

REVIEW ARTICLES AND TEXTBOOKS

Department of Theoretical Studies

S. NAGASE and K. HIRAO, *Advance in Molecular Theory. Introduction to Modern Chemistry* (in Japanese), Iwanami; Tokyo (2002).

K. KOBAYASHI, "Theoretical Prediction and Design of Endohedral Metallofullerenes," *Chemical Industry* (in Japanese) **53**, 617 (2002).

Y. SUGITA and Y. OKAMOTO, "Free-Energy Calculations in Protein Folding by Generalized-Ensemble Algorithms," *Lecture Notes in Computational Science and Engineering*, T. Schlick and H. H. Gan, Eds. Springer-Verlag; Berlin, 304 (2002).

Y. OKAMOTO, "Computer Simulations of Protein Folding," *Computational Science* (in Japanese), *Japanese Scientific Monthly (GAKUJUTSU GEPPU)* **55**, 28 (2002).

K. NAGAYA, Y. TERANISHI and H. NAKAMURA, "Selective Excitation Among Closely Lying Multi-Levels," in *Laser Control and Manipulation of Molecules*, A. Bandrauk, R. J. Gordon and Y. Fujimura, Eds., ACS Symposium Series 821, American Chemical Society (2002).

H. NAKAMURA, *Nonadiabatic Transition: Concepts, Basic Theories and Applications*, World Scientific/Imperial College Press; Singapore (2002).

T. NAKAJIMA, T. TSUNEDA, H. NAKANO and K. HIRAO, "Recent Advances in Electronic Structure Theory," *J.Theor.Comput.Chem.* **1**, 109 (2002).

H. NAKANO, K. SORAKUBO, K. NAKAYAMA and K. HIRAO, "Complete Active Space Valence Bond (CASVB) Method and its Application to Chemical Reactions," *Valence Bond Theory*, David Cooper, Ed., Elsevier, 55 (2002).

T. NAKAJIMA, T. YANAI and K. HIRAO, "Relativistic Electronic Structure Theory," *J. Comput. Chem.* **23**, 847 (2002).

Department of Molecular Structure

T. YOKOYAMA, "Theory of XAFS," in *X-ray Absorption Spectroscopy: XAFS and its Applications* (in Japanese), T. Ohta, Ed., IPC Inc.; Tokyo, 7 (2002).

T. KATO, T. AKASAKA, K. TASHIRO and T. AIDA, "An Inclusion Complex of a Cyclic Dimmer of Metalloporphyrin with La@C₈₂," *Proceedings of the International Symposium on Fullerenes, Nanotubes, and Carbon Nanoclusters*, P. V. Kamat, D. M. Guldi and K. M. Kadish, Eds., The Electrochemical Society, Inc.; Pennington, **11**, 354 (2001).

S. OKUBO and T. KATO, "Spin Dynamics of Lanthanum Metallofullerenes," *The Proceedings of the International Symposium on Nanonetwork Materials, Fullerenes, Nanotubes, and Related Systems*, S. Saito et al., Eds., AIP Conference Proceedings, **590**, 469 (2001).

Department of Electronic Structure

T. SUZUKI, L. WANG and H. KOHGUCHI, "Femtosecond Time-Resolved Photoelectron Imaging," in *Imaging in Chemical Dynamics*, ACS Symposium Series 770 (2001).

T. SUZUKI and B. J. WHITAKER, "Non-Adiabatic Dynamics Effects in Chemistry Revealed by Time-Resolved Charged Particle Imaging," *International Reviews of Physical Chemistry* **20**, 313 (2001).

H. KOHGUCHI and T. SUZUKI, "Rotational Inelastic Scattering of Free Radicals," *Annual Report on the Progress of Chemistry* (2002).

T. SUZUKI, "Femtosecond Time-Resolved Photoelectron Imaging," in *Advances in Physical Chemistry*, World Scientific; Singapore (2002).

T. SUZUKI and S. NANBU, "Non-Adiabatic Bending Dissociation of OCS," in *Low-Lying Potential Energy Surfaces*, ACS Symposium Series 828 (2002).

T. YAMASE, "Current Topics on Antiviral Drugs, Topics 4: Antiviral Activity of Polyoxometalates for a Novel Typed Inorganic Drug," *J. Clinical & Experimental Medicine* **201**, 262 (2002).

T. YAMASE, "Time-Resolved ESR-Spectroscopic Investigation of Polyoxometalate Photochemistry," *Catalysts & Catalysis* **44**, 340 (2002).

Department of Molecular Assemblies

T. NAKAMURA, M. TANIGUCHI, Y. MISAKI, K. TANAKA and Y. NOGAMI, "ESR Investigation of Organic Conductor with Itinerant and Local Spins, (CHTM-TTP)₂TCNQ," in *EPR in the 21st Century*, A.

Kawamori, J. Yamauchi and H. Ohta, Eds., Elsevier Science; Amsterdam, 192 (2002).

Department of Applied Molecular Science

H. IWAMURA and K. INOUE, "Magnetic Ordering in Metal Coordination Complexes with Aminoxyl Radicals," *Magnetism: Molecules to Materials II, Molecule-Based Materials*, J. S. Miller and M. Drillon, Eds., 61 (2001).

K. INOUE, "Nitroxide Radical-Metal-Based Molecular Magnets," *π -Electron Magnetism-From Molecules to Magnetic Materials-, Structure & Bonding*, J. Veciana Ed., Springer-Verlag; Heidelberg, **100**, 61 (2001).

M. HASHIMOTO, T. YUZAWA, C. KATO, K. IWATA and H. HAMAGUCHI, "Fast Time-Resolved Mid-Infrared Spectroscopy Using Grating Spectrometers," in *Handbook of Vibrational Spectroscopy*, J. M. Chