus, Sulfur Silicon Relat. Elem.* **177**, 1671 (2002).
- T. NAKAZAWA, S. BAN, Y. OKUDA, M. MASUYA, A. MITSUTAKE and Y. OKAMOTO**, "A PH-Dependent Variation in  $\alpha$ -Helix Structure of the S-Peptide of Ribonuclease A Studied by Monte Carlo Simulated Annealing," *Biopolymers* **63**, 273 (2002).
- T. NAGASIMA, Y. SUGITA, A. MITSUTAKE and Y. OKAMOTO**, "Generalized-Ensemble Simulations of Spin Systems and Protein Systems," *Comput. Phys. Commun.* **146**, 69 (2002).
- G. V. MIL'NIKOV and H. NAKAMURA**, "Use of Diabatic Basis in the Adiabatic-by-Sector R-Matrix Propagation Method in Time-Independent Reactive Scattering Calculations," *Comput. Phys. Commun.* **140**, 381 (2001).
- G. V. MIL'NIKOV and H. NAKAMURA**, "Practical Implementation of the Instanton Theory for the Ground State Tunneling Splitting," *J. Chem. Phys.* **115**, 6881 (2001).
- C. ZHU, H. KAMISAKA and H. NAKAMURA**, "Significant Improvement of the Trajectory Surface Hopping Method by the Zhu-Nakamura Theory," *J. Chem. Phys.* **115**, 11036 (2001).
- G. V. MIL'NIKOV and H. NAKAMURA**, "Regularization of Scattering Calculations at R-Matrix Poles," *J. Phys. B: At. Mol. Opt. Phys.* **34**, L791 (2001).
- H. KAMISAKA, W. BIAN, K. NOBUSADA and H. NAKAMURA**, "Accurate Quantum Dynamics of Electronically Nonadiabatic Chemical Reactions in the  $\text{DH}_2^+$  System," *J. Chem. Phys.* **116**, 654 (2002).
- C. ZHU, H. KAMISAKA and H. NAKAMURA**, "New Implementation of the Trajectory Surface Hopping Method with Use of the Zhu-Nakamura Theory. II. Application to the Charge Transfer Processes in the  $3\text{D DH}_2^+$

System," *J. Chem. Phys.* **116**, 3234 (2002).

**P. KOLORENC, M. CÍZEK, J. HORÁČEK, G. V. MIL'NIKOV and H. NAKAMURA**, "Study of Dissociative Electron Attachment to HI Molecule by using R-matrix Representation for Green's Function," *Physica Scripta* **65**, 328 (2002).

**Y. SUZUKI and Y. TANIMURA**, "Probing a Colored-Noise Induced Peak of a Strongly Damped Brownian System by One- and Two-Dimensional Spectroscopy," *Chem. Phys. Lett.* **358**, 51 (2002).

**Y. TANIMURA, V. B. P. LEITE and J. N. ONUCHIC**, "The Energy Landscape for Solvent Dynamics in Electron Transfer Reactions: a Minimalist Model," *J. Chem. Phys.* **117**, 2172 (2002).

**O. HINO, Y. TANIMURA and S. TEN-NO**, "Biorthogonal Approach for Explicitly Correlated Calculations Using the Transcorrelated Hamiltonian," *J. Chem. Phys.* **115**, 7865 (2001).

**O. HINO, Y. TANIMURA and S. TEN-NO**, "Application of the Transcorrelated Hamiltonian to the Linearized Coupled Cluster Singles and Doubles Model," *Chem. Phys. Lett.* **353**, 317 (2002).

**A. MASUHARA, H. KASAI, T. KATO, S. OKADA, H. OIKAWA, Y. NOZUE, S.K. TRIPATHY and H. NAKANISHI**, "Hetero-Multilayered Thin Films Made Up of Polydiacetylene Microcrystals and Metal Fine Particles," *J. Macromol. Sci.-Pure appl. Chem. A* **38**, 1371 (2002).

**S. SAITO**, "Electronic Properties of Nanotube Based Materials," *Tours 2000 Symposium on Nuclear Physics IV*, M. Amould, *et al.*, Eds., American Institute of Physics Conference Proceedings **561**, 214 (2001).

**N. HAMADA, M. YAMAJI, S. OKADA and S. SAITO**, "Dielectric Function of C<sub>60</sub>-Encapsulating Nanotube," *Proc. International Symposium on Nanonetwork Materials: Fullerenes, Nanotubes, and Related Systems* (Kamakura, 15–18 January 2001), S. Saito *et al.*, Eds., American Institute of Physics Conference Proceedings **590**, 201 (2001).

**S. OKADA, S. SAITO, A. OSHIYAMA and Y. MIYAMOTO**, "Electronic Structure and Energetics of Carbon Nanotubes Encapsulating C<sub>60</sub>," *Proc. International Symposium on Nanonetwork Materials: Fullerenes, Nanotubes, and Related Systems* (Kamakura, 15–18 January 2001), S. Saito *et al.*, Eds., American Institute of Physics Conference Proceedings **590**, 173 (2001).

**S. OKADA, S. SAITO and A. OSHIYAMA**, "Semiconducting Form of the First-Row Elements: C<sub>60</sub> Chain Encapsulated in BN Nanotubes," *Phys. Rev. B* **64**, 20130 (2001).

**K. UMEMOTO, S. SAITO, S. BERBER and D. TOMANEK**, "Carbon Foam: Spanning the Phase Space between Graphite and Diamond," *Physical Review B* **64**, 193409-1 (2001).

**Y. MIYAMOTO, S. SAITO and D. TOMANEK**, "Electronic Interwall Interactions and Charge Redistribution in Multiwall Nanotubes," *Phys. Rev. B* **65**, 041402-1 (2001).

**K. UMEMOTO and S. SAITO**, "Electronic Structure of Ba<sub>4</sub>C<sub>60</sub> and Cs<sub>4</sub>C<sub>60</sub>," *Proc. International Symposium on Nanonetwork Materials: Fullerenes, Nanotubes, and Related Systems* (Kamakura, 15–18 January 2001), S. Saito *et al.*, Eds., American Institute of Physics Conference Proceedings **590**, 305 (2001).

**A. Oshiyama, S. Okada and S. Saito**, "Prediction of Electroic Properties of Carbon-Based Nanotstructures," *Physica B* **323**, 21 (2002).

**T. MIYAKE and S. SAITO**, "Electronic Structure of Potassium-Doped Carbon Nanotubes," *Physica B* **323**, 219 (2002).

**S. OKADA, S. SAITO and A. OSHIYAMA**, "Electronic and Geometric Structures of Multi-Walled BN Nanotubes," *Physica B* **323**, 224 (2002).

**K. KANAMITSU and S. SAITO**, "Geometries, Electronic Properties, and Energetics of Isolated Single Walled Carbon Nanotubes," *J. Phys. Soc. Jpn.* **71**, 483 (2002).

**S. OKADA, S. SAITO and A. OSHIYAMA**, "Interwall Interaction and Electronic Structure of Double-Walled BN Nanotubes," *Phys. Rev. B* **65**, 165410 (2002).

**T. MIYAKE and S. SAITO**, "Electronic Structure of Potassium-Doped Carbon Nanotubes," *Phys. Rev. B* **65**, 165419 (2002).

**M. KAMIYA, T. TSUNEDA and K. HIRAO**, "A Density Functional Study of van der Waals Interactions," *J. Chem. Phys.* **117**, 6010 (2002).

**W. LIE, D. G. FEDROV and K. HIRAO**, "Theoretical Study of the Reaction XY<sub>4</sub> = XY<sub>3</sub> + Y, where X = C, Si, Ge, Sn, Pb and Y = CH<sub>3</sub>, C<sub>2</sub>H<sub>5</sub>," *J. Phys. Chem. A* **106**, 7057 (2002).

**J. PAULOVIC, T. NAKAJIMA, K. HIRAO and L. SELJO**, "Third-Order Douglas-Kroll Ab Initio Model Potential for Actinides," *J. Chem. Phys.* **117**, 3597 (2002).

**M. DUPUIS, Y. KAWASHIMA and K. HIRAO**, "The QM/MM-pol-vib/CAV Solvation Model with Polarizable MM for Excited States: II. Application to the Blue Shift in H<sub>2</sub>CO <sup>1</sup>(π\* ← n) Excitation," *J. Chem. Phys.* **117**, 1255 (2002).

**M. DUPUIS, M. AIDA, Y. KAWASHIMA and K. HIRAO**, "The QM/MM-pol-vib/CAV Solvation Model With Polarizable MM for Excited States: I. Energy and Gradients Formulation and Implementation," *J. Chem. Phys.* **117**, 1242 (2002).

**Y. KAWASHIMA, M. DUPUIS and K. HIRAO**, "The QM/MM-pol-vib/CAV Solvation Model Extended to the Monte Carlo Method: Application to the Blue Shift of the H<sub>2</sub>CO <sup>1</sup>(π\* ← n) Excitation," *J. Chem. Phys.* **117**, 248 (2002).

- T. TSUCHIYA, T. NAKAJIMA, K. HIRAO and L. SEIJO**, "A Third-Order Douglas-Kroll Ab Initio Model Potential for Lanthanides," *Chem. Phys. Lett.* **361**, 334 (2002).
- T. YANAI, T. NAKAJIMA, Y. ISHIKAWA, and K. HIRAO**, "Highly Efficient Algorithm for Electron Repulsion Integrals over Relativistic Four-Component Gaussian-Type Spinors," *J. Chem. Phys.* **116**, 10122 (2002).
- H. A. WITEK, D. G. FEDOROV, A. VIEL, P-O. WIDMARK and K. HIRAO**, "Theoretical Study of the Unusual Potential Energy Curve of the  $A^1\Sigma^+$  State of AgH," *J. Chem. Phys.* **116**, 8396 (2002).
- T. NAKAJIMA and K. HIRAO**, "Accurate Relativistic Gaussian Basis Sets Determined by the Third-Order Douglas-Kroll Approximation with a Finite-Nucleus Model," *J. Chem. Phys.* **116**, 8270 (2002)
- K. YAGI, T. TAKETSUGU and K. HIRAO**, "A New Analytic Form of Ab Initio Potential Energy Function: An Application to H<sub>2</sub>O," *J. Chem. Phys.* **116**, 3963 (2002).
- H. NAKANO, R. UCHIYAMA and K. HIRAO**, "Quasi-Degenerate Perturbation Theory with General Multiconfiguration Self-Consistent Field Reference Functions," *J. Comput. Chem.* **23**, 1166 (2002).
- Y. NAKAO, Y. K. CHOE and K. HIRAO**, "A CASCI-MRMP Method Based on Kohn-Sham Orbitals," *Mol. Phys. (Davidson Special Issue)* **100**, 729 (2002).
- R. C. DEKA and K. HIRAO**, "Lewis Acidity and Basicity of Cation-Exchanged Zeolites: QM/MM and Density Functional Studies," *J. Mol. Catal. A-Chem.* **181**, 275 (2002).
- H. A. WITEK, Y. -K. CHOE, J. P. FINLEY and K. HIRAO**, "Intruder-State Avoidance Multireference Møller-Plesset Perturbation Theory," *J. Comput. Chem.* **23**, 957 (2002).
- K. YAGI, T. TAKETSUGU and K. HIRAO**, "Generation of Full-Dimensional Potential Energy Surface of Intramolecular Hydrogen Atom Transfer in Malonaldehyde and Tunneling Dynamics," *J. Chem. Phys.* **115**, 10647 (2001).
- D. AJITHA and K. HIRAO**, "Dipole Moments of  $^2\Sigma$  and  $^2\Pi$  Ktates of CN Radical at Different Internuclear Distances *via* Fock Space Multi-Reference Coupled Cluster Linear Response Approach," *Chem. Phys. Lett.* **347**, 121 (2001).
- T. NAKAJIMA and K. HIRAO**, "Relativistic Effects for Polarizabilities and Hyperpolarizabilities of Rare Gas Atoms," *Chem. Lett.* 766 (2001).
- Y. KUROSAKI and T. TAKAYANAGI**, "Ab initio Molecular Orbital Study of O(<sup>1</sup>D) Insertion into C–C Bond in Cyclopropane and Ethane," *Chem. Phys. Lett.* **355**, 424 (2002).
- T. TAKAYANAGI**, "Quantum Scattering Calculations of the O(<sup>1</sup>D) + N<sub>2</sub>(X<sup>1</sup> $\Sigma_g^+$ )  $\rightarrow$  O(<sup>3</sup>P) + N<sub>2</sub>(X<sup>1</sup> $\Sigma_g^+$ ) Spin-Forbidden Electronic Quenching Collision," *J. Phys. Chem. A* **106**, 4914 (2002).
- T. TAKAYANAGI and H. AKAGI**, "Translational Energy Dependence of NO + NO / N<sub>2</sub> + O<sub>2</sub> Product Branching in the O(<sup>1</sup>D) + N<sub>2</sub>O Reaction: a Classical Trajectory Study on a New Global Potential Energy Surface for the Lowest <sup>1</sup>A' State," *Chem. Phys. Lett.* **363**, 298 (2002).
- T. TAKAYANAGI and M. SHIGA**, "Path Integral Molecular Dynamics Combined with Discrete-Variable-Representation Approach: the Effect of Solvation Structures on Vibrational Spectra of Cl<sub>2</sub> in Helium Clusters," *Chem. Phys. Lett.* **362**, 504 (2002).
- A. KOVALENKO and F. HIRATA**, "A Replica Reference Interaction Site Model Theory for a Polar Molecular Liquid Sorbed in a Disordered Microporous Material with Polar Chemical Groups," *J. Chem. Phys.* **115**, 8620 (2001).
- H. SATO and F. HIRATA**, "Realization of Three-Dimensional Solvation-Structure from Site-Site Radial Distribution Functions in Liquids," *Bull. Chem. Soc. Jpn.* **74**, 1831 (2001).
- T. IMAI, Y. HARANO, A. KOVALENKO and F. HIRATA**, "Theoretical Study for Volume Changes Associated with the Helix-Coil Transition of Polypeptides," *Biopolymers* **59**, 512 (2001).
- T. SUMI, T. IMAI and F. HIRATA**, "Integral Equations for Molecular Fluids Based on Interaction Site Model: Density-Functional Formulation," *J. Chem. Phys.* **115**, 6653 (2001).
- T. YAMAZAKI, H. SATO and F. HIRATA**, "Solvent Effect on the Nuclear Magnetic Shielding: Ab Initio Study by the Combined Reference Interaction Site Model and Electronic Structure Theories," *J. Chem. Phys.* **115**, 8949 (2001).
- F. HIRATA and S-H. CHONG**, "Collective Density Fluctuations and Dynamics of Ions in Water Studied by the Interaction-Site Model of Liquids," *Cond. Matter Phys.* **4**, 261 (2001).
- T. YAMAGUCHI and F. HIRATA**, "Site-Site Mode-Coupling Theory for the Shear Viscosity of Molecular Liquids," *J. Chem. Phys.* **115**, 9340 (2001).
- A. KOVALENKO and F. HIRATA**, "First Principle Realization of a van der Waals-Maxwell Theory for Water," *Chem. Phys. Lett.* **349**, 496 (2001).
- A. KOVALENKO and F. HIRATA**, "Description of a Polar Molecular Liquid in a Disordered Microporous Material with Activating Chemical Groups by a Replica RISM Theory," *Cond. Matter Phys.* **4**, 643 (2001).
- M. KINOSHITA, T. IMAI, A. KOVALENKO and F. HIRATA**, "Improvement of the Reference Interaction Site Model Theory for Calculating the Partial Molar Volume of Amino Acids and Polypeptides," *Chem. Phys. Lett.* **348**, 337 (2001).
- T. YAMAGUCHI and F. HIRATA**, "Translational Diffusion and Reorientational Relaxation of Water Analyzed by Site-Site Generalized Langevin Theory," *J. Chem. Phys.* **116**, 2502 (2002).
- H. SATO and F. HIRATA**, "Equilibrium and Nonequilibrium Solvation Structure of Hexammineruthenium (II,III)



in Aqueous Solution: Ab Initio RISM-SCF Study," *J. Phys. Chem. A* **106**, 2300 (2002).

**K. YOSHIDA, KOVALENKO, T. YAMAGUCHI and F. HIRATA**, "Structure of *tert*-Butyl Alcohol-Water Mixtures Studied by the RISM Theory," *J. Phys. Chem. B* **106**, 5042 (2002).

**T. IMAI, H. NOMURA, M. KINOSHITA and F. HIRATA**, "Partial Molar Volumes and Compressibilities of Alkali-Halide Ions in Aqueous Solution: Hydration Shell Analysis with an Integral Equation Theory of Molecular Liquids," *J. Phys. Chem.* **106**, 7308 (2002).

**T. YAMAGUCHI and F. HIRATA**, "Interaction-Site Model Description of the Reorientational Relaxation of Molecular Liquids: Incorporation of the Interaxial Coupling into the Site-Site Generalized Langevin/Mode-Coupling Theory," *J. Chem. Phys.* **117**, 2216 (2002).

**M. KUWABARA and K. YONEMITSU**, "Ground State Phases and Optical Properties in Extended Peierls-Hubbard Models for Halogen-Bridged Binuclear Metal Complexes," *J. Mater. Chem.* **11**, 2163 (2001).

**X. SUN, R. L. FU, K. YONEMITSU and K. NASU**, "Photoinduced Phenomenon in Polymers," *Phys. Rev. A* **64**, 032504 (2001).

**K. YONEMITSU**, "Intra- and Inter-Chain Excitations near a Quantum Phase Transition in Quasi-One-Dimensional Conductors," *Mol. Cryst. Liq. Cryst.* **376**, 53 (2002).

**M. MORI and K. YONEMITSU**, "Optical Conductivity for Possible Ground States of Dimerized Two-Band Pd(dmit)<sub>2</sub> Salts," *Mol. Cryst. Liq. Cryst.* **376**, 141 (2002).

**M. KUWABARA and K. YONEMITSU**, "Optical Excitations in XMMX Monomers and MMX Chains," *Mol. Cryst. Liq. Cryst.* **376**, 251 (2002).

**J. KISHINE, P. A. LEE and X. G. WEN**, "Signature of the Staggered Flux State around a Superconducting Vortex in Underdoped Cuprates," *Phys. Rev. B* **65**, 064526 (2002).

**K. YONEMITSU**, "Quantum and Thermal Charge-Transfer Fluctuations for Neutral-Ionic Phase Transitions in the One-Dimensional Extended Hubbard Model with Alternating Potentials," *Phys. Rev. B* **65**, 085105 (2002).

**K. YONEMITSU**, "Finite-Temperature Phase Diagram of Mixed-Stack Charge-Transfer Complexes," *J. Phys. Chem. Solids* **63**, 1495 (2002).

**J. KISHINE**, "Underlying SU(2) Gauge Structure and Hidden Staggered Flux State in the Lightly Doped Spin Liquid," *J. Phys. Chem. Solids* **63**, 1559 (2002).

**J. KISHINE and K. YONEMITSU**, "Dimensional Crossovers and Phase Transitions in Strongly Correlated Low-Dimensional Electron Systems: Renormalization-Group Study," *Int. J. Mod. Phys. B* **16**, 711 (2002).

**K. YONEMITSU**, "Lattice and Magnetic Instabilities near the Neutral-Ionic Phase Transition of the One-Dimensional Extended Hubbard Model with Alternating Potentials in the Thermodynamic Limit," *Phys. Rev. B* **65**, 205105 (2002).

**K. YONEMITSU, M. KUWABARA and N. MIYASHITA**, "Variation Mechanisms of Ground-State and Optical-Excitation Properties in Quasi-One-Dimensional Two-Band Electron Systems," *Mol. Cryst. Liq. Cryst.* **379**, 467 (2002).

**K. YONEMITSU**, "Collective Excitations and Confinement in the Excitation Spectra of the Spinless Fermion Model on a Ladder," *Phys. Rev. B* **66**, 035121 (2002).

### Department of Molecular Structure

**H. OKAMOTO and M. KINOSHITA**, "Picosecond Infrared Spectrum of 4-(Pyrrol-1-yl)benzoxazole: Structure of the Excited Charge-Transfer States of Donor-Acceptor Systems," *J. Phys. Chem. A* **106**, 3485 (2002).

**H. OKAMOTO, M. KINOSHITA, S. KOHTANI, R. NAKAGAKI and K. A. ZACHARIASSE**, "Picosecond Infrared Spectra and Structure of Locally Excited and Charge Transfer Excited States of Isotope-Labeled 4-(Dimethylamino)benzoxazoles," *Bull. Chem. Soc. Jpn.* **75**, 957 (2002).

**T. YAMAZAKI, N. MORITA, R. S. HAYANO, E. WIDMANN and J. EADES**, "Antiprotonic Helium," *Phys. Rep.* **366**, 183 (2002).

**K. TOZAWA, H. YAGI, K. HISAMATSU, K. OZAWA, M. YOSHIDA and H. AKUTSU**, "Functions and ATP-Binding Responses of the Twelve Histidine Residues in the TF<sub>1</sub>-ATPase  $\beta$  Subunit," *J. Biochem.* **130**, 527 (2001).

**K. SUGASE, Y. OYAMA, K. KITANO, T. IWASHITA, T. FUJIWARA, H. AKUTSU and M. ISHIGURO**, "Designing Analogs of Mini Atrial Natriuretic Peptide Based on Structural Analysis by NMR and Restrained Molecular Dynamics," *J. Med. Chem.* **45**, 881 (2002).

**E. HARADA, Y. FUKUOKA, T. OHMURA, A. FUKUNISHI, G. KAWAI, T. FUJIWARA and H. AKUTSU**, "Redox-Coupled Conformational Alternations in Cytochrome *c*<sub>3</sub> from *D. vulgaris* Miyazaki F on the Basis of its Reduced Solution Structure," *J. Mol. Biol.* **319**, 767 (2002).

**A. BANDARA, S. S. KANO, K. ONDA, S. KATANO, J. KUBOTA, K. DOMEN, C. HIROSE and A. WADA**, "SFG Spectroscopy of CO/Ni(111): UV Pumping and Transient Hot Band Transition of Adsorbed CO," *Bull. Chem. Soc. Jpn.* **75**, 1125 (2002).

**K. ONDA, M. NAKAGAWA, T. ASAKAI, R. WATASE, A. WADA, K. ICHIMURA and C. HIROSE**,

“Controlling Packing Structure of Hydrophobic Alkyl Tails of Monolayered Films of Ion-Paired Macrocyclic Amphiphiles as Studied by Sum-Frequency Generation Spectroscopy,” *J. Phys. Chem. B* **106**, 3855 (2002).

**A. FURUBE, T. SHIOZAWA, A. ISHIKAWA, A. WADA, K. DOMEN and C. HIROSE**, “Femtosecond Transient Absorption Spectroscopy on Photocatalysts,  $K_4Nb_6O_{17}$  and  $Ru(bpy)_3^{2+}$  Intercalated  $K_4Nb_6O_{17}$  Thin Films,” *J. Phys. Chem. B* **106**, 3065 (2002).

**K. KUSAFUKA, H. NOGUCHI, K. ONDA, C. HIROSE, K. DOMEN and A. WADA**, “Time-Resolved Study of Formate/Ni(111) Surface by Picosecond SFG Spectroscopy,” *Surf. Sci.* **502/503**, 313 (2002).

**K. ONDA, A. WADA, K. DOMEN and C. HIROSE**, “Realtime Observation of Desorption Process of Isobutene in Zeolite Using Picosecond Infrared Lasers,” *Surf. Sci.* **502/503**, 319 (2002).

**H. TAKABA, K. KUSAFUKA, M. N. GAMO, Y. SATO, T. ANDO, J. KUBOTA, A. WADA and C. HIROSE**, “Vibrational Sum-Frequency Observation of Synthetic Diamonds,” *Diam. Rel. Mater.* **10**, 1643 (2001).

**K. ONDA, K. TANABE, H. NOGUCHI, A. WADA, T. SHIDO, A. YAMAGUCHI and Y. IWASAWA**, “Surface Hydroxyl Group and Adsorbed Water on  $\gamma$ - $Al_2O_3$  Studied by Picosecond Infrared Pump-Probe Experiment,” *J. Phys. Chem. B* **105**, 11456 (2001).

**D. MATSUMURA, T. YOKOYAMA, K. AMEMIYA, S. KITAGAWA and T. OHTA**, “X-Ray Magnetic Circular Dichroism Study on Spin Reorientation Transition of Magnetic Thin Films Induced by Surface Chemisorption,” *Phys. Rev. B* **66**, 024402 (2002).

**S. OKUBO, T. KATO, M. INAKUMA and H. SHINOHARA**, “Separation and Characterization of ESR-Active Lanthanum Endohedral Fullerenes,” *New Diamond and Frontier Carbon Technology* **11**, 285 (2001).

**S. S. SEOMUN, J. K. VIJI, N. HAYASHI, T. KATO and A. FUKUDA**, “Surface Molecular Alignment by In-Plane Anchoring in the Cell Showing the V-Shaped Switching,” *Appl. Phys. Lett.* **79**, 940 (2001).

**T. IKOMA, Q. ZHANG, F. SAITO, K. AKIYAMA, S. TERO-KUBOTA and T. KATO**, “Radicals in the Mechanochemical Dechlorination of Hazardous Organochlorine Using CaO Nanoparticles,” *Bull. Chem. Soc. Jpn.* **74**, 2303 (2001).

**A. ITO, H. INO, K. TANAKA, K. KANEMOTO and T. KATO**, “Facile Synthesis, Crystal Structures, and High-Spin Cationic States of All-para-Brominated Oligo(*N*-phenyl-*m*-aniline)s,” *J. Org. Chem.* **67**, 491 (2002).

**T. KATO, S. OKUBO, M. INAKUMA and H. SHINOHARA**, “Electronic State of Scandium Trimer Encapsulated in  $C_{82}$  Cage,” *Phys. Solid State* **44**, 410 (2002).

#### Department of Electronic Structure

**K. HINO, Y. INOKUCHI, K. KOSUGI, H. SEKIYA, Y. HOSOKOSHI, K. INOUE and N. NISHI**, “Photochemical Generation of High Spin Clusters in Solution: Cyclopentadienyl-Vanadium $_mO_n$ ,” *J. Phys. Chem. B* **106**, 1290 (2002).

**H. MORI, H. KUGISAKI, Y. INOKUCHI, N. NISHI, E. MIYOSHI, K. SAKOTA, K. OHASHI and H. SEKIYA**, “Structure and Intermolecular Hydrogen Bond of Jet-Cooled *p*-Aminophenol- $(H_2O)_1$  Studied by Electronic and IR-Dip Spectroscopy and Density Functional Theory Calculations,” *Chem. Phys.* **277**, 105 (2002).

**T. NAKABAYASHI and N. NISHI**, “States of Molecular Associates in Binary Mixtures of Acetic Acid with Protic and Aprotic Polar Solvents: A Raman Spectroscopic Study,” *J. Phys. Chem. A* **106**, 3491 (2002).

**Y. INOKUCHI and N. NISHI**, “Infrared Photodissociation Spectroscopy of Protonated Formic Acid-Water Binary Clusters,  $H^+(HCOOH)_nH_2O$  ( $n = 1-5$ ). Spectroscopic Study of Ion Core Switch Model and Magic Number,” *J. Phys. Chem. A* **106**, 4529 (2002).

**T. NAKABAYASHI, S. KAMO, K. WATANABE, H. SAKURAGI and N. NISHI**, “Observation of Formation Dynamics of Solvated Aromatic Cation Radicals Following Photoionization,” *Chem. Phys. Lett.* **355**, 241 (2002).

**H. MORI, H. KUGISAKI, Y. INOKUCHI, N. NISHI, E. MIYOSHI, K. SAKOTA, K. OHASHI and H. SEKIYA**, “LIF and IR Dip Spectra of Jet-Cooled *p*-Aminophenol- $M$  ( $M = CO, N_2$ ): Hydrogen-Bonded or van der Waals-Bonded Structure?” *J. Phys. Chem. A* **106**, 4886 (2002).

**K. OHASHI, Y. INOKUCHI, N. NISHI and H. SEKIYA**, “Intermolecular Interaction in Aniline-Benzene Hetero-Trimer and Aniline Homo-Trimer Ions,” *Chem. Phys. Lett.* **357**, 223 (2002).

**Y. INOKUCHI, K. OHASHI, H. SEKIYA and N. NISHI**, “Intracluster Proton Transfer in Aniline-Amine Complex Ions,” *Chem. Phys. Lett.* **359**, 288 (2002).

**Y. HONKAWA, Y. INOKUCHI, K. OHASHI, N. NISHI and H. SEKIYA**, “Infrared Photodissociation Spectroscopy of Aniline $^+$ -(water) $_{1,2}$  and Aniline $^+$ -(methanol) $_{1,2}$ ,” *Chem. Phys. Lett.* **358**, 419 (2002).

**M. SAKAI, K. DAIGOKU, S. ISHIUCHI, M. SAEKI, K. HASHIMOTO and M. FUJII**, “Structures of Carbazole- $(H_2O)_n$  ( $n = 1-3$ ) Clusters Studied by IR Dip Spectroscopy and a Quantum Chemical Calculation,” *J. Phys. Chem. A* **105**, 8651 (2001).

**H. YOKOYAMA, H. WATANABE, T. OMI, S. ISHIUCHI and M. FUJII**, “Structure of Hydrogen-Bonded Clusters of 7-Azaindole Studied by IR Dip Spectroscopy and Ab Initio Molecular Orbital Calculation,” *J. Phys. Chem. A* **105**, 9366 (2001).

**S. ISHIUCHI, M. SAKAI, K. DAIGOKU, T. UEDA, T. YAMANAKA, K. HASHIMOTO and M. FUJII**,

“Picosecond Time-Resolved Infrared Spectra of Photo-Excited Phenol-(NH<sub>3</sub>)<sub>3</sub> Cluster,” *Chem. Phys. Lett.* **347**, 87 (2001).

**M. SAEKI, S. ISHIUCHI, M. SAKAI and M. FUJII**, “Structure of 1-Naphthol/Alcohol Clusters Studied by IR Dip Spectroscopy and Ab Initio Molecular Orbital Calculations,” *J. Phys. Chem. A* **105**, 10045 (2001).

**S. KINOSHITA, H. KOJIMA, T. SUZUKI, T. ICHIMURA, K. YOSHIDA, M. SAKAI and M. FUJII**, “Pulsed Field Ionization Zero Kinetic Energy Photoelectron Study on Methylanisole Molecules in a Supersonic Jet,” *Phys. Chem. Chem. Phys.* **3**, 4889 (2001).

**H. G. KJAERGAARD, D. L. HOWARD, D. P. SCHOFIELD, T. W. ROBINSON, S. ISHIUCHI and M. FUJII**, “OH- and CH-Stretching Overtone Spectra of Catechol,” *J. Phys. Chem. A* **106**, 258 (2002).

**K. YOSIDA, K. SUZUKI, S. ISHIUCHI, M. SAKAI, M. FUJII, C. E. H. DESSENT and K. MÜLLER-DETHLEFS**, “The PFI-ZEKE Photoelectron Spectrum of m-Fluorophenol and its Aqueous Complexes: Comparing Intermolecular Vibrations in Rotational Isomers,” *Phys. Chem. Chem. Phys.* **4**, 2534 (2002).

**H. KATAYANAGI and T. SUZUKI**, “Non-Adiabatic Bending Dissociation of OCS: The Effect of Bending Excitation on the Transition Probability,” *Chem. Phys. Lett.* **360**, 104 (2002).

**B. BOTAR, T. YAMASE and E. ISHIKAWA**, “Synthesis and Structure of a Novel Vanadium-Containing Tungstobismustate(III) K<sub>12</sub>[(VO)<sub>3</sub>(BiW<sub>9</sub>O<sub>33</sub>)<sub>2</sub>].30H<sub>2</sub>O,” *Inorg. Chem. Commun.* **4**, 551 (2001).

**H. NARUKE and T. YAMASE**, “Crystallization and Structural Characterization of Two Europium Molybdates, Eu<sub>4</sub>Mo<sub>7</sub>O<sub>27</sub> and Eu<sub>6</sub>Mo<sub>10</sub>O<sub>39</sub>,” *J. Solid State Chem.* **160**, 85 (2001).

**H. MURAKAMI, T. KOZEKI, Y. SUZUKI, S. ONO, H. OHTAKE, N. SARUKURA, E. ISHIKAWA and T. YAMASE**, “Nanocluster Crystals of Lacunary Polyoxometalates: Novel application as Structure Design-Flexible, Inorganic Nonlinear Materials,” *Appl. Phys. Lett.* **79**, 3564 (2001).

**L. YANG, H. NARUKE and T. YAMASE**, “A 3-D Inorganic/Organic Hybrid Vanadium Oxide with Pentacoordinate Co(II) Complex, [Co(4,4'-bipy)V<sub>2</sub>O<sub>6</sub>],” *Acta Crystallogr., Sect. C: Cryst. Struct. Commun.* **57**, 1378 (2001).

**H. NARUKE and T. YAMASE**, “Tb<sub>2</sub>Mo<sub>4</sub>O<sub>15</sub>,” *Acta Crystallogr., Sect. E* **57**, i106 (2001).

**F. GAO, T. YAMASE and H. SUZUKI**, “H<sub>2</sub>O<sub>2</sub>-Based Epoxidation of Bridged-Cyclic Alkenes with [P{Ti(O<sub>2</sub>)<sub>2</sub>W<sub>10</sub>O<sub>38</sub>}<sup>7-</sup> in Monophasic Systems: Active Site and Kinetics,” *J. Mol. Catal., A* **180**, 97 (2002).

**T. YAMASE and P. PROKOP**, “Photochemical Formation of Tire-Shaped Molybdenum Blues: Topology of a Defect Anion, [Mo<sub>142</sub>O<sub>432</sub>H<sub>28</sub>(H<sub>2</sub>O)<sub>58</sub>]<sup>12-</sup>,” *Angew. Chem. Int. Ed. Engl.* **41**, 466 (2002).

**H. NARUKE and T. YAMASE**, “Size-Dependent Population of Trivalent Rare Earth (RE<sup>3+</sup>) in [RE<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>(SbW<sub>9</sub>O<sub>33</sub>)(W<sub>5</sub>O<sub>18</sub>)<sub>2</sub>]<sup>15-</sup>, and Structural Characterization of a Lanthanum-Polyoxotungstate Complex [Lu<sub>3</sub>(H<sub>2</sub>O)<sub>4</sub>(SbW<sub>9</sub>O<sub>33</sub>)<sub>2</sub>(W<sub>5</sub>O<sub>18</sub>)<sub>2</sub>]<sup>21-</sup>,” *Bull. Chem. Soc. Jpn.* **75**, 1275 (2002).

**H. NARUKE and T. YAMASE**, “Gd<sub>4</sub>Mo<sub>7</sub>O<sub>27</sub>, a Novel Phase in the Gd<sub>2</sub>O<sub>3</sub>-MoO<sub>3</sub> System,” *Acta Crystallogr., Sect. E* **58**, i62 (2002).

**T. IIMORI and Y. OHSHIMA**, “S<sub>1</sub>-S<sub>0</sub> Vibronic Spectra of Benzene Clusters Revisited: I. The Tetramer,” *J. Chem. Phys.* **117**, 3656 (2002).

**T. IIMORI, Y. AOKI and Y. OHSHIMA**, “S<sub>1</sub>-S<sub>0</sub> Vibronic Spectra of Benzene Clusters Revisited: II. The Trimer,” *J. Chem. Phys.* **117**, 3675 (2002).

## Department of Molecular Assemblies

**I. SHIROTANI, J. HAYASHI, K. YAKUSHI, K. TAKEDA, T. YOKOTA, K. SHIMIZU, K. AMAYA, A. NAKAYAMA and K. AOKI**, “Pressure-Induced Insulator-to-Metal Transition and Superconductivity in Iodanil, C<sub>6</sub>I<sub>4</sub>O<sub>2</sub>,” *Physica B* **304**, 6 (2001).

**M. MAKSIMUK, K. YAKUSHI, H. TANIGUCHI, K. KANODA and A. KAWAMOTO**, “The C=C Stretching Vibrations of κ-(BEDT-TTF)<sub>2</sub>Cu[N(CN)<sub>2</sub>]Br and its Deuterated Analogues,” *J. Phys. Soc. Jpn.* **70**, 3728 (2001).

**K. YAMAMOTO, K. YAKUSHI, K. MIYAGAWA, K. KANODA and A. KAWAMOTO**, “Charge Ordering in θ-(BEDT-TTF)<sub>2</sub>RbZn(SCN)<sub>4</sub> Studied by Vibration Spectroscopy,” *Phys. Rev. B* **65**, 85110 (2002).

**J. OUYANG, K. YAKUSHI, T. KINOSHITA, N. NANBU, M. AOYAGI, Y. MISAKI and K. TANAKA**, “The Assignment of the In-Plane Molecular Vibrations of the BDT-TTP Electron-Donor Molecule Based on the Polarized Raman and Infrared Spectra, where BDT-TTP is 2,5-bis(1,3-dithiol-2-ylidene)-1,3,4,6-Tetrathiapentalene,” *Spectrochim. Acta, Part A* **58**, 1643 (2002).

**T. NAKAMURA, K. TAKAHASHI, T. ISE, T. SHIRAHATA, M. URUICHI, K. YAKUSHI and T. MORI**, “Magnetic Properties of Organic Spin-Ladder Systems, (BDTFP)<sub>2</sub>X(PhCl)<sub>0.5</sub>,” *Mol. Cryst. Liq. Cryst.* **376**, 95 (2002).

**O. DROZDOVA, H. YAMOCHI, K. YAKUSHI, M. URUICHI and G. SAITO**, “Charge Transfer Degree of BO Complexes,” *Mol. Cryst. Liq. Cryst.* **376**, 135 (2002).

**Y. YAMASHITA, M. TOMURA, M. URUICHI and K. YAKUSHI**, “Synthesis and Properties of π-Extended TTF Analogues and their Cation Radical and Dication Salts,” *Mol. Cryst. Liq. Cryst.* **376**, 19 (2002).

**K. YAKUSHI, J. OUYANG, M. SIMONYAN, Y. MISAKI and K. TANAKA**, “Charge Order in θ-(BDT-



- TTP)<sub>2</sub>Cu(NCS)<sub>2</sub>,” *Mol. Cryst. Liq. Cryst.* **380**, 53 (2002).
- Y. DING, M. SIMONYAN, Y. YONEHARA, M. URUICHI and K. YAKUSHI**, “Formation of Mixed Crystal System Co<sub>x</sub>Ni<sub>1-x</sub>Pc(AsF<sub>6</sub>)<sub>0.5</sub>,” *Mol. Cryst. Liq. Cryst.* **380**, 283 (2002).
- K. YAMAMOTO, K. YAKUSHI, M. INOKUCHI, M. KINOSHITA and G. SAITO**, “Charge Disproportionation and its Ordering Pattern in  $\theta$  and  $\alpha$  Types of BEDT-TTF Salts Studied by Raman and Infrared Spectroscopy,” *Mol. Cryst. Liq. Cryst.* **380**, 221 (2002).
- G. SAITO, H. SASAKI, T. AOKI, Y. YOSHIDA, A. OTSUKA, H. YAMOCHI, O. O. DROZDOVA, K. YAKUSHI, H. KITAGAWA and T. MITANI**, “Complex Formation of Ethylenedioxyethylenedithio-tetrathiafulvalene (EDOEDT-TTF: EOET) and its Self-Assembling Ability,” *J. Mater. Chem.* **12**, 1640 (2002).
- T. YAMAMOTO, H. TAJIMA, R. KATO, M. URUICHI and K. YAKUSHI**, “Raman Spectra of (Me<sub>2</sub>-DCNQI)<sub>2</sub>Cu<sub>x</sub>Li<sub>1-x</sub> ( $0 < x < 1$ ). The Evidence of Charge Separation at Room Temperature in a One-Dimensional Conductor Having a Quarter-Filled Band,” *J. Phys. Soc. Jpn.* **71**, 1956 (2002).
- T. NAKAMURA, K. TAKAHASHI, T. SHIRAHATA, M. URUICHI, K. YAKUSHI and T. MORI**, “Magnetic Investigation of Possible Quasi-One-Dimensional Two-Leg Ladder Systems, (BDTFP)<sub>2</sub>X(PhCl)<sub>0.5</sub> (X = PF<sub>6</sub>, AsF<sub>6</sub>),” *J. Phys. Soc. Jpn.* **71**, 2022 (2002).
- M. URUICHI, K. YAKUSHI, T. SHIRAHATA, K. TAKAHASHI, T. MORI and T. NAKAMURA**, “Structural Phase Transition in Quasi-1D Conductors, (BDTFP)<sub>2</sub>X(PhCl)<sub>0.5</sub> (X = PF<sub>6</sub>, AsF<sub>6</sub>) [BDTFP = 5,7-bis(1,3-dithiol-2-ylidene)-5,7-dihydrofuro[3,4-*b*]pyrazine],” *J. Mater. Chem.* **12**, 2696 (2002).
- T. NAKAMURA, T. TAKAHASHI, S. AONUMA and R. KATO**, “EPR Investigation of the Electronic States in  $\beta'$ -Type [Pd(dmit)<sub>2</sub>]<sub>2</sub> Compounds (Where dmit is the 1,3-Dithia-2-Thione-4,5-Dithiolato),” *J. Mater. Chem.* **11**, 2159 (2001).
- T. NAKAMURA, K. TAKAHASHI, T. ISE, T. SHIRAHATA, M. URUICHI, K. YAKUSHI and T. MORI**, “Magnetic Properties of Organic Spin-Ladder Systems, (BDTFP)<sub>2</sub>X(PhCl)<sub>0.5</sub>,” *Mol. Cryst. Liq. Cryst.* **376**, 95 (2002).
- S. FUJIYAMA and T. NAKAMURA**, “NMR Study of Charge Localized States of (TMTTF)<sub>2</sub>Br,” *J. Phys. Chem. Solids* **63**, 1259 (2002).
- S. FUJIYAMA, M. TAKIGAWA, S. HORII, N. MOTOYAMA, H. EISAKI and S. UCHIDA**, “NMR Observation of Charge Fluctuations in Quasi-One-Dimensional Cuprates,” *J. Phys. Chem. Solids* **63**, 1119 (2002).
- T. NAKAMURA, K. TAKAHASHI, T. SHIRAHATA, M. URUICHI, K. YAKUSHI and T. MORI**, “Magnetic Investigation of Possible Quasi-One-Dimensional Two-Leg Ladder Systems, (BDTFP)<sub>2</sub>X(PhCl)<sub>0.5</sub> (X = PF<sub>6</sub>, AsF<sub>6</sub>),” *J. Phys. Soc. Jpn.* **71**, 2022 (2002).
- T. NAITO, T. INABE, H. KOBAYASHI and A. KOBAYASHI**, “A New Molecular Metal Based on Pd(dmit)<sub>2</sub>: Synthesis, Structure and Electrical Properties of (C<sub>7</sub>H<sub>13</sub>NH)[Pd(dmit)<sub>2</sub>]<sub>2</sub> (dmit<sup>2-</sup> = 2-thioxo-1,3-dithiole-4,5-dithiolate),” *J. Mater. Chem.* **11**, 2199 (2001).
- V. GRITSENKO, H. TANAKA, H. KOBAYASHI and A. KOBAYASHI**, “A New Molecular Superconductor,  $\kappa$ -(BETS)<sub>2</sub>TiCl<sub>4</sub> (BETS = bis(ethylenedithio)tetraselenafulvalene),” *J. Mater. Chem.* **11**, 2410 (2001).
- R. B. LYUBOVSKII, S. I. PESOTSKII, S. V. KONOVALIKHIN, G. V. SHILOV, A. KOBAYASHI, H. KOBAYASHI, V. I. NIZHANKOVSKII, J. A. A. J. PERENBOOM, O. A. BOGDANOVA, E. I. ZHILYAEVA and R. N. LYUBOVSKAYA**, “Crystal Structure, Electrical Transport, Electronic Band structure and Quantum Oscillations Studies of the Organic Conducting Salt,  $\theta$ -(BETS)<sub>4</sub>HgBr<sub>4</sub>(C<sub>6</sub>H<sub>5</sub>Cl),” *Synth. Met.* **123**, 149 (2001).
- H. MORIYAMA, S. NAGAYAMA, T. MOCHIDA and H. KOBAYASHI**, “Nickel Complexes with Extended Tetrathiafulvalene Dithiolate Ligands,” *Synth. Met.* **120**, 973 (2001).
- C. PALASSIS, M. MOLA, J. TRITZ, S. HILL, S. UJI, K. KAWANO, M. TAMURA, T. NAITO and H. KOBAYASHI**, “Periodic Orbit Resonances in  $\kappa$ -ET<sub>2</sub>I<sub>3</sub>,” *Synth. Met.* **120**, 999 (2001).
- H. SHINAGAWA, S. UJI, T. TERASHIMA, H. TANAKA, H. KOBAYASHI, A. KOBAYASHI and M. TOKUMOTO**, “Phase Transition in Magnetic Field Parallel to the Conducting Plane for  $\lambda$ -(BETS)<sub>2</sub>FeCl<sub>4</sub>,” *Synth. Met.* **120**, 929 (2001).
- E. ZHILYAEVA, O. BOGDANOVA, R. LYUBOVSKAYA, S. PESOTSKII, J. PERENBOOM, S. KONOVALIKHIN, G. SHILOV, A. KOBAYASHI and H. KOBAYASHI**, “New BETS Based Molecular Conductors with Bromomercurate Anions,” *Synth. Met.* **120**, 1089 (2001).
- T. I. MAKAROVA, P. SCHARFF, B. SUNDQVIST, B. NARYMBETOV, H. KOBAYASHI, M. TOKUMOTO, V. A. DAVYDOV, A. V. RAKHMANINA and L. S. KASHEVAROVA**, “Anisotropic Metallic Properties of Highly-Oriented Rhombohedral C<sub>60</sub> Polymer,” *Synth. Met.* **121**, 1099 (2001).
- B. NARYMBETOV, A. OMERZU, V. V. KABANOV, M. TOKUMOTO, H. KOBAYASHI and D. MIHAJLOVIC**, “C<sub>60</sub> Molecular Configurations Leading Ferromagnetic Exchange Interactions in TDAE-C<sub>60</sub>,” *Trans. Mater. Res. Soc. Jpn.* **26**, 1143 (2001).
- D. Z. KURMAEV, A. MOEWES, U. SCHWINGENSCHLOGL, R. CLAESSEN, M. I. KATSNELSON, H. KOBAYASHI, S. KAGOSHIMA, Y. MISAKI, D. L. EDERER, K. ENDO and M. YANAGIHARA**, “Electronic Structure of Charge Transfer Salts,” *Phys. Rev. B* **64**, 233107-1 (2001).
- S. UJI, H. KOBAYASHI, L. BALICAS and J. S. BROOKS**, “Superconductivity in an Organic Conductor Stabilized by a High Magnetic Field,” *Adv. Mater.* **14**, 243 (2002).

- S. UJI, C. TERAKURA, T. TERASHIMA, T. YAKABE, Y. TERAII, M. TOKUMOTO, A. KOBAYASHI, F. SAKAI, H. TANAKA and H. KOBAYASHI, "Fermi Surface and Internal Magnetic Field of Organic Conductors  $\lambda$ -(BETS)<sub>2</sub>Fe<sub>x</sub>Ga<sub>1-x</sub>Cl<sub>4</sub>," *Phys. Rev. B* **65**, 113101 (2002).
- B. NARYMBETOV, A. OMERZU, V. KAVANOV, M. TOKUMOTO, H. KOBAYASHI and D. MIHAJLOVIC, "C<sub>60</sub> Molecular Configurations Leading to Ferromagnetic Exchange Interactions in TDAE·C<sub>60</sub>," *Russian, J. Solid. State Phys.* **44**, 422 (2002).
- E. FUJIWARA, V. GRITSENKO, H. FUJIWARA, I. TAMURA, H. KOBAYASHI, M. TOKUMOTO and A. KOBAYASHI, "Magnetic Molecular Conductors Based on BETS Molecules and Divalent Magnetic Anions [BETS = Bis(ethylenedithio)tetraselenafulvalene]," *Inorg. Chem.* **41**, 3230 (2002).
- H. FUJIWARA, H. KOBAYASHI, E. FUJIWARA and A. KOBAYASHI, "An indication of Magnetic-Field-Induced Superconductivity in a Bi-Functional Layered Organic Conductor,  $\kappa$ -(BETS)<sub>2</sub>FeBr<sub>4</sub>," *J. Am. Chem. Soc.* **124**, 6816 (2002).
- B. ZHANG, H. TANAKA, H. FUJIWARA, H. KOBAYASHI, E. FUJIWARA and A. KOBAYASHI, "Dual-Action Molecular Superconductors with Magnetic Anions," *J. Am. Chem. Soc.* **124**, 9982 (2002).
- H. TANAKA, H. KOBAYASHI and A. KOBAYASHI, "A Conducting Crystal Based on A Single-Component Paramagnetic Molecule, [Cu(dmdt)<sub>2</sub>] (dmdt = dimethyltetrathiafulvalenedithiolate)," *J. Am. Chem. Soc.* **124**, 10002 (2002).
- V. GRITSENKO, E. FUJIWARA, H. FUJIWARA and H. KOBAYASHI, "Stable Molecular Metals Based on Bis(ethylenedithio)tetraselenafulvalene and Halogen Ions:  $\kappa$ -(BETS)<sub>2</sub>X·C<sub>2</sub>H<sub>4</sub>(OH)<sub>2</sub> (X = Br, Cl)," *Synth. Met.* **128**, 273 (2002).
- H. KOBAYASHI, E. FUJIWARA, H. FUJIWARA, H. TANAKA, H. AKUTSU, I. TAMURA, T. OTSUKA, A. KOBAYASHI, M. TOKUMOTO and P. CASSOUX, "Development and Physical Properties of Magnetic Organic Superconductors Based on BETS Molecules [BETS = bis(ethylenedithio)tetraselenafulvalene]," *J. Phys. Chem. Solids* **63**, 1235 (2002).
- I. TAMURA, H. KOBAYASHI and A. KOBAYASHI, "X-Ray Diffraction Study of  $\alpha$ -(BEDT-TTF)<sub>2</sub>I<sub>3</sub> Single Crystal under High Pressure," *J. Phys. Chem. Solids* **63**, 1255 (2002).
- S. I. PESOTSKII, R. B. LYUBOVSKII, W. BIEBERRACHER, M. V. KARTSOVNIK, V. I. NIZHANKOPVSKII, N. D. KUSHCH, H. KOBAYASHI and A. KOBAYASHI, "On the Possibility of a Radical Decrease in the Strength of Many-Body Interactions in the Organic Metal  $\alpha$ -(BETS)<sub>2</sub>KHg(SCN)<sub>4</sub>," *J. Exp. Theor. Phys.* **94**, 431 (2002).
- H. KOBAYASHI, E. FUJIWARA, H. FUJIWARA, H. TANAKA, I. TAMURA, B. ZHANG, V. GRITSENKO, T. OTSUKA, A. KOBAYASHI, M. TOKUMOTO and P. CASSOUX, "Magnetic Organic Superconductor—Interplay of Conductivity and Magnetism," *Mol. Cryst. Liq. Cryst.* **379**, 9 (2002).
- A. KOBAYASHI, W. SUZUKI, E. FUJIWARA, T. OTSUKA, H. TANAKA, Y. OKANO and H. KOBAYASHI, "Molecular Design and Development of Single-Component Molecular Metals with Extended TTF Ligands," *Mol. Cryst. Liq. Cryst.* **379**, 19 (2002).
- H. KOBAYASHI, E. FUJIWARA, H. FUJIWARA, H. TANAKA, T. OTSUKA, A. KOBAYASHI, M. TOKUMOTO and P. CASSOUX, "Antiferromagnetic Organic Superconductors, BETS<sub>2</sub>FeX<sub>4</sub> (X = Br, Cl)," *Mol. Cryst. Liq. Cryst.* **380**, 139 (2002).
- E. OJIMA, H. FUJIWARA, H. TOKUMOTO and A. KOBAYASHI, "New Organic Conductors Based on Tellurium-Containing Dobor Molecules," *Mol. Cryst. Liq. Cryst.* **380**, 175 (2002).
- H. FUJIWARA, E. FUJIWARA and H. KOBAYASHI, "Synthesis, Structures and Physical Properties of the Cation Radical Salts Based on Tempo Radical Containong Electron Donors," *Mol. Cryst. Liq. Cryst.* **380**, 269 (2002).
- W. SUZUKI, E. FUJIWARA, A. KOBAYASHI, A. HASAGAWA, T. MIYAMOTO and H. KOBAYASHI, "Syntheses, Structure and Physical Properties of Palladium Complexes with an Extended-TTF Dithiolate Ligand, Bis(di-n-propylthiotetrathiafulvalenedithiolato)palladate," *Chem. Lett.* 936 (2002).
- S. UJI, C. TERAKURA, T. TERASHIMA, Y. OKANO and R. KATO, "Anisotropic Superconductivity and Dimensional Crossover in (TMET-STF)<sub>2</sub>BF<sub>4</sub>," *Phys. Rev. B* **64**, 214517 (2001).
- E. WATANABE, M. FUJIWARA, J. -I. YAMAURA and R. KATO, "Synthesis and Properties of Novel Donor-Type Metal-Dithiolene Complexes Based on 5,6-dihydro-1,4-dioxine-2,3-dithiol (edo) Ligand," *J. Mater. Chem.* **11**, 2131 (2001).
- T. NAKAMURA, T. TAKAHASHI, S. AONUMA and R. KATO, "EPR Investigation of the Electronic States in  $\beta'$ -Type [Pd(dmit)<sub>2</sub>] Compounds (where dmit is 2-thioxo-1,3-dithiole-4,5-dithiolate)," *J. Mater. Chem.* **11**, 2159 (2001).
- K. OSHIMA, T. SASAKI, M. MOTOKAWA and R. KATO, "Quantized Hall Effect-Like Behavior in (DMET-TSeF)<sub>2</sub>AuI<sub>2</sub>," *Synth. Met.* **120**, 943 (2001).
- M. TAMURA, K. YAMANAKA, Y. MORI, Y. NISHIO, K. KAJITA, H. MORI, S. TANAKA, J. -I. YAMAURA, T. IMAKUBO, R. KATO, Y. MISAKI and K. TANAKA, " $\pi$ -f Composite Metals," *Synth. Met.* **120**, 1041 (2001).
- M. TAMURA, T. IMAKUBO, K. YAMANAKA, Y. MORI, Y. NISHIO, K. KAJITA, Y. MISAKI, K. TANAKA, H. MORI, S. TANAKA, J. -I. YAMAURA and R. KATO, "Preparation, Structure and Electronic Properties of Some Organic Donor Salts of Rare-Earth Complex Anions: Novel 4f- $\pi$  Composite Conductors," *Mol.*



*Cryst. Liq. Cryst.* **379**, 35 (2002).

**S. OHIRA, M. TAMURA and R. KATO**, "Superconductivity of [Pd(dmit)<sub>2</sub>] Salts under Pressure Studied by an RF Technique," *Mol. Cryst. Liq. Cryst.* **379**, 41 (2002).

**J. -I. YAMAURA and R. KATO**, "High Pressure X-Ray Crystal Structure Analysis of Pd(dmit)<sub>2</sub> Salts," *Mol. Cryst. Liq. Cryst.* **379**, 47 (2002).

**T. NAKAMURA, T. TAKAHASHI, S. AONUMA and R. KATO**, "g-Tensor Analyses of β'-Type Pd(dmit)<sub>2</sub> Metal Complexes," *Mol. Cryst. Liq. Cryst.* **379**, 53 (2002).

**T. IMAKUBO, N. TAJIMA, M. TAMURA, R. KATO, Y. NISHIO and K. KAJITA**, "A Supramolecular Superconductor θ-(DIETS)<sub>2</sub>[Au(CN)<sub>4</sub>]," *J. Mater. Chem.* **12**, 159 (2002).

**T. KAWAMOTO, M. ASHIZAWA, T. MORI, J. -I. YAMAURA, R. KATO, Y. MISAKI and K. TANAKA**, "Dimerization Effect on the Physical Properties in New One-Dimensional Organic Conductors: (ChTM-TTP)<sub>2</sub>AuBr<sub>2</sub>, (ChTM-TTP)<sub>2</sub>GaCl<sub>4</sub>, and (ChTM-TTP)ReO<sub>4</sub>," *Bull. Chem. Soc. Jpn.* **75**, 435 (2002).

**Y. SHIMOJO, M. A. TANATAR, T. ISHIGURO and R. KATO**, "Superconductivity and Magnetoresistance Oscillations in Weakly Pressurized Quasi One-Dimensional Superconductor (DMET-TSeF)<sub>2</sub>AuI<sub>2</sub>," *J. Phys. Soc. Jpn.* **71**, 393 (2002).

**Y. OSHIMA, H. OHTA, K. KOYAMA, M. MOTOKAWA, H. M. YAMAMOTO and R. KATO**, "Observation of High-Order Harmonic Resonances in Magneto-optical Measurement of (BEDT-TTF)<sub>2</sub>Br(DIA)," *J. Phys. Soc. Jpn.* **71**, 1031 (2002).

### Department of Applied Molecular Science

**K. INOUE, H. IMAI, P. S. GHALSASI, K. KIKUCHI, M. OHBA, H. OKAWA and J. V. YAKHMI**, "A Three-Dimensional Ferrimagnet with High Magnetic Transition Temperature ( $T_C$ ) of 53 K Based on a Chiral Molecule," *Angew. Chem. Int. Ed. Engl.* **40**, 4242 (2001).

**N. V. BARANOV, T. GOTO, Y. HOSOKOSHI, K. INOUE, F. IWAHORI and N. V. MUSHNIKOV**, "Magnetic Viscosity at the Metamagnetic Phase Transition in Organic Mn<sup>II</sup>(hfac)<sub>2</sub> Compound with the One-Dimensional Chain Structure," *Mater. Sci. Forum* **373-376**, 441 (2001).

**K. INOUE, A. S. MARKOSYAN, H. KUMAGAI and P. S. GHALSASI**, "Synthesis and Magnetic Properties of Chiral Molecule Based Magnets," *Mater. Sci. Forum* **373-376**, 449 (2001).

**I. S. DUBENCO, I. YU. GAIDUKOVA, K. INOUE, ASHOT S. MARKOSYAN and V. E. RODIMIN**, "Instability of Co Magnetism and Magnetoelastic Properties of the (Ho, Y)Co<sub>3</sub> Compounds," *Mater. Sci. Forum* **373-376**, 633 (2001).

**K. SUZUKI, Y. HOSOKOSHI and K. INOUE**, "Pressure-induced Metamagnetic Behavior in a Quasi-One-Dimensional Molecule-Based Ferrimagnet," *Chem. Lett.* 316 (2002).

**K. SUZUKI, Y. HOSOKOSHI and K. INOUE**, "Pressure Effects on Molecular Magnets of Mn Complexes with Bisaminoxylbenzene Derivatives," *Mol. Cryst. Liq. Cryst.* **379**, 247 (2001).

**N. AZUMA, N. SENBA, K. OKUDA, K. OHARA, Y. HOSOKOSHI, K. INOUE and K. MUKAI**, "Synthesis and Magnetic Property of the Salts of Positively Charged Verdazyl Radicals and TCNQF<sub>4</sub><sup>-</sup> Anion Radical," *Mol. Cryst. Liq. Cryst.* **376**, 341 (2001).

**M. INOKUCHI, K. SUZUKI, M. KINOSHITA, Y. HOSOKOSHI and K. INOUE**, "Magnetic Properties of Cs and N(CH<sub>3</sub>)<sub>4</sub> Salts of TCNQ," *Mol. Cryst. Liq. Cryst.* **376**, 507 (2001).

**K. MUKAI, M. YANAGIMOTO, Y. SHIMOBÉ, K. KINDO and T. HAMAMOTO**, "High-Field Magnetization and Magnetic Susceptibility Studies of the Doping Effect of Nonmagnetic Impurities on the Organic Spin-Peierls System: p-CyDOV Radical Crystal," *J. Phys. Chem. B* **106**, 3687 (2002).

**H. KUMAGAI, K. INOUE and M. KURMOO**, "Self-Organized Metallo-Helicates and -Ladder with 2,2'-Biphenyldicarboxylate (C<sub>14</sub>H<sub>8</sub>O<sub>4</sub>)<sub>2</sub><sup>-</sup>: Synthesis, Crstal Structures, and Magnetic Properties," *Bull. Chem. Soc. Jpn.* **75**, 1283 (2002).

**K. KATOH, Y. HOSOKOSHI, K. INOUE, M. I. BARTASHEVICH, H. NAKANO and T. GOTO**, "Magnetic Properties of Organic Two-Leg Spin-Ladder Systems with  $S = 1/2$  and  $S = 1$ ," *J. Phys. Chem. Solids* **63**, 1277 (2002).

**H. KUMAGAI, N. KYRITSAKAS, Y. OKA, K. INOUE and M. KURMOO**, "Hydrothermal Synthesis and Structural and Magnetic Characterization of the Coordination Bonding Network Co<sup>II</sup>(H<sub>2</sub>O)<sub>2</sub>Carboxy-Cinnamate," *Mol. Cryst. Liq. Cryst.* **379**, 217 (2002).

**Y. OKA, H. KUMAGAI, K. INOUE and M. KURMOO**, "Hydrothermal Synthesis and Characterization of a Two-Dimensional Cobalt (II) Complex Containing Cinnamate Anion," *Mol. Cryst. Liq. Cryst.* **379**, 265 (2002).

**S. HAYAMI, Y. HOSOKOSHI, K. INOUE, Y. EINAGA, O. SATO and Y. MAEDA**, "Pressure-Stabilized Low-Spin State for Binuclear Iron(III) Spin-Crossover Compounds," *Bull. Chem. Soc. Jpn.* **74**, 2361 (2001).

**M. TANAKA, Y. HOSOKOSHI, A. S. MARKOSYAN, K. INOUE and H. IWAMURA**, "Metal (3d)-Organic (2p)-Hybrid Magnets Made of Mn(II) Ions with Tris(aminoxyl) Radicals (R) as Bridging Ligands. 2D Complexes [Mn(hfac)<sub>2</sub>]<sub>3</sub>•R<sub>2</sub>," *Synth. Met.* **122**, 463 (2001).

**H. KUMAGAI, Y. OKA, M. AKITA-TANAKA and K. INOUE**, "Hydrothermal Synthesis and Characterization of a Two-Dimensional Nickel(II) Complex Containing Benzenehexacarboxylic Acid(mellitic acid)," *Inorg. Chim. Acta* **332**, 176 (2002).

**K. HINO, Y. INOKUCHI, K. KOSUGI, H. SEKIYA, Y. HOSOKOSHI, K. INOUE and N. NISHI**,

“Photochemical Generation of High Spin Clusters in Solution: (Cyclopentadienyl-Vanadium)<sub>m</sub>O<sub>n</sub>,” *J. Phys. Chem. B* **106**, 1290 (2002).

**S. AONUMA, H. CASELLAS, B. GARREAU De BONNEVAL, I. MALFANT, C. FAULMAN, P. CASSOUX, Y. HOSOKOSHI and K. INOUE**, “Structure and Property of M(dmit)<sub>2</sub> Salt with Trimethylammonio-TEMPO and Related Magnetic Organic Cations,” *Mol. Cryst. Liq. Cryst.* **130**, 263 (2002).

**K. JITSUKAWA, T. IRISA, H. EINAGA and H. MASUDA**, “A Substrate-Specific  $\alpha$ -Hydroxylation of Dipeptides Mediated upon a Co(III)-Terpyridine Complex: A Functional Model for Peptidylglycine  $\alpha$ -Hydroxylating Monooxygenase,” *Chem. Lett.* **30** (2001).

**H. KUMITA, T. MORIOKA, T. OZAWA, K. JITSUKAWA, H. EINAGA and H. MASUDA**, “Site-Selective Recognition of Amino Acids by The Co(III) Complexes Containing (N)(O)<sub>3</sub>-Type Tripodal Tetradentate Ligand,” *Bull. Chem. Soc. Jpn.* **74**, 1035 (2001).

**K. MATSUMOTO, T. OZAWA, K. JITSUKAWA, H. EINAGA and H. MASUDA**, “Crystal Structure and Redox Behavior of a Novel Siderophore Model System: A Trihydroxamate-Iron(III) Complex with Intra- and Interstrand Hydrogen Bonding Networks,” *Inorg. Chem.* **40**, 190 (2001).

**H. KUMITA, K. JITSUKAWA, H. EINAGA and H. MASUDA**, “Characterization of an NH- $\pi$  Interaction in Co(III) Ternary Complexes with Aromatic Amino Acids,” *Inorg. Chem.* **40**, 3936 (2001).

**K. JITSUKAWA, Y. OKA, H. EINAGA and H. MASUDA**, “Reverse Reactivity in Hydroxylation of Adamantane and Epoxidation of Cyclohexene Catalyzed by the Mononuclear Ruthenium-oxo Complexes with 6-Substituted Tripodal Polypyridine Ligands,” *Tetrahedron Lett.* **42**, 3467 (2001).

**K. MATSUMOTO, T. OZAWA, K. JITSUKAWA, H. EINAGA and H. MASUDA**, “A Structural Model of the Ferrichrome Type Siderophore: Chiral Preference Induced by Intramolecular Hydrogen Bonding Networks in Ferric Trihydroxamate,” *Chem. Commun.* 978 (2001).

**K. MATSUMOTO, N. SUZUKI, T. OZAWA, K. JITSUKAWA and H. MASUDA**, “Crystal Structure and Solution Behavior of the Iron(III) Complex of the Artificial Trihydroxamate Siderophore with Tris(3-aminopropyl)-Amine Backbone,” *Eur. J. Inorg. Chem.* **10**, 2481 (2001).

**K. JITSUKAWA, M. HARATA, H. ARII, H. SAKURAI and H. MASUDA**, “SOD Activities of the Copper Complexes with Tripodal Polypyridylamine Ligands Having a Hydrogen Bonding Site,” *Inorg. Chim. Acta* **324**, 108 (2001).

**S. OGO, R. YAMAHARA, T. FUNABIKI, H. MASUDA and Y. WATANABE**, “Biomimetic Intradiol-Cleavage of Catechols with Incorporation of Both Atoms of O<sub>2</sub>: The Role of the Vacant Coordination Site on the Iron Center,” *Chem. Lett.* 1062 (2001).

**M. ISHIDA, M. Takai, H. Okabayashi, H. Masuda, M. Furusaka, and C. J. O’Connor**, “Supramolecular Aggregates formed by L-Glutamic Acid-Oligomers: SANS and SAXS Studies of the Hydrogen Bonded Self-Assembly,” *Phys. Chem. Chem. Phys.* **3**, 3140 (2001).

**M. ISHIDA, M. TAKAI, H. OKABAYASHI, H. MASUDA, M. FURUSAKA and C. J. O’CONNOR**, “Micellar Structure of an Oligopeptide Surfactant “Trimeric *N*-Dodecanoyl-L-Proline Potassium Salt” in Aqueous Solution—Small-Angle Neutron Scattering Study,” *Colloid Polym. Sci.* **279**, 1034 (2001).

**A. YOSHINO, M. ISHIDA, H. YUKI, H. OKABAYASHI, H. MASUDA and C. J. O’CONNOR**, “Structure of Liquid-Crystalline Phases Formed by *N*-Acetyl-L-Glutamic Acid Oligomeric Benzyl Esters—<sup>2</sup>H NMR Study,” *Colloid Polym. Sci.* **279**, 1144 (2001).

**M. ISHIDA, M. TAKAI, H. OKABAYASHI, H. MASUDA, E. NISHIO and C. J. O’CONNOR**, “FTIR Evidence for Antiparallel  $\beta$ -Sheet Structures of Long Oligomeric *N*-Acetyl-L-Glutamic Acid Benzyl Esters,” *Vibrational Spectroscopy* **27**, 135 (2001).

**M. ISHIDA, M. TAKAI, H. OKABAYASHI, H. MASUDA, E. NISHIO and C. J. O’CONNOR**, “Long Acyl Chain Induces Conformational Changes in Oligomeric *N*-Acyl-L-Proline Anions: a FTIR Study,” *Vibrational Spectroscopy* **27**, 109 (2001).

**K. IZAWA, T. OGASAWARA, H. MASUDA, H. OKABAYASHI and I. NODA**, “Application of Generalized Two-Dimension Correlation Theory to Gel Permeation Chromatographic Analysis,” *Phys. Chem. Commun.* **12**, 1 (2001).

**K. IZAWA, T. OGASAWARA, H. MASUDA, H. OKABAYASHI and I. NODA**, “Two-Dimensional Correlation Gel Permeation Chromatography Study of Octyltriethoxysilane Sol-Gel Polymerization Process,” *Macromolecules* **35**, 92 (2002).

**H. OKABAYASHI, K. IZAWA, T. YAMAMOTO, H. MASUDA, E. NISHIO and C. J. O’CONNOR**, “Surface Structure of Silica Gel Reacted with 3-Mercaptopropyltriethoxysilane and 3-Aminotriethoxysilane: Formation of the S-S Bridge Structure and its Characterization by Raman Scattering and Diffuse Reflectance Fourier Transform Spectroscopic Studies,” *Colloid Polym. Sci.* **280**, 135 (2002).

**M. TAKANI, T. YAJIMA, H. MASUDA and O. YAMAUCHI**, “Spectroscopic and Structural Characterization of Copper(II) and Palladium(II) Complexes of a Lichen Substance Usnic Acid and its Derivatives. Possible Forms of Environmental Metals Retained in Lichens,” *J. Inorg. Biochem.* **91**, 139 (2002).

**K. JITSUKAWA, H. SHIOZAKI and H. MASUDA**, “Epoxidation Activities of Mononuclear Ruthenium-oxo Complexes with a Square Planar 6,6’-bis(benzoylamino)-2,2’-bipyridine and Axial Ligands,” *Tetrahedron Lett.* **43**, 1491 (2002).

**A. WADA, S. OGO, S. NAGATOMO, T. KITAGAWA, Y. WATANABE, K. JITSUKAWA and H.**

**MASUDA**, "Reactivity for a Hydroperoxide Bound to Mononuclear Non-Heme Iron Site," *Inorg. Chem.* **41**, 616 (2002).

**K. IZAWA, T. OGASAWARA, H. MASUDA, H. OKABAYASHI, C. J. O'CONNOR and I. NODA**, "Two-Dimensional Correlation Gel Permeation Chromatography (2D GPC) Study of 1H,1H,2H,2H-Perfluorooctyltriethoxysilane Sol-Gel Polymerization Process," *J. Phys. Chem. B* **106**, 2867 (2002).

**K. IZAWA, T. OGASAWARA, H. MASUDA, H. OKABAYASHI, C. J. O'CONNOR and I. NODA**, "Growth Process of Polymer Aggregates Formed by Perfluorooctyltriethoxysilane. -Resolved Near-IR and Two-Dimensional Near-IR Correlation Studies," *Colloid Polym. Sci.* **280**, 380 (2002).

**R. YAMAHARA, S. OGO, H. MASUDA and Y. WATANABE**, "(Catecholato)iron(III) Complexes: Structural and Functional Models for the Catechol-Bound Iron(III) Form of Catechol Dioxygenases," *J. Inorg. Biochem.* **88**, 284 (2002).

**K. IZAWA, T. OGASAWARA, H. MASUDA, H. OKABAYASHI, C. J. O'CONNOR and I. NODA**, "2D Gel Permeation Chromatography (2D GPC) Correlation Studies of the Growth Process for Perfluorooctyltriethoxysilane Polymer Aggregates," *Phys. Chem. Chem. Phys.* **4**, 1053 (2002).

**K. IZAWA, T. OGASAWARA, H. MASUDA, H. OKABAYASHI, C. J. O'CONNOR and I. NODA**, "TWO-Dimensional Correlation Gel Permeation Chromatography (2D correlation GPC) Study of the Sol-Gel Polymerization of Octyltriethoxysilane. HCl-Concentration Dependence," *Phys. Chem. Commun. [online computer file]* No. 2 (2002).

**H. OKABAYASHI, M. ISHIDA, H. YUKI, N. HATTORI, H. MASUDA and C. J. O'CONNOR**, "Phase Structures of the *N*-Acetyl-L-Glutamic Acid Oligomeric Benzyl Esters (Exact Residue Numbers 4, 6, 8, and 12)-Dioxane Systems and their Optical Properties," *Colloid Polym. Sci.* **280**, 599 (2002).

**K. IWATA and H. TAKAHASHI**, "Photoinduced Cl Transfer Reaction between Biphenyl and Carbon Tetrachloride Studied by Nanosecond Time-Resolved Infrared Spectroscopy and Picosecond Time-Resolved Fluorescence Spectroscopy," *J. Mol. Struct.* **598**, 97 (2001).

**K. IWATA, S. TAKEUCHI and T. TAHARA**, "Photochemical Bimolecular Reaction between Biphenyl and Carbon Tetrachloride: Observed Ultrafast Kinetics and Diffusion-Controlled Reaction Model," *Chem. Phys. Lett.* **347**, 331 (2001).

**H. ISHIKAWA, K. IWATA and H. HAMAGUCHI**, "Picosecond Dynamics of Stepwise Double Proton Transfer Reaction in the Excited State of the 2-Aminopyridine/Acetic Acid System," *J. Phys. Chem. A* **106**, 2305 (2002).

**K. IWATA, R. OZAWA and H. HAMAGUCHI**, "Analysis of the Solvent- and Temperature-Dependent Raman Spectral Changes of *S*<sub>1</sub> *Trans*-Stilbene and the Mechanism of the *Trans* to *Cis* Isomerization: Dynamic Polarization Model of Vibrational Dephasing and the C=C Double-Bond Rotation," *J. Phys. Chem. A* **106**, 3614 (2002).

**K. IWATA**, "Effects of Pump and Probe Light Field on Picosecond Time-Resolved Resonance Raman Spectra of *S*<sub>1</sub> *Trans*-Stilbene. Disagreement between Stokes- and Anti-Stokes Scattering Frequencies," *Bull. Chem. Soc. Jpn.* **75**, 1075 (2002).

**J. YAMADA, T. TOITA, H. AKUTSU, S. NAKATSUJI, H. NISHIKAWA, I. IKEMOTO and K. KIKUCHI**, "The Crystal Structure and Physical Properties of β-(BDA-TTP)<sub>2</sub>FeCl<sub>4</sub> [BDA-TTP = 2,5-bis(1,3-dithian-2-ylidene)-1,3,4,6-tetrathiapentalene]," *Chem. Commun.* 2538 (2001).

**T. KODAMA, M. KUSUDA, N. OZAWA, R. FUJII, K. SAKAGUCHI, H. NISHIKAWA, I. IKEMOTO, K. KIKUCHI, Y. MIYAKE and Y. ACHIBA**, "Spectroscopic Studies of Endohedral Metallofullerenes," *New diamond and Frontier Carbon Technology* **11**, 367 (2001).

**K. INOUE, H. IMAI, P. S. GHALSASI, K. KIKUCHI, M. OHBA, H. KAWA, and J. V. YAKHMI**, "A Three-Dimensional Ferrimagnet with a High Magnetic Transition Temperature (*T*<sub>C</sub>) of 53 K Based on a Chiral Molecule," *Angew. Chem., Int. Ed. Engl.* **40**, 4242 (2001).

**T. ISHII, R. KANEHAMA, N. AIZAWA, M. YAMASHITA, H. MATSUZAKA, K. SUGIURA, H. MIYASAKA, T. KODAMA, K. KIKUCHI, I. IKEMOTO, H. TANAKA, K. MARUMOTO and S. KURODA**, "Fullerene C<sub>60</sub> Exhibiting a Strong Intermolecular Interaction in a Cocrystallite with C<sub>4</sub> Symmetrical Cobalt Tetrakis(di-*tert*-butylphenyl)porphyrin," *J. Chem. Soc., Dalton Trans.* 2975 (2001).

**H. NISHIKAWA, T. MORIMOTO, T. KODAMA, I. IKEMOTO, K. KIKUCHI, J. YAMADA, H. YOSHINO and K. MURATA**, "New Organic Superconductors Consisting of an Unprecedented π-Electron Donor," *J. Am. Chem. Soc.* **124**, 730 (2002).

**T. KODAMA, N. OZAWA, Y. MIYAKE, K. SAKAGUCHI, H. NISHIKAWA, I. IKEMOTO, K. KIKUCHI and Y. ACHIBA**, "Structural Study of Three Isomers of Tm@C<sub>82</sub> by <sup>13</sup>C NMR Spectroscopy," *J. Am. Chem. Soc.* **124**, 1452 (2002).

**J. YAMADA, M. WATANABE, T. TOITA, H. AKUTSU, S. NAKATSUJI, H. NISHIKAWA, I. IKEMOTO and K. KIKUCHI**, "2-(1,3-Dithiolan-2-ylidene)-5-(1,3-dithian-2-ylidene)-1,3,4,6-Tetrathiapentalene (DHDA-TTP), a Hybrid of BDH-TTP and BDA-TTP, and Its Metallic Cation-Radical Salts," *Chem. Commun.* 1118 (2002).

**S. OKADA, H. OHOYAMA and T. KASAI**, "Stereo-Selectivity in the Penning Ionization Reaction of CH<sub>3</sub>X (X = Cl, Br, I) + Ar(<sup>3</sup>P) → CH<sub>3</sub>X<sup>+</sup> + Ar + e<sup>-</sup>," *Chem. Phys. Lett.* **355**, 77 (2002).

**A. OKANO, H. OHOYAMA and T. KASAI**, "Focusing and Selecting the Linear Type HBr-N<sub>2</sub>O by Using a 2 m Long Electrostatic Hexapole Field," *J. Chem. Phys.* **116**, 1325 (2002).



**M. HASHINOKUCHI, R. KOUMURA, D. -C. CHE and T. KASAI**, "A New Channel of Hydrogen Elimination in the 121.6-nm Photodissociation of Formic Acid Detected by a Doppler-Selected TOF Mass Spectrometry," *J. Mass Spectrom. Soc. Jpn.* **50**, 7 (2002).

**D. -C. CHE, M. HASHINOKUCHI, Y. SHIMIZU, H. OHOYAMA and T. KASAI**, "Photodissociation of DCI Dimer Selected by an Electrostatic Hexapole Field Combined with a Doppler-Selected Time-of-Flight Technique: Observation of [CIDCI] Transient Species," *Phys. Chem. Chem. Phys.* **3**, 4979 (2001).

**K. MORITANI, M. OKADA, M. NAKAMURA, T. KASAI and Y. MURATA**, "Hydrogen-Exchange Reactions via Hot Hydrogen Atoms Produced in the Dissociation Process of Molecular Hydrogen on Ir{100}," *J. Chem. Phys.* **115**, 9947 (2001).

**K. IMURA, H. OHOYAMA and T. KASAI**, "Evidence for the  $\text{HCl}^+(\text{A})$  Formation in the Reaction of  $\text{Ne}(^3\text{P})$  with the Size-Selected HCl Dimer Using an Electrostatic Hexapole field," *Chem. Lett.* 1136 (2001).

**M. NOSAKA, M. TAKASU and K. KATOH**, "Characterization of Gels by Monte Carlo Method Using a Model of Radical Polymerization with Cross Linkers," *J. Chem. Phys.* **115**, 11333 (2001).

**H. NOGUCHI and M. TAKASU**, "Self-Assembly of Amphiphiles into Vesicles: a Brownian Dynamics Simulation," *Phys. Rev. E* **64**, 041913 (2001).

**H. NOGUCHI and M. TAKASU**, "Fusion Pathways of Vesicles, a Brownian Dynamics Simulation," *J. Chem. Phys.* **115**, 9547 (2001).

**H. NOGUCHI and M. TAKASU**, "Adhesion of Nanoparticles to Vesicles: a Brownian Dynamics Simulation," *Biophys. J.* **83**, 299 (2002).

**H. NOGUCHI and M. TAKASU**, "Structural Changes of Pulled Vesicles: a Brownian Dynamics Simulation," *Phys. Rev. E* **65**, 051907 (2002).

#### Department of Vacuum UV Photoscience

**T. KINOSHITA, H. GUNASEKARA, Y. TAKATA, S. KIMURA, M. OKUNO, Y. HARUYAMA, N. KOSUGI, K. G. NATH, H. WADA, A. MITSUDA, M. SHIGA, T. OKUDA, A. HARASAWA, H. OGASAWARA and A. KOTANI**, "Spectroscopy Studies of Temperature-Induced Valence Transition on  $\text{Eu}_2(\text{Si}_{1-x}\text{Ge}_x)_2$  around Eu 3d-4f, 4d-4f and Ni 2p-3d Excitation Regions," *J. Phys. Soc. Jpn.* **71**, 148 (2002).

**E. RÜHL, R. FLESCHE, W. TAPPE, D. NOVIKOV and N. KOSUGI**, "Sulfur 1s Excitation of S-2 and S-8: Core-Valence- and Valence- Valence-Exchange Interaction and Geometry-Specific Transitions," *J. Chem. Phys.* **116**, 3316 (2002).

**M. MIZUNO, H. HAMAGUCHI and T. TAHARA**, "Observation of Resonance Hyper-Raman Scattering from *all-trans*-Retinal," *J. Phys. Chem. A* **106**, 3599 (2002).

**T. FUJINO, S. Yu. ARZHANTSEV and T. TAHARA**, "Femtosecond/picosecond Time-Resolved Spectroscopy of *Trans*-Azobenzene: Isomerization Mechanism Following  $\text{S}_2(\pi\pi^*) \leftarrow \text{S}_0$  Photoexcitation," *Bull. Chem. Soc. Jpn.* **75**, 1031 (2002).

**D. MANDAL, T. TAHARA, N. M. WEBBER and S. R. MEECH**, "Ultrafast Fluorescence of the Chromophore of the Green Fluorescent Protein in Alcohol Solutions," *Chem. Phys. Lett.* **358**, 495 (2002).

**D. MANDAL, S. SOHBAN, T. TAHARA and K. BHATTACHARYA**, "Femtosecond Study of Solvation Dynamics of DCM in Micelles," *Chem. Phys. Lett.* **359**, 77 (2002).

**Z. WANG, H. NODA, Y. NONOGAKI, N. YABUMOTO and T. URISU**, "IR Line Width Broadening at Nearly Ideal H-Terminationregion on Si(100)-(2x1) Surfaces," *Surf. Sci.* **502**, 86 (2002).

**Z. WANG, H. NODA, Y. NONOGAKI, N. YABUMOTO and T. URISU**, "Hydrogen Diffusion and Chemical Reactivity with Water on Nearly Ideally H-terminated Si(100) Surface," *Jpn. J. Appl. Phys.* **41**, 4275 (2002).

**Y. TAKABAYASHI, Y. KUBOZONO, T. KANBARA, S. FUJIKI, K. SHIBATA, Y. HARUYAMA, T. HOSOKAWA, Y. RIKIISHI and S. KASHINO**, "Pressure and Temperature Dependences of the Structural Properties of  $\text{Dy}@C_{82}$  Isomer I," *Phys. Rev. B* **65**, 73405 (2002).

**S. FUJIKI, Y. KUBOZONO, M. KOBAYASHI, Y. RIKIISHI, S. KASHINO, K. ISHII, H. SUEMATSU and A. FUJIWARA**, "Structure and Physical Properties of  $\text{Cs}_{3+\alpha}\text{C}_{60}$  ( $\alpha = 0.0-1.0$ ) under Ambient and High Pressures," *Phys. Rev. B* **65**, 235425 (2002).

**S. D. MORE, H. GRAAF, M. BAUNE, C. WANG and T. URISU**, "Influence of Substrate Roughness on the Formation of Aliphatic Self-Assembled Monolayers (SAM) on Silicon(100)," *Jpn. J. Appl. Phys.* **41**, 4390 (2002).

**S. MORE, W. BERNDT, A. SEITSONNEN and A. M. BRADSHAW**, "Adsorption of Pt(111) ( $\sqrt{3} \times \sqrt{3}$ )R30° and (2x2)-Na: Experiment and Theory," *Phys. Rev. B* **63**, 075406 (2001).

**S. TANAKA, S. D. MORE, J. MURAKAMI, M. ITOH and M. KAMADA**, "Surface Photovoltage Effects on p-GaAs (100) from Core-Level Photoelectron Spectroscopy Using Synchrotron Radiation and a Laser," *Phys. Rev. B* **64**, 155308 (2001).

**S. MIYAKE, I. SHIMIZU, R. MANORY, T. MORI and G. KIMMEL**, "Structural Modifications of Hafnium Oxide Films Prepared by Ion Beam Assisted Deposition under High Energy Oxygen Irradiation," *Surf. Coat. Technol.* **146-147**, 237 (2001).

- S. SAKABE, K. NISHIHARA, N. NAKASHIMA, J. KOU, S. SHIMIZU, V. ZHAKHOVSKII, H. AMITANI and F. SATO**, "The Interactions of Ultra-Short High-Intensity Laser Pulses with Large Molecules and Clusters: Experimental and Computational Studies," *Physics of Plasmas* **8**, 2517 (2001).
- Y. HIKOSAKA and K. MITSUKE**, "Formation and Autoionization of a Dipole-Forbidden Superexcited State of CS<sub>2</sub>," *J. Phys. Chem. A* **105**, 8130 (2001).
- H. NAKANO, T. MORI, T. HORIKUBI and N. KAMEGASHIRA**, "Structural Analysis of a New Layered Compound: La<sub>0.05</sub>Sr<sub>0.95</sub>MnO<sub>3</sub>," *J. Am. Ceram. Soc.* **85**, 1576 (2002).
- T. MORI, N. KAMEGASHIRA, K. AOKI, T. SHISHIDO and T. FUKUDA**, "Crystal Growth and Crystal Structures of the LnMnO<sub>3</sub> Perovskites: Ln = Nd, Sm, Eu and Gd," *Mater. Lett.* **54**, 238 (2002).
- R. MANORY, T. MORI, I. SHIMIZU, S. MIYAKE and G. KIMMEL**, "Growth and Structure Control of HfO<sub>2-x</sub> Films with Cubic and Tetragonal Structures Obtained by Ion Beam Assisted Deposition," *J. Vac. Sci. Technol., A* **20**, 549 (2002).
- K. IWASAKI and K. MITSUKE**, "Development of a Conical Energy Analyzer for Angle-Resolved Photoelectron Spectroscopy," *Surf. Rev. Lett.* **9**, 583 (2002).

### Coordination Chemistry Laboratories

- Y. UOZUMI, M. KAWATSURA and T. HAYASHI**, "(R)-2-Diphenylphosphino-2'-methoxy-1,1'-binaphthyl," *Org. Syn.* **78**, 1 (2002).
- Y. UOZUMI and M. NAKAZONO**, "Amphiphilic Resin-Supported Rhodium-Phosphine Catalysts for C-C Bond Forming Reactions in Water," *Adv. Synth. Catal.* **344**, 274 (2002).
- S. NAGAI, S. TAKEMOTO, T. UEDA, K. MIZUTANI, Y. UOZUMI and H. TOKUDA**, "Studies on the Chemical Transformations of Rotenoids. 6 Synthesis and Antitumor-Promoting Activity of [1]Benzofuro[2,3-d]pyridazines Fused with 1,2,4-Triazole, 1,2,4-Triazine and 1,2,4-Triazepine," *J. Heterocyclic Chem.* **38**, 1097 (2001).
- S. NAGAI, T. MIYACHI, T. NAKANE, T. UEDA and Y. UOZUMI**, "Synthesis and Potential Central Nervous System Stimulant Activity of 5,8-Methanoquinazolines and Bornano[1,2,4]triazines Fused with Imidazole and Pyrimidine," *J. Heterocyclic Chem.* **38**, 379 (2001).
- Y. UOZUMI, T. ARII and T. WATANABE**, "Double Carbonylation of Aryl Iodides with Primary Amines under Atmospheric Pressure Conditions Using Pd/PPh<sub>3</sub>/DABCO/THF System," *J. Org. Chem.* **66**, 5272 (2001).
- T. HAYASHI, J. W. HAN, A. TAKEDA, J. TANG, K. NOHMI, K. MUKAIDE, H. TSUJI and Y. UOZUMI**, "Modification of Chiral Monodentate Phosphine Ligands (MOP) for Palladium-Catalyzed Asymmetric Hydrosilylation of Cyclic 1,3-Dienes," *Adv. Synth. Catal.* **343**, 279 (2001).
- T. HAYASHI, S. HIRATE, K. KITAYAMA, H. TSUJI, A. TORII and Y. UOZUMI**, "Asymmetric Hydrosilylation of Styrenes Catalyzed by Palladium-MOP Complexes: Ligand Modification and Mechanistic Studies," *J. Org. Chem.* **66**, 1441 (2001).
- K. NISHIYAMA, A. KUBO, I. TANIGUCHI, M. YAMADA and H. NISHIHARA**, "Effects of Alkyl Chain as a Spacer on Electrochemical Reaction and SEIRA Spectra for Self-Assembled Monolayer Having Anthraquinone Redox Center," *Electrochemistry* **69**, 980 (2001).
- I. TANIGUCHI**, "Analysis of Biological Functions of Metalloproteins Using Biocompatible Modified Electrodes," *Anal. Sci.* **17**, 1355 (2001).
- T. SAWAGUCHI, F. MIZUTANI and I. TANIGUCHI**, "Interfacial Structures of Self-Assembled Monolayers of 2-pyridinethiol on Au(111) Studied by In Situ Tunneling Microscopy," *Anal. Sci.* **17**, 1383 (2001).
- K. NISHIYAMA, H. IKEBE, Y. HOSHIDE, H. NAGAI and I. TANIGUCHI**, "NADP<sup>+</sup> Sensor on *Chrorella* Ferredoxin/Ferredoxin-NADP<sup>+</sup>-Reductase Modified Indium Oxides," *Chem. Sens.* **17**, 92 (2001).
- K. NISHIYAMA, A. KUBO, A. UEDA and I. TANIGUCHI**, "Surface pK<sub>a</sub> of Amine-Terminated Self-Assembled Monolayers Evaluated by Direct Observation of Counter Anion by FT-Surface Enhanced Raman Spectroscopy," *Chem. Lett.* **80** (2002).
- I. TANIGUCHI, K. HARA, H. ISHIMOTO, M. IWAI and S. RANGARAJAN**, "Ion Selectivity for Electrode Reactions on Functionalized Monolayer Modified Electrode," *Chem. Sens.* **18**, 133 (2002).
- S. UEMURA, M. SAKATA, I. TANIGUCHI, C. HIRAYAMA and M. KUNITAKE**, "In-Situ STM Observation of Coronene Epitaxial Adlayers on Au(111) Surfaces Prepared by the Transfer of Langmuir Films," *Thin Solid Films* **409**, 206 (2002).
- G. P. -J. HAREAU, S. NEYA, N. FUNASAKI and I. TANIGUCHI**, "New Route to Protoporphyrins III and XIII from Common Starting Pyrroles," *Tetrahedron Lett.* **43**, 3109 (2002).
- M. YAMASHITA, K. YOKOYAMA, S. FURUKAWA, T. MANABE, T. ONO, K. NAKATA, C. KACHI-TERAJIMA, F. IWAHORI, T. ISHII, H. MIYASAKA, K. SUGIURA, H. MATSUZAKI, H. KISHIDA, H. OKAMOTO, H. TANAKA, Y. HASEGAWA, K. MARUMOTO, H. ITO and S. KURODA**, "Tuning of Electronic Structures of Quasi-One-Dimensional Bromo-Bridged Ni(III) Complexes with Strong Electron-Correlation by Doping of Co(III) Ions, [Ni<sub>1-x</sub>Co<sub>x</sub>(chxn)<sub>2</sub>Br]Br<sub>2</sub>," *Inorg. Chem.* **41**, 1998 (2002).
- S. FUJIMORI, A. INO, T. OKANE, A. FUJIMORI, K. OKADA, T. MANABE, M. YAMASHITA, H. KISHIDA and H. OKAMOTO**, "Angle-Resolved Photoemission Study of Halogen-Bridged MX-Chain

Compound  $[\text{Ni}(\text{chxn})_2\text{Br}]_2\text{Br}_2$ ," *Phys. Rev. Lett.* **88**, 247601-1(2002).

**H. TANAKA, K. MARUMOTO, S. KURODA, T. MANABE and M. YAMASHITA**, "ESR Detection of Induced Spin Moments in Halogen-Bridged Mixed-Metal Complexes  $\text{Ni}_{1-x}\text{Pd}_x(\text{chxn})_2\text{Br}_3$ ," *J. Phys. Soc. Jpn.* **71**, 1370 (2002).

**K. NAKATA, H. MIYASAKA, K. SUGIMOTO, T. ISHII, K. SUGIURA and M. YAMASHITA**, "Construction of a One-Dimensional Chain Composed of  $\text{Mn}_6$  Clusters and 4,4'-bipyridine Linkers: The First Step for Creating of "Nano-Dots-Wires," *Chem. Lett.* 658 (2002).

**T. KURODA-SOWA, S. FUKUDA, S. MIYOSHI, M. MAEKAWA, M. MUNAKATA, H. MIYASAKA and M. YAMASHITA**, "A Chemical Modification of a  $\text{Mn}_{12}$  Single-Molecule Magnet by Replacing Carboxylate Anion with Diphenylphosphate Anions," *Chem. Lett.* 682 (2002).

**S. NORO, R. KITAJIMA, M. KONDO, S. KITAGAWA, T. ISHII, H. MATSUZAKA and M. YAMASHITA**, "Framework Engineering by Anions and Porous Functionalities of  $\text{Cu}(\text{II})/4,4'$ -bpy Coordination Polymers," *J. Am. Chem. Soc.* **124**, 2568 (2002).

**H. TANAKA, K. MARUMOTO, S. KURODA, T. ISHII, R. KANEHAMA, N. AIZAWA, H. MATSUZAKA, K. SUGIURA, H. MIYASAKA, T. KODAMA, K. KIKUCHI, I. IKEMOTO and M. YAMASHITA**, "ESR Studies of  $\text{Co}(\text{tbp})\cdot\text{C}_{60}$  Single Crystal," *J. Phys.: Condens. Matter* **14**, 3993 (2002).

**S. NORO, S. KITAGAWA, M. YAMASHITA and T. WADA**, "New Microporous Coordination Polymer Affording Guest-Coordination Sites at Channel Walls," *Chem. Commun.* 222 (2002).

**F. KAKIUCHI, H. OHTAKI, M. SONODA, N. CHATANI and S. MURAI**, "Mechanistic Study of the  $\text{Ru}(\text{H})_2(\text{CO})(\text{PPh}_3)_3$ -Catalyzed Addition of C-H Bonds in Aromatic Esters to Olefins," *Chem. Lett.* 918 (2001).

**N. CHATANI, T. ASAUMI, S. YORIMITSU, T. IKEDA, F. KAKIUCHI and S. MURAI**, " $\text{Ru}_3(\text{CO})_{12}$ -Catalyzed Coupling Reaction of  $sp^3$  C-H Bonds Adjacent to a Nitrogen Atom in Alkylamines with Alkenes," *J. Am. Chem. Soc.* **123**, 10935 (2001).

**N. CHATANI, A. KAMITANI, M. OSHITA, Y. FUKUMOTO and S. MURAI**, "Catalytic Carbonylation Reactions of Benzyne Derivatives," *J. Am. Chem. Soc.* **123**, 12686 (2001).

**H. INOUE, N. CHATANI and S. MURAI**, "Cycloisomerization of  $\omega$ -Aryl-1-Alkynes:  $\text{GaCl}_3$  as a Highly Electrophilic Catalyst for Alkyne Activation," *J. Org. Chem.* **67**, 1414 (2002).

**F. KAKIUCHI, K. IGI, M. MATSUMOTO, T. HAYAMIZU, N. CHATANI and S. MURAI**, "A New Chelation-Assistance Mode for a Ruthenium-Catalyzed Silylation at the C-H Bond in Aromatic Ring with Hydrosilanes," *Chem. Lett.* 396 (2002).

**F. FUKUMOTO, K. SAWADA, N. CHATANI and S. MURAI**, " $\text{Ir}_4(\text{CO})_{12}$ -Catalyzed Coupling Reaction of Imidazoles with Aldehydes in the Presence of a Hydrosilane to Give 2-Substituted Imidazoles," *Angew. Chem., Int. Ed. Engl.* **41**, 2779 (2002).

**T. WADA, K. TSUGE and K. TANAKA**, "Synthesis and Redox Properties of Bis(ruthenium-hydroxo)complexes with Quinone and Bipyridine Ligand as a Water-Oxidation Catalysts," *Inorg. Chem.* **40**, 329 (2001).

**H. SUGIMOTO and K. TANAKA**, "Ruthenium Terpyridine Complexes with Mono- and Bidentate Dithiolene Ligands," *J. Chem. Soc., Dalton Trans.* 57 (2001).

**T. TOMON, D. OYAMA, T. WADA, S. KAZUSHI and K. TANAKA**, "A Ru-Carbene Complex with a Metallacycle Involving a 1,8-naphthylidene Framework," *Chem. Commun.* 1100 (2001).

**K. ITO, T. NAGATA and K. TANAKA**, "Synthesis and Electrochemical Properties of Transition Metal Complexes of 2,2':6',2''-Terpyridine 1,1''-Dioxide," *Inorg. Chem.* **40**, 6331 (2001).

**H. SUGIMOTO and K. TANAKA**, "Synthesis of New Ruthenium Carbonyl Terpyridine *o*-Phenylene Complexes: Strong Interaction between carbonyl and *o*-Phenylene Ligands," *J. Organomet. Chem.* **622**, 280 (2001).

**K. KOBAYASHI, H. OHTSU, T. WADA and K. TANAKA**, "Ruthenium Oxy Radical Complex Containing *o*-Quinone Ligand Detected by ESR Measurements of Spin Trapping Technique," *Chem. Lett.* 868 (2002).

**Y. SUNADA, Y. HAYASHI, H. KAWAGUCHI and K. TATSUMI**, "Alkynethiolato and Alkyneselenolato Ruthenium Half-Sandwich Complexes: Synthesis, Structures, and Reactions with  $(\eta^5\text{-C}_5\text{H}_5)_2\text{Zr}$ ," *Inorg. Chem.* **40**, 7072 (2001).

**Y. ARIKAWA, H. KAWAGUCHI, K. KASHIWABARA and K. TATSUMI**, "Trithiotungsten(VI) Complexes Having Phosphine-Thiolate Hybrid Ligands: Synthesis and Cluster Forming Reactions with  $\text{CuBr}$ ,  $\text{FeCl}_2$ , and  $[\text{Fe}(\text{CH}_3\text{CN})_6](\text{ClO}_4)_2$ ," *Inorg. Chem.* **41**, 513 (2002).

**H. KAWAGUCHI and T. MATSUO**, "Binuclear Iron(II) Complex from a Linked-bis(amidinate) Ligand: Synthesis and its Reaction with Carbon Monoxide," *Chem. Commun.* 958 (2002).

**T. KOMURO, T. MATSUO, H. KAWAGUCHI and K. TATSUMI**, "Palladium Dimethylsilanedithiolato Complex: a Precursor for Ti-Pd and Ti-Pd<sub>2</sub> Heterometallic Complexes," *Chem. Commun.* 988 (2002).

**T. MATSUO, H. KAWAGUCHI and M. SAKAI**, "Synthesis and Structures of Ti(III) and Ti(IV) Complexes Supported by a Tridentate Aryloxy Ligand," *J. Chem. Soc., Dalton Trans.* 2536 (2002).

**J. -P. LANG, H. KAWAGUCHI and K. TATSUMI**, "Reactions of Tetrathiotungstate and Tetrathiomolybdate with Substituted Haloalkanes," *J. Chem. Soc., Dalton Trans.* 2573 (2002).

**H. KAWAGUCHI and T. MATSUO**, "Dinitrogen-Bond Cleavage in a Niobium Complex Supported by a Tridentate Aryloxy Ligand," *Angew. Chem., Int. Ed. Engl.* **41**, 2792 (2002).



- N. NAKATA, N. TAKEDA and N. TOKITOH**, "Synthesis and Structure of a Kinetically Stabilized 2-Germanaphthalene: the First Stable Neutral Germaaromatic Compound," *Organometallics* **20**, 5507 (2001).
- S. YASUI, K. ITOH, A. OHNO and N. TOKITOH**, "Kinetic Deuterium Isotope Effect in Single-Electron Transfer Occurring from Tributylphosphine to Viologens," *Chem. Lett.* 1056 (2001).
- N. TAKEDA, T. KAJIWARA and N. TOKITOH**, "Reaction of Stable Silylene-Isocyanide Complexes with Boranes: Synthesis and Properties of the First Stable Silylborane-Isocyanide Complexes," *Chem. Lett.* 1076 (2001).
- M. ITOH, K. TAKENAKA, R. OKAZAKI, N. TAKEDA and N. TOKITOH**, "The First Stable Aromatic S-Nitrosothiol: Synthesis, Structure and Reactivity," *Chem. Lett.* 1206 (2001).
- K. NAGATA, N. TAKEDA and N. TOKITOH**, "Syntheses and Crystal Structures of the First Disulfur and Diselenium Complexes of Platinum," *Angew. Chem. Int. Ed. Engl.* **41**, 136 (2002).
- T. SASAMORI, N. TAKEDA, M. FUJIO, M. KIMURA, S. NAGASE and N. TOKITOH**, "Synthesis and Structure of the First Stable Phosphabismuthene," *Angew. Chem. Int. Ed. Engl.* **41**, 139 (2002).
- N. TOKITOH, T. SADAHIRO, K. HATANO, T. SASAKI, N. TAKEDA and R. OKAZAKI**, "Synthesis of Kinetically Stabilized Silaneselone and Silanetellone," *Chem. Lett.* 34 (2002).
- N. TAKEDA, A. SHINOHARA and N. TOKITOH**, "The First Stable 9-Silaanthracene," *Organometallics* **21**, 256 (2002).
- N. TOKITOH, K. KISHIKAWA, R. OKAZAKI, T. SASAMORI, N. NAKATA and N. TAKEDA**, "Synthesis and Characterization of an Extremely Hindered Tetraaryl-Substituted Digermene and Its Unique Properties in the Solid State and in Solution," *Polyhedron* **21**, 563 (2002).
- T. SASAMORI, Y. ARAI, N. TAKEDA, R. OKAZAKI, Y. FURUKAWA, M. KIMURA, S. NAGASE and N. TOKITOH**, "Syntheses, Structures and Properties of Kinetically Stabilized Distibenes and Dibismuthenes, Novel Doubly Bonded Systems between Heavier Group 15 Elements," *Bull. Chem. Soc. Jpn.* **75**, 661 (2002).
- N. NAKATA, N. TAKEDA and N. TOKITOH**, "Synthesis and Properties of the First Stable Germabenzene," *J. Am. Chem. Soc.* **124**, 6914 (2002).
- N. TOKITOH, T. SASAMORI, N. TAKEDA and S. NAGASE**, "Systematic Studies on Homo- and Heteronuclear Doubly Bonded Compounds of Heavier Group 15 Elements," *Phosphorus, Sulfur Silicon Relat. Elem.* **177**, 1473 (2002).
- K. NAGATA, N. TAKEDA and N. TOKITOH**, "Synthesis of Novel Platinum Dichalcogenido-Complexes by Taking Advantage of Bulky Phosphine Ligands," *Phosphorus, Sulfur Silicon Relat. Elem.* **177**, 1859 (2002).
- S. YASUI, K. ITOH, A. OHNO and N. TOKITOH**, "Reaction of Trivalent Phosphorus Compounds with Viologens," *Phosphorus, Sulfur Silicon Relat. Elem.* **177**, 2001 (2002).
- T. SASAMORI, N. TAKEDA and N. TOKITOH**, "Synthesis and Reaction of the First Stable Phosphabismuthene, a Novel Compound with Phosphorus-Bismuth Double Bond," *Phosphorus, Sulfur Silicon Relat. Elem.* **177**, 2003 (2002).
- N. NAKATA, N. TAKEDA and N. TOKITOH**, "Reactions of 2-Germanaphthalene with Elemental Sulfur and Selenium: Synthesis of Novel Cyclic Polychalcogenides Containing a Germanium, Trichalcogenagermolanes," *Chem. Lett.* 818 (2002).
- F. TAKEI, H. HAYASHI, K. ONITSUKA and S. TAKAHASHI**, "Helical Poly(aryl isocyanide)s Possessing Chiral Alkoxy carbonyl Groups," *Polym. J.* **33**, 310 (2001).
- F. FENG, T. MIYASHITA, F. TAKEI, K. ONITSUKA and S. TAKAHASHI**, "Formation of an Optically Active Helical Polyisocyanide Langmuir-Blodgett Film," *Chem. Lett.* 764 (2001).
- F. TAKEI, H. HAYASHI, K. ONITSUKA, N. KOBAYASHI and S. TAKAHASHI**, "Helical Chiral Polyisocyanides Possessing Porphyrin Pendants: Determination of Helicity by Exciton Coupled Circular Dichroism," *Angew. Chem., Int. Ed.* **40**, 4092 (2001).

#### Laser Research Center for Molecular Science

- Z. LIU, T. KOZEKI, Y. SUZUKI, N. SARUKURA, K. SHIMAMURA, T. FUKUDA, M. HIRANO and H. HOSONO**, "Ce<sup>3+</sup>:LiCaAlF<sub>6</sub> Crystal for High-Gain or High-Peak-Power Amplification of Ultraviolet Femtosecond Pulses and New Potential Ultraviolet Gain Medium: Ce<sup>3+</sup>:LiSr<sub>0.8</sub>Ca<sub>0.2</sub>AlF<sub>6</sub>," *IEEE J. Sel. Top. Quantum Electron.* **7**, 542 (2001).
- M. OTO, S. KIKUGAWA, N. SARUKURA, M. HIRANO and H. HOSONO**, "Optical Fiber for Deep Ultraviolet Light," *IEEE Photonics Technol. Lett.* **13**, 978 (2001).
- K. SHIMAMURA, H. SATO, A. BENSALAH, V. SUDESH, H. MACHIDA, N. SARUKURA and T. FUKUDA**, "Crystal Growth of Fluorides for Optical Applications," *Cryst. Res. Technol.* **36**, 801 (2001).
- H. MURAKAMI, T. KOZEKI, Y. SUZUKI, S. ONO, H. OHTAKE, N. SARUKURA, E. ISHIKAWA and T. YAMASE**, "Nanocluster Crystals of Lacunary Polyoxometalates as Structure-Design-Flexible, Inorganic Nonlinear Materials," *Appl. Phys. Lett.* **79**, 3564 (2001).
- H. OHTAKE, Y. SUZUKI, N. SARUKURA, S. ONO, T. TSUKAMOTO, A. NAKANISHI, S. NISHIZAWA, M. L. STOCK, M. YOSHIDA and H. ENDERT**, "THz-Radiation Emitter and Receiver System Based on a 2T Permanent Magnet, 1040 nm Compact Fiber Laser and Pyroelectric Thermal Receiver," *Jpn. J. Appl. Phys., Part 2* **40**, L1223 (2001).

- K. SHIMAMURA, H. SATO, A. BENSALAH, H. MACHIDA, N. SARUKURA and T. FUKUDA**, "Growth of Ce-Doped Colquiriite- and Scheelite-Type Single Crystals for UV Laser Applications," *Opt. Mater.* **19**, 109 (2002).
- Z. LIU, K. SHIMAMURA, T. FUKUDA, T. KOZEKI, Y. SUZUKI and N. SARUKURA**, "High-Energy Pulse Generation from Solid-State Ultraviolet Lasers Using Large Ce:Fluoride Crystals," *Opt. Mater.* **19**, 123 (2002).
- K. KAWAMURA, N. ITO, N. SARUKURA, M. HIRANO and H. HOSONO**, "New Adjustment Technique for Time Coincidence of Femtosecond Laser Pulses Using Third Harmonic Generation in Air and its Application to Holograph Encoding System," *Rev. Sci. Instrum.* **73**, 1711 (2002).
- Y. SUZUKI, T. KOZEKI, S. ONO, H. MURAKAMI, H. OHTAKE, N. SARUKURA, T. NAKAJYO, F. SAKAI and Y. AOKI**, "Hybrid Time-Resolved Spectroscopic System for Evaluating Laser Material Using a Table-Top-Sized, Low-Jitter, 3-MeV Picosecond Electron-Beam Source with a Photocathode," *Appl. Phys. Lett.* **80**, 3280 (2002).
- H. OHTAKE, Y. SUZUKI, S. ONO, N. SARUKURA, T. HIROSUMI and T. OKADA**, "Simultaneous Measurement of Thickness and Water Content of Thin Black Ink Films for the Printing Using THz Radiation," *Jpn. J. Appl. Phys., Part 2* **41**, L475 (2002).
- K. YAMAMOTO, K. TOMINAGA, H. SASAKAWA, A. TAMURA, H. MURAKAMI, H. OHTAKE and N. SARUKURA**, "Far-Infrared Absorption Measurements of Polypeptides and Cytochrome *c* by THz Radiation," *Bull. Chem. Soc. Jpn.* **75**, 1083 (2002).
- Y. SUZUKI, S. ONO, H. MURAKAMI, T. KOZEKI, H. OHTAKE, N. SARUKURA, G. MASADA, H. SHIRAIISHI and I. SEKINE**, "0.43 J, 10 Hz Fourth Harmonic Generation of Nd:YAG Laser Using Large Li<sub>2</sub>B<sub>4</sub>O<sub>7</sub> Crystals," *Jpn. J. Appl. Phys., Part 2* **41**, L823 (2002).
- T. KOZEKI, Y. SUZUKI, M. SAKAI, H. OHTAKE, N. SARUKURA, K. SHIMAMURA, T. FUKUDA, T. NAKAJYO, F. SAKAI and Y. AOKI**, "Electron-Beam Excitation of a Ce<sup>3+</sup>:LiCaAlF<sub>6</sub> Crystal for Future High-Peak-Power UV lasers," *Appl. Phys. B* **74**, S185 (2002).
- V. LUPEI, A. LUPEI, S. GEORGESCU, T. TAIRA, Y. SATO and A. IKESUE**, "The Effect of Nd Concentration on the Spectroscopic and Emission Decay Properties of Highly Doped Nd:YAG Ceramics," *Phys. Rev. B* **64**, 092102 (2001).
- V. LUPEI, N. PAVEL and T. TAIRA**, "Laser Emission in Highly-Doped Nd:YAG Crystals under <sup>4</sup>F<sub>5/2</sub> and <sup>4</sup>F<sub>3/2</sub> Pumping," *Opt. Lett.* **26**, 1678 (2001).
- V. LUPEI, A. LUPEI, N. PAVEL, T. TAIRA and A. IKESUE**, "Comparative Investigation of Spectroscopic and Laser Emission Characteristics under Direct 885-nm Pump of Concentrated Nd:YAG Ceramics and Crystals," *Appl. Phys. B* **73**, 757 (2001).
- V. LUPEI, N. PAVEL and T. TAIRA**, "Highly Efficient Laser Emission in Concentrated Nd:YVO<sub>4</sub> Components under Direct Pumping into the Emitting Level," *Opt. Commun.* **201**, 431 (2002).
- J. SAIKAWA, S. KURIMURA, I. SHOJI and T. TAIRA**, "Tunable Frequency-Doubled Yb:YAG Microchip Lasers," *Opt. Mater.* **19**, 169 (2002).
- I. SHOJI, Y. SATO, S. KURIMURA, V. LUPEI, T. TAIRA, A. IKESUE and K. YOSHIDA**, "Thermal-Birefringence-Induced Depolarization in Nd:YAG Ceramics," *Opt. Lett.* **27**, 234 (2002).
- V. LUPEI, N. PAVEL and T. TAIRA**, "Efficient Laser Emission in Concentrated Nd Laser Materials under Pumping into the Emitting Level," *IEEE J. Quantum Electron.* **38**, 240 (2002).
- V. LUPEI, A. LUPEI, S. GEORGESCU, B. DIACONESCU, T. TAIRA, Y. SATO, S. KURIMURA and A. IKESUE**, "High-Resolution Spectroscopy and Emission Decay in Concentrated Nd:YAG Ceramics," *J. Opt. Soc. Am. B* **19**, 360 (2002).
- I. SHOJI and T. TAIRA**, "Intrinsic Reduction of the Depolarization Loss in Solid-State Lasers by Use of a (110)-cut Y<sub>3</sub>Al<sub>5</sub>O<sub>12</sub> Crystal," *Appl. Phys. Lett.* **80**, 3048 (2002).
- V. LUPEI, N. PAVEL and T. TAIRA**, "1064-nm Laser Emission of Highly Doped Nd: Yttrium Aluminum Garnet under 885-nm Diode Laser Pumping," *Appl. Phys. Lett.* **80**, 4309 (2002).
- N. E. YU, J. H. RO, M. CHA, S. KURIMURA and T. TAIRA**, "Broadband Quasi-Phase-Matched Second Harmonic Generation in MgO-Doped Periodically Poled LiNbO<sub>3</sub> at the Communications Band," *Opt. Lett.* **27**, 1046 (2002).
- T. DASCALU, T. TAIRA and N. PAVEL**, "Diode Edge-Pumped Microchip Composite Yb:YAG Laser," *Jpn. J. Appl. Phys.* **41**, L606 (2002).

#### Research Center for Molecular-scale Nanoscience

- N. TROMBACH, H. TADA, S. HILLER, D. SCHLETTWEIN and D. WOHRLE**, "Photovoltaic Junction Properties of Ultrathin Films of Phthalocyaninatooxovanadium (PcVO) on H-Terminated N-Si(111)," *Thin Solid Films* **396**, 109 (2001).
- K. OKAMOTO, T. TOJO, H. TADA, M. TERAZIMA and K. MATSUSIGE**, "Microscopic Patterning on The Polysilane Films by The Laser Induced Grating Technique," *Mol. Cryst. Liq. Cryst.* **370**, 379 (2001).
- M. TAKADA, H. YOSHIOKA, H. TADA and K. MATSUSHIGE**, "Electrical Characteristics of Phthalocyanine Films Prepared by Electrophoretic Deposition," *Jpn. J. Appl. Phys.* **41**, L73 (2002).
- M. TAKADA, H. GRAAF, Y. YAMASHITA and H. TADA**, "BTQBT (bis-(1, 2, 5-thiadiazolo)-p-quinobis(1, 3-dithiole)) Thin Films; A Promising Candidate for High Mobility Organic Transistors," *Jpn. J. Appl. Phys.* **41**, L4

(2002).

**M. ARA, H. GRAAF and H. TADA**, "Nanopatterning of Alkyl Monolayers Covalently Bound to Si(111) with An Atomic Force Microscope," *Appl. Phys. Lett.* **80**, 2565 (2002).

**M. ARA, H. GRAAF and H. TADA**, "Atomic Force Microscope Anodization of Si(111) Covered with Alkyl," *Jpn. J. Appl. Phys.* **41**, 4894 (2002).

**H. GRAAF, M. ARA and H. TADA**, "Force Curve Measurement of Self-Assembled Organic Monolayers Bound Covalently on Silicon (111)," *Mol. Cryst. Liq. Cryst.* **377**, 33 (2002).

**M. TACHIBANA, S. TANAKA, Y. YAMASHITA and K. YOSHIZAWA**, "Small Bandgap Polymers Involving Tricyclic Nonclassical Thiophene as a Building Block," *J. Phys. Chem. B* **106**, 3549 (2002).

**M. B. ZAMAN, M. TOMURA and Y. YAMASHITA**, "Crystal Engineering Using Anilic Acids and Dipyridyl Compounds through a New Supramolecular Synthon," *J. Org. Chem.* **66**, 5987 (2001).

**M. TOMURA and Y. YAMASHITA**, "Bis(tetra-n-butylammonium) Bis(2-dicyanomethylene-4,5-dimercapto-1,3-dithiole)nickel(II)," *Acta Crystallogr., Sect. E* **58**, m133 (2002).

**K. ONO, K. SAITO, H. UCHIUMI and M. TOMURA**, "<sup>1</sup>H NMR Analysis and Crystal Structures of 1,1',3,3'-Tetramethyl-2,2'-bi-1*H*-Imidazolium Bis(tetraphenylborate): Ion-Associative Interactions Containing Ketone, Aldehyde, and Nitrile," *Chem. Lett.* 622 (2002).

**M. TOMURA, M. AKHTARUZZAMAN, K. SUZUKI and Y. YAMASHITA**, "4,7-Diiodo-2,1,3-benzothiadiazole and 7,7'-Diiodo-4,4'-bis(2,1,3-benzothiadiazole)," *Acta Crystallogr., Sect. C: Cryst. Struct. Commun.* **58**, o373 (2002).

**Y. YAMASHITA, M. TOMURA, M. URUICHI and K. YAKUSHI**, "Synthesis and Properties of  $\pi$ -Extended TTF Analogues and Their Cation Radical and Dication Salts," *Mol. Cryst. Liq. Cryst.* **376**, 19 (2002).

**K. ITO, T. NAGATA and K. TANAKA**, "Synthesis and Electrochemical Properties of Transition Metal Complexes of 2,2':6',2''-Terpyridine 1,1''-Dioxide," *Inorg. Chem.* **40**, 6331 (2001).

**M. SAEKI, T. TSUKUDA and T. NAGATA**, "Ab initio Study of  $\text{CO}_2^- \cdot \text{CO}_2 \leftrightarrow \text{C}_2\text{O}_4^-$  Isomerization," *Chem. Phys. Lett.* **348**, 461 (2001).

**L. ZHU, K. TAKAHASHI, M. SAEKI, T. TSUKUDA and T. NAGATA**, "Photodissociation of Gas-Phase  $\text{I}_3^-$ : Product Branching in the Visible and UV Regions," *Chem. Phys. Lett.* **350**, 233 (2001).

**T. TSUKUDA, L. ZHU, M. SAEKI and T. NAGATA**, "Photochemistry of  $(\text{NO})_n^-$  as Studied by Photofragment Mass Spectrometry," *Int. J. Mass Spectrom.* **220**, 137 (2002).

**H. SAKURAI, T. TSUKUDA and T. HIRAO**, "Pd/C as a Reusable Catalyst for the Coupling Reaction of Halophenols and Arylboronic Acids in Aqueous Media," *J. Org. Chem.* **67**, 2721 (2002).

**H. SAKURAI, T. HIRAO, Y. NEGISHI, H. TSUNAKAWA and T. TSUKUDA**, "Palladium Clusters Stabilized by Cyclodextrins Catalyze Suzuki-Miyaura Coupling Reactions in Water," *Trans. Mater. Res. Soc. Jpn.* **27**, 185 (2002).

**D. KUWAHARA, T. NAKAI, J. ASHIDA and S. MIYAJIMA**, "Novel Structure Discovered on Two-Dimensional Spin-Echo NMR Spectra for a Homonuclear Two-Spins System in Rotating Solids," *Proceedings of 14th Conference of the International Society of Magnetic Resonance* 130 (2001).

**M. KOMIYAMA, M. GU and H.-M. WU**, "Determination of Extra-framework Cation Positions and Their Occupancies on Heulandite(010) by Atomic Force Microscopy," *J. Phys. Chem. B* **105**, 4680 (2001).

**M. KOMIYAMA, T. UCHIHASHI, Y. SUGAWARA and S. MORITA**, "Molecular Orbital Interpretation of Thymine/graphite NC-AFM Images," *Surf. Interface Anal.* **29**, 53 (2001).

**M. KOMIYAMA and D. YIN**, "Apparent Local Structural Change Caused by Ultraviolet Light on a  $\text{TiO}_2$  Surface Observed by Scanning Tunneling Microscopy," *Jpn. J. Appl. Phys.* **40**, 4281 (2001).

**M. KOMIYAMA and T. SHIMAGUCHI**, "Partial Reduction of Si(IV) in  $\text{SiO}_2$  Thin Film by Deposited Metal Particles - An XPS Study," *Surf. Interface Anal.* **29**, 189 (2001).

**N. GU and M. KOMIYAMA**, "Various Phases on Natural Stilbite (010) Surface Observed by Atomic Force Microscopy under Aqueous Conditions," *Jpn. J. Appl. Phys.* **40**, 4285 (2001).

**S. HASEGAWA, K. YAKUSHI, H. INOKUCHI, K. K. OKUDAIRA, N. UENO, K. SEKI, E. MORIKAWA and V. SAILE**, "Calculated Photoelectron Angular Distributions of  $\omega$ -(*n*-pyrrolyl)alkanethiol Self-Assembled Monolayers for Distinguishing Between Different Arrangements of Pyrrole Groups," *J. Electron Spectrosc. Relat. Phenom.* **120**, 121 (2001).

**S. HASEGAWA, T. HORIGOME, K. YAKUSHI, H. INOKUCHI, K. K. OKUDAIRA, N. UENO, K. SEKI, R. J. WILLCUT, R. L. McCARLEY, E. MORIKAWA and V. SAILE**, "Angle-Resolved Photoemission Measurements of  $\nu$ -(*n*-pyrrolyl)alkanethiol Self-Assembled Monolayers Using In-Situ Sample Preparation Apparatus," *J. Electron Spectrosc. Relat. Phenom.* **113**, 101 (2001).

**K. K. OKUDAIRA, E. MORIKAWA, S. HASEGAWA, H. ISHII, Y. AZUMA, M. IMAMURA, H. SHIMADA, K. SEKI and N. UENO**, "Surface Electronic Structure and Molecular Orientation of Poly(9-vinylcarbazole) Thin Film: ARUPS and NEXAFS," *Nucl. Instrum. Methods Phys. Res., Sect. A* **467-468**, 1233



(2001).

**K. K. OKUDAIRA, S. KERA, H. SETOYAMA, E. MORIKAWA and N. UENO**, "Electronic Structure and Molecular Orientation at Thin Film Surfaces of Pendant-Group Polymers Studied by Outermost Surface Spectroscopy Using Metastable Atoms," *J. Electron Spectrosc. Relat. Phenom.* **121**, 225 (2001).

**H. YAMANE, H. SETOYAMA, S. KERA, K. K. OKUDAIRA and N. UENO**, "Low-Energy Electron Transmission Experiments on Graphite," *Phys. Rev. B* **64**, 113407 (2001).

**Y. AZUMA, K. IWASAWA, T. KURIHARA, K. K. OKUDAIRA, Y. HARADA and N. UENO**, "Low Energy Electron Diffraction of the System In-[perylene-3,4,9, 10-tetracarboxylic Dianhydride] on MoS<sub>2</sub>," *J. Appl. Phys.* **91**, 5024 (2002).

**D. YOSHIMURA, H. ISHII, T. MIYAMAE, S. HASEGAWA, K. K. OKUDAIRA, N. UENO and K. SEKI**, "Intramolecular Energy-Band Dispersion in Oriented Thin Film of n-CF<sub>3</sub>(CF<sub>2</sub>)<sub>22</sub>CF<sub>3</sub> Observed by Angle-Resolved UV Photoemission and its Theoretical Simulation," *Surf. Rev. Lett.* **9**, 407 (2002).

**Y. TAKABAYASHI, Y. KUBOZONO, T. KANBARA, S. FUJIKI, K. SHIBATA, Y. HARUYAMA, T. HOSOKAWA, Y. RIKIISHI and S. KASHINO**, "Pressure and Temperature Dependences of the Structural Properties of Dy@C<sub>82</sub> Isomer I," *Phys. Rev. B* **65**, 73405 (2002).

**K. ISHII, A. FUJIWARA, H. SUEMATSU and Y. KUBOZONO**, "Ferromagnetism and Giant Magnetoresistance in the Rare-Earth Fullerides Eu<sub>6-x</sub>Sr<sub>x</sub>C<sub>60</sub>," *Phys. Rev. B* **65**, 134431 (2002).

**D. H. CHI, Y. IWASA, X. H. CHEN, T. TAKENOBŪ, T. ITO, T. MITANI, E. NISHIBORI, M. TAKATA, M. SAKATA and Y. KUBOZONO**, "Bridging Fullerenes with Metals," *Chem. Phys. Lett.* **359**, 177 (2002).

**S. FUJIKI, Y. KUBOZONO, M. KOBAYASHI, T. KAMBE, Y. RIKIISHI, S. KASHINO, K. ISHII, H. SUEMATSU and A. FUJIWARA**, "Structure and Physical Properties of Cs<sub>3+α</sub>C<sub>60</sub> (α = 0.0–1.0) under Ambient and High Pressures," *Phys. Rev. B* **65**, 235425 (2002).

**Y. NAGAO, R. IKEDA, S. KANDA, Y. KUBOZONO and H. KITAGAWA**, "Complex-Plane Impedance Study on a Hydrogen-Doped Copper Coordination Polymer: *N,N'*-bis-(2-hydroxy-ethyl)-Dithiooxamidato-Copper(II)," *Mol. Cryst. Liq. Cryst.* **379**, 89 (2002).

**Y. TANIMOTO, Y. AKIMOTO, Y. FUJIWARA, M. MUKAI, T. TAKUI, T. KINOSHITA and K. ITOH**, "Magnetic Field Effect on the Fluorescence of *m*-Phenylenebis(phenylmethylene) in a Rigid Glass at 77 K," *Bull. Chem. Soc. Jpn.* **74**, 2325 (2001).

**Y. TANIMOTO, R. YAMAGUCHI, Y. KANAZAWA and M. FUJIWARA**, "Magnetic Orientation of *Lysozyme* Crystals," *Bull. Chem. Soc. Jpn.* **75**, 1133 (2002).

**S. KOHTANI, M. SUGIYAMA, Y. FUJIWARA, Y. TANIMOTO and R. NAKAGAKI**, "Asymmetric Photolysis of 2-Phenylcycloalkanones with Circularly Polarized Light: A Kinetic Model for Magnetic Field Effects," *Bull. Chem. Soc. Jpn.* **75**, 1223 (2002).

**Y. FUJIWARA, J. HAMADA, T. AOKI, T. SHIMIZU, Y. TANIMOTO, H. YONEMURA, S. YAMADA, T. UJIE and H. NAKAMURA**, "Chain Length Dependence of High Magnetic Field Effects on Lifetimes of Radical Ions Pairs Linked by a Methylene Chain: Interpretation by both Spin-Lattice and Spin-Spin Relaxations," *Mol. Phys.* **100**, 1405 (2002).

**M. FUJIWARA, K. KAWAKAMI and Y. TANIMOTO**, "Magnetic Orientation of Carbon Nanotubes at Temperatures of 231 K and 314 K," *Mol. Phys.* **100**, 1085 (2002).

**H. YOSHIKAWA, S. NISHIKIORI, T. WATANABE, T. ISHIDA, G. WATANABE, M. MURAKAMI, K. SUWINSKA, R. LUBORADZKI and J. LIPKOWSKI**, "Polycyano-Polycadmate Host Clathrates Including a Methylviologen Dication. Syntheses, Crystal Structures and Photo-Induced Reduction of Methylviologen Dication," *J. Chem. Soc., Dalton Trans.* 1907 (2002).

**K. KONOSHIMA, T. GOTO, T. ISHIDA, K. URABE and M. KITAO**, "IR Absorption Spectra of Electrochromic WO<sub>3</sub> Films," *Trans. Mater. Res. Soc. Jpn.* **27**, 349 (2002).

#### UVSOR (Ultraviolet Synchrotron Orbital Radiation) Facility

**S. ASAKA, M. ITOH and M. KAMADA**, "Ultraviolet Light Amplification within a Nanometer-Sized Layer," *Phys. Rev. B* **63**, 81104 (2001).

**S. TANAKA, S. D. MORÉ, J. MURAKAMI, M. ITOH, Y. FUJII and M. KAMADA**, "Surface Photovoltage Effects on p-GaAs(100) from Core-Level Photoelectron Spectroscopy Using Synchrotron Radiation and a Laser," *Phys. Rev. B* **64**, 155308 (2001).

**M. ITOH and M. KAMADA**, "Comparative Study of Auger-Free Luminescence and Valence-Band Photoemission in Wide-Gap Materials," *J. Phys. Soc. Jpn.* **70**, 3446 (2001).

**M. KAMADA and M. ITOH**, "Nonradiative Decay of Core Excitons in the Auger-Free Luminescence Materials CsCl and BaF<sub>2</sub>," *Phys. Rev. B* **65**, 245104 (2002).

**T. TSUJIBAYASHI, K. TOYODA, S. SAKURAGI, M. KAMADA, and M. ITOH**, "Spectral Profile of the Two-Photon Absorption Coefficients in CaF<sub>2</sub>," *Appl. Phys. Lett.* **80**, 2883 (2002).

**K. KANDA, T. KITAGAWA, Y. SHIMIZUGAWA, Y. HARUYAMA, S. MATSUI, M. TERASAWA, H. TSUBAKINO, I. YAMADA, T. GEJO and M. KAMADA**, "Characterization of Hard Diamond-Like Carbon

- Films Formed by Ar-Gas Cluster Ion Beam-Assisted Fullerene Deposition," *Jpn. J. Appl. Phys.* **41**, 4295 (2002).
- M. KAMADA, S. TANAKA, K. TAKAHASHI, Y. DOI, K. FUKUI, T. KINOSHITA, Y. HARUYAMA, S. ASAKA, Y. FUJII and M. ITOH**, "Beam-line Systems for Pump-Probe Photoelectron Spectroscopy Using SR and Laser," *Nucl. Instrum. Methods Phys. Res., Sect. A* **467/468**, 1441 (2001).
- S. ASAKA, J. AZUMA, T. TSUJIBAYASHI, M. ITOH, M. WATANABE, O. ARIMOTO, S. NAKANISHI, H. ITOH and M. KAMADA**, "Optical Detection System Using Time Structure of UVSOR for Combined Laser-SR Experiments," *Nucl. Instrum. Methods Phys. Res., Sect. A* **467/468**, 1455 (2001).
- M. KAMADA**, "Experiments with Combined Laser and SR at the UVSOR Facility," *LSWAVE Proceedings* 11 (2001).
- S. D. MORÉ, S. TANAKA, T. NISHITANI, T. NAKANISHI and M. KAMADA**, "Cesiumoxide-GaAs Interface and Layer Thickness in NEA Surface Formation," *SPIN2000* 916 (2001).
- S. TANAKA, K. TAKAHASHI, S. D. MORÉ, T. NISHITANI, T. NAKANISHI, and M. KAMADA**, "Surface Photo-Voltage Effect on Clean and NEA Surfaces of GaAs and Its Superlattice," *SPIN2000* 1000 (2001).
- M. KAMADA, K. TAKAHASHI, Y. DOI, F. FUKUI, T. TAYAGAKI and K. TANAKA**, "Photoelectron Spectroscopic Study on Photo-Induced Phase Transition of Spin-Crossover Complex," *Phase Transition* **41** (2002).
- S. TANAKA, K. TAKAHASHI, J. AZUMA, K. HAYAKAWA, M. ITOH and M. KAMADA**, "New Spectroscopy for Photo-Induced Phenomena Using Combination of Synchrotron Radiation and Laser," *Phase Transition* **51** (2002).
- K. TAKAHASHI, M. KAMADA, Y. DOI, K. FUKUI, T. TAYAGAKI and K. TANAKA**, "Photo-Induced Phase Transition of Spin-Crossover Complex Studied with the Combination of SR and Laser," *Surf. Rev. Lett.* **9**, 319 (2002).
- S. TANAKA, S. D. MORÉ, T. NISHITANI, K. TAKAHASHI, T. NAKANISHI and M. KAMADA**, "Surface-Photovoltage Effect on GaAs-GaAsP Super-Lattice Studied with Combination of Synchrotron Radiation and Laser," *Surf. Rev. Lett.* **9**, 1297 (2002).
- R. GUILLEMIN, E. SHIGEMASA, K. LE GUEN, D. CEOLIN, C. MIRON, N. LECLERCQ, P. MORIN and M. SIMON**, "Dynamical Angular Correlation in Molecular Auger Decay," *Phys. Rev. Lett.* **87**, 203001 (2001).
- R. GUILLEMIN, O. HEMMERS, D. W. LINDLE, E. SHIGEMASA, K. LE GUEN, D. CEOLIN, C. MIRON, N. LECLERCQ, P. MORIN, M. SIMON and P. W. LANGHOFF**, "Nondipolar Electron Angular Distributions from Fixed-in-Space Molecules," *Phys. Rev. Lett.* **89**, 033002 (2002).
- E. SHIGEMASA, T. GEJO, M. NAGASONO, T. HATSUI and N. KOSUGI**, "Double and Triple Excitations near the K-Shell Ionization Threshold of N<sub>2</sub> Revealed by Symmetry-Resolved Spectroscopy," *Phys. Rev. A* **66**, 022508 (2002).
- S. KODA, M. HOSAKA, J. YAMAZAKI, M. KATOH and H. HAMA**, "Development of Longitudinal Feedback System for a Storage Ring Free Electron Laser," *Nucl. Instrum. Methods Phys. Res., Sect. A* **475**, 211 (2001).
- M. HOSAKA, S. KODA, M. KATOH, J. YAMAZAKI and H. HAMA**, "FEL Induced Electron Bunch Heating Observed by a Method Based on Synchronous Phase Detection," *Nucl. Instrum. Methods Phys. Res., Sect. A* **475**, 217 (2002).
- M. HOSAKA, S. KODA, M. KATOH, J. YAMAZAKI, K. HAYASHI, K. TAKASHIMA, T. GEJO and H. HAMA**, "From the Operation of an SRFEL to a User Facility," *Nucl. Instrum. Methods Phys. Res., Sect. A* **483**, 146 (2002).
- S. KIMURA, T. NISHI, M. OKUNO, H. IWATA, H. AOKI and A. OCHIAI**, "Charge Ordering Effect of Electronic Structure of Yb<sub>4</sub>(As<sub>1-x</sub>Sb<sub>x</sub>)<sub>3</sub>," *J. Phys. Soc. Jpn.* **71**, 300 (2002).
- S. KIMURA, M. OKUNO, H. IWATA, T. SAITOH, T. OKUDA, A. HARASAWA, T. KINOSHITA, A. MITSUDA, H. WADA and M. SHIGA**, "Temperature-Induced Valence Transition of EuNi<sub>2</sub>(Si<sub>0.25</sub>Ge<sub>0.75</sub>)<sub>2</sub> Studied by Eu 4d-4f Resonant Photoemission and Optical Conductivity," *J. Phys. Soc. Jpn.* **71**, 255 (2002).
- H. OKAMURA, M. MATSUNAMI, S. KIMURA, T. NANBA, F. IGA and T. TAKABATAKE**, "Optical Conductivity of Diluted Kondo Semiconductors Yb<sub>1-x</sub>Lu<sub>x</sub>B<sub>12</sub>," *J. Phys. Soc. Jpn.* **71**, 303 (2002).
- S. O. HONG, B. H. MIN, H. J. LEE, S. KIMURA, M. H. JUNG, T. TAKABATAKE and Y. S. KWON**, "Influence of Electronic Structure of CeSbNi<sub>0.15</sub> on its Optical Conductivity," *Physica B* **312-313**, 251 (2002).
- H. OKAMURA, M. MATSUNAMI, S. KIMURA, T. NANBA, F. IGA and T. TAKABATAKE**, "Optical Gap in the Diluted Kondo Semiconductors Yb<sub>1-x</sub>Lu<sub>x</sub>B<sub>12</sub>: Lattice and Single-Site Effects," *Physica B* **312-313**, 157 (2002).
- H. OKAMURA, T. KORETSUNE, M. MATSUNAMI, S. KIMURA, T. NANBA, H. IMAI, Y. SHIMAKAWA and Y. KUBO**, "Magneto-Optical Study of the Colossal Magnetoresistance Pyrochlore Tl<sub>2</sub>Mn<sub>2</sub>O<sub>7</sub>," *Physica B* **312-313**, 714 (2002).
- S. KIMURA, M. OKUNO, H. IWATA, H. KITAZAWA and G. KIDO**, "Low-Energy Electronic Structure of Ce<sub>1-x</sub>La<sub>x</sub>Sb (x = 0, 0.1) in the Magnetically Ordered States," *Physica B* **312-313**, 228 (2002).
- S. KIMURA, M. OKUNO, H. IWATA, T. NISHI, H. AOKI and A. OCHIAI**, "Low-Energy Optical Conductivity of Yb<sub>4</sub>As<sub>3</sub>," *Physica B* **312-313**, 356 (2002).
- T. KINOSHITA, H. P. N. J. GUNASEKARA, Y. TAKATA, S. KIMURA, M. OKUNO, Y. HARUYAMA, N. KOSUGI, K. G. NATH, H. WADA, A. MITSUDA, M. SHIGA, T. OKUDA, A. HARASAWA, H. OGASAWARA and A. KOTANI**, "Spectroscopy Studies of Temperature-Induced Valence Transition Material

- EuNi<sub>2</sub>(Si<sub>1-x</sub>Ge<sub>x</sub>)<sub>2</sub> around Eu 3d-4f, Eu 4d-4f and Ni 2p-3d Excitation Regions,” *J. Phys. Soc. Jpn.* **71**, 148 (2002).
- H. OKAMURA, T. KORETSUNE, M. MATSUNAMI, S. KIMURA, T. NANBA, H. IMAI, Y. SHIMAKAWA and Y. KUBO**, “Charge Dynamics in the Colossal Magneto-Resistance Pyrochlore Ti<sub>2</sub>Mn<sub>2</sub>O<sub>7</sub>,” *Phys. Rev. B* **64**, 180409(R) (2001).
- S. KIMURA, M. OKUNO, H. IWATA, H. AOKI and A. OCHIAI**, “Temperature Dependence of Low-Energy Optical Conductivity of Yb<sub>4</sub>(As<sub>1-x</sub>P<sub>x</sub>)<sub>3</sub> (x = 0, 0.05, 0.15),” *J. Phys. Soc. Jpn.* **70**, 2829 (2001).

### Computer Center

- I. TOKUE, H. TANAKA, K. YAMASAKI and S. NANBU**, “Formation of HCl<sup>+</sup>(A<sup>2</sup>Σ<sup>+</sup>) and HBr<sup>+</sup>(A<sup>2</sup>Σ<sup>+</sup>) Resulting from He(2<sup>3</sup>S) Penning Ionization of HCl and HBr,” *J. Phys. Chem. A* **106**, 6068 (2002).
- J. -I. CHOE, S. -K. CHANG and S. NANBU**, “Ab Initio Study of Conformers of p-tert-Butylcalix[4]crown-6-Ether Complexed with Alkyl Ammonium Cations,” *Bull. Korean Chem. Soc.* **23**, 891 (2002).
- J. OUYANG, K. YAKUSHI, T. KINOSHITA, S. NANBU, M. AOYAGI, Y. MISAKI and K. TANAKA**, “The Assignment of the In-Plane Molecular Vibrations of the BDT-TTP Electron-Donor Molecule Based on the Polarized Raman and Infrared Spectra, where BDT-TTP is 2,5-bis(1,3-dithiol-2-ylidene)-1,3,4,6-Tetrathiapentalene,” *Spectrochim. Acta, Part A* **58**, 1643 (2002).

### Center for Integrative Bioscience

- S. OGO, S. MAKIHARA, Y. KANEKO and Y. WATANABE**, “pH-Dependent Transfer Hydrogenation, Reductive Amination, and Dehalogenation of Water-Soluble Carbonyl Compounds and Alkyl Halides Promoted by Cp\*Ir Complexes,” *Organometallic* **20**, 4903 (2001).
- S. OGO, R. YAMAHARA, T. FUNABIKI, H. MASUDA and Y. WATANABE**, “Biomimetic Intradiol-Cleavage of Catechols with Incorporation of Both Atoms of O<sub>2</sub>: The Role of the Vacant Coordination Site on the Iron Center,” *Chem. Lett.* 1062 (2001).
- T. TOMITA, S. OGO, T. EGAWA, H. SHIMADA, N. OKAMOTO, Y. IMAI, Y. WATANABE, Y. ISHIMURA and T. KITAGAWA**, “Elucidation of the Differences between the 430 and 455-nm Absorbing Forms of P450-Isocyanide Adducts by Resonance Raman Spectroscopy,” *J. Biol. Chem.* **276**, 36261 (2001).
- I. HARA, T. UENO, S. OZAKI, S. ITOH, K. LEE, N. UEYAMA and Y. WATANABE**, “Oxidative Modification of Tryptophan-43 in the Heme Vicinity of the F43W/H64L Myoglobin Mutant,” *J. Biol. Chem.* **276**, 36067 (2001).
- S. OGO, T. ABURA and Y. WATANABE**, “pH-Dependent Transfer Hydrogenation of Ketones with HCOONa as a Hydrogen Donor Promoted by (η<sup>6</sup>-C<sub>6</sub>Me<sub>6</sub>)Ru Complexes,” *Organometallics* **21**, 2964 (2002).
- S. OGO, H. NAKAI and Y. WATANABE**, “pH-Dependent H<sub>2</sub>-Activation Cycle to Reduction of Nitrate Ion by Metal Complexes,” *J. Am. Chem. Soc.* **124**, 597 (2002).
- H. NAKAI, S. OGO and Y. WATANABE**, “pH-Dependent Cross-Coupling Reactions of Water-Soluble Organic Halides with Organoboron Compounds Catalyzed by an Organometallic Aqua Complex [(SCS)Pd<sup>II</sup>(H<sub>2</sub>O)]<sup>+</sup> {SCS = C<sub>6</sub>H<sub>3</sub>-2,6-(CH<sub>2</sub>SBu<sup>t</sup>)<sub>2</sub>},” *Organometallics* **21**, 1674 (2002).
- A. WADA, S. OGO, S. NAGATOMO, T. KITAGAWA, Y. WATANABE, K. JITSUKAWA and H. MASUDA**, “Reactivity of Hydrogen Peroxide Bound to a Mononuclear Non-Heme iron Site,” *Inorg. Chem.* **41**, 616 (2002).
- K. HASHIMOTO, S. NAGATOMO, S. FUJINAMI, H. FURUTACHI, S. OGO, M. SUZUKI, A. UEHARA, Y. MAEDA, Y. WATANABE and T. KITAGAWA**, “A New Mononuclear Iron(III) Complex Containing a Peroxocarbonate Ligand,” *Angew. Chem. Int. Ed. Engl.* **41**, 1201 (2002).
- S. KATO, H. -J. YANG, T. UENO, S. OZAKI, G. N. PHILLIPS, Jr., S. FUKUZUMI and Y. WATANABE**, “Asymmetric Sulfoxidation and Amine Binding by H64D/V68A and H64D/V68S Mb: Mechanistic Insight into the Chiral Discrimination Step,” *J. Am. Chem. Soc.* **124**, 8506 (2002).
- K. OHKUBO, R. TAYLOR, O. V. BOLTALINA, S. OGO and S. FUKUZUMI**, “Electron Transfer Reduction of a Highly Electron-Deficient Fullerene, C<sub>60</sub>F<sub>18</sub>,” *Chem. Commun.* **41**, 1202 (2002).
- M. Y. ALI, S. UEMURA, K. ADACHI, H. ITOH, K. KINOSITA, Jr. and S. ISHIWATA**, “Myosin V is a Left-Handed Spiral Motor on the Right-Handed Actin Helix,” *Nature Struct. Biol.* **9**, 464 (2002).
- T. MASAIKE, E. MUNAYUKI, H. NOJI, K. KINOSITA, Jr. and M. YOSHIDA**, “F<sub>1</sub>-ATPase Changes its Conformations upon Phosphate Release,” *J. Biol. Chem.* **277**, 21643 (2002).
- Y. HIRONO-HARA, H. NOJI, M. NISHIMURA, E. MUNAYUKI, K. Y. HARA, R. YASUDA, K. KINOSITA, Jr. and M. YOSHIDA**, “Pause and Rotation of F<sub>1</sub>-ATPase during Catalysis,” *Proc. Natl. Acad. Sci. U.S.A.* **98**, 13649 (2001).

**H. NAKAJIMA, E. NAKAGAWA, K. KOBAYASHI, S. TAGAWA and S. AONO**, “Ligand-Switching Intermediates for the CO-Sensing Transcriptional Activator CooA Measured by Pulse Radiolysis,” *J. Biol. Chem.* **276**, 37895 (2001).

**V. RUBTSOV, T. ZHANG, H. NAKAJIMA, S. AONO, G. I. RUBTSOV, S. KUMAZAKI and K. YOSHIHARA**, “Conformational Dynamics of Transcriptional Regulator CooA Protein Studied by Subpicosecond



Mid-Infrared Vibrational Spectroscopy," *J. Am. Chem. Soc.* **123**, 10056 (2001).

**S. AONO, T. KATO, M. MATSUKI, H. NAKAJIMA, T. OHTA, T. UCHIDA and T. KITAGAWA**, "Resonance Raman and Ligand Binding Studies of the Oxygen Sensing Signal Transducer Protein HemAT from *Bacillus subtilis*," *J. Biol. Chem.* **277**, 13528 (2002).

**R. DAVYDOV, V. KOFMAN, H. FUJII, T. YOSHIDA, M. IKEDA SAITO and B. M. HOFFMAN**, "Catalytic Mechanism of Heme Oxygenase Through EPR and ENDOR of Cryoreduced Oxy-Heme Oxygenase and its Asp140 Mutants," *J. Am. Chem. Soc.* **124**, 1798 (2002).

**H. FUJII**, "<sup>13</sup>C-NMR Signal Detection of Iron Bound Cyanide Ions in Ferric Cyanide Complexes of Heme Proteins," *J. Am. Chem. Soc.* **124**, 5936 (2002).

**N. OKISHIO, T. TANAKA, M. NAGAI, R. FUKUDA, S. NAGATOMO and T. KITAGAWA**, "Identification of Tyrosine Residues Involved in Ligand Recognition by the Phosphatidylinositol 3-Kinase Src Homology 3 Domain: Circular Dichroism and UV Resonance Raman Studies," *Biochemistry* **40**, 15797 (2001).

**S. ITOH, H. BANDO, M. NAKAGAWA, S. NAGATOMO, T. KITAGAWA, K. D. KARLIN and S. FUKUZUMI**, "Formation, Characterization, and Reactivity of Bis( $\mu$ -oxo)dinickel(III) Complexes Supported by A Series of Bis[2-(2-pyridyl)ethyl]amine Ligands," *J. Am. Chem. Soc.* **123**, 11168 (2001).

**S. ITOH, H. KUMEI, M. TAKI, S. NAGATOMO, T. KITAGAWA and S. FUKUZUMI**, "Oxygenation of Phenols to Catechols by A ( $\mu$ - $\eta^2$ : $\eta^2$ -Peroxo)dinickel(II) Complex: Mechanistic Insight into the Phenolase Activity of Tyrosinase," *J. Am. Chem. Soc.* **123**, 6708 (2001).

**Y. MIZUTANI and T. KITAGAWA**, "Ultrafast Structural Relaxation of Myoglobin Following Photodissociation of Carbon Monoxide Probed by Time-Resolved Resonance Raman Spectroscopy," *J. Phys. Chem. B* **105**, 10992 (2001).

**Y. MIZUTANI and T. KITAGAWA**, "Ultrafast Dynamics of Myoglobin Probed by Time-Resolved Resonance Raman Spectroscopy," *Chem. Records* **1**, 258 (2001).

**T. TOMITA, S. OGO, T. EGAWA, H. SHIMADA, N. OKAMOTO, Y. IMAI, Y. WATANABE, Y. ISHIMURA and T. KITAGAWA**, "Elucidation of the Differences between the 430- and 455-nm Absorbing Forms of P450-Isocyanide Adducts by Resonance Raman Spectroscopy," *J. Biol. Chem.* **276**, 36261 (2001).

**A. WADA, S. OGO, S. NAGATOMO, T. KITAGAWA, Y. WATANABE, K. JITSUKAWA and H. MASUDA**, "Reactivity of Hydroperoxide Bound to a Mononuclear Non-Heme Iron Site," *Inorg. Chem.* **41**, 616 (2002).

**S. AONO, T. KATO, M. MATSUKI, H. NAKAJIMA, T. OHTA, T. UCHIDA and T. KITAGAWA**, "Resonance Raman and Ligand Binding Studies of the Oxygen-Sensing Signal Transducer Protein HemAT from *Bacillus Subtilis*," *J. Biol. Chem.* **277**, 13528 (2002).

**M. AKI, T. OGURA, Y. NARUTA, T. H. LE, T. SATO and T. KITAGAWA**, "UV Resonance Raman Characterization of Model Compounds of Tyr244 of Bovine Cytochrome *c* Oxidase in Its Neutral, Deprotonated Anionic, and Deprotonated Neutral Radical Forms: Effects of Covalent Binding between Tyrosine and Histidine," *J. Phys. Chem. A* **106**, 3436 (2002).

**N. HARUTA and T. KITAGAWA**, "Time-Resolved UV Resonance Raman Investigation of Protein Folding Using a Rapid Mixer: Characterization of Kinetic Folding Intermediates of Apomyoglobin," *Biochemistry* **41**, 6595 (2002).

**K. HASHIMOTO, S. NAGATOMO, S. FUJINAMI, H. FURUTACHI, S. OGO, S. SUZUKI, A. UEHARA, Y. MAEDA, Y. WATANABE and T. KITAGAWA**, "A New Mononuclear Iron(III) Complex Containing a Peroxocarbonate Ligand," *Angew. Chem. Int. Ed. Engl.* **41**, 1202 (2002).

**H. HAYASHI, K. UOZUMI, S. FUJINAMI, S. NAGATOMO, K. SHIREN, H. FURUTACHI, M. SUZUKI, A. UEHARA and T. KITAGAWA**, "Modulation of the Copper-Dioxygen Reactivity by Stereochemical Effect of Tetradentate Tripodal Ligands," *Chem. Lett.* 416 (2002).

**S. HIROTA, Y. MIZOGUCHI, O. YAMAUCHI and T. KITAGAWA**, "Observation of an Isotope-Sensitive Low-Frequency Raman Band Specific to Metmyoglobin," *J. Biol. Inorg. Chem.* **7**, 217 (2002).

**T. KITAGAWA, N. HARUTA and Y. MIZUTANI**, "Time-Resolved Resonance Raman Study on Ultrafast Structural Relaxation and Vibrational Cooling of Photodissociated Carbonmonoxy Myoglobin," *Biopolymers* **67**, 207 (2002).

**Y. MIZUTANI and T. KITAGAWA**, "Mode Dependence of Vibrational Energy Redistribution in Nickel Tetraphenylporphyrin Probed by Picosecond Time-Resolved Resonance Raman Spectroscopy: Slow IVR to Phenyl Peripherals," *Bull. Chem. Soc. Jpn.* **75**, 965 (2002).

**S. NAGATOMO, Y. JIN, M. NAGAI, H. HORI and T. KITAGAWA**, "Changes in the Abnormal  $\alpha$ -Subunit upon CO-Binding to the Normal  $\beta$ -Subunit of Hb M Boston: Resonance Raman, EPR and CD Study," *Biophys. Chem.* **98**, 217 (2002).

**S. NAGATOMO, M. NAGAI, N. SHIBAYAMA and T. KITAGAWA**, "Differences in Changes of the  $\alpha$ 1- $\beta$ 2 Subunit Contacts between Ligand Binding to the  $\alpha$  and  $\beta$  Subunits of Hemoglobin A: UV Resonance Raman Analysis Using Ni-Fe Hybrid Hemoglobin," *Biochemistry* **41**, 10010 (2002).

**A. SATO, Y. SASAKURA, S. SUGIYAMA, I. SAGAMI, T. SHIMIZU, Y. MIZUTANI and T. KITAGAWA**, "Stationary and Time-Resolved Resonance Raman Spectra of His77 and Met95 Mutants of the Isolated Heme Domain of a Direct Oxygen Sensor from *E. coli*," *J. Biol. Chem.* **277**, 32650 (2002).

**M. TAKI, S. TERAMAE, S. NAGATOMO, Y. TACHI, T. KITAGAWA, S. ITOH and S. FUKUZUMI**, "Fine-

Tuning of Copper(I)-Dioxygen Reactivity by 2-(2-Pyridyl)ethylamine Bidentate Ligands," *J. Am. Chem. Soc.* **124**, 6367 (2002).

**B. VENKATESH, H. HORI, G. MIYAZAKI, S. NAGATOMO, T. KITAGAWA and H. MORIMOTO**, "Coordination Geometry of Cu-Porphyrin in Cu(II)-Fe(II) Hybrid Hemoglobins Studied by Q-Band EPR and Resonance Raman Spectroscopies," *J. Inorg. Biochem.* **88**, 310 (2002).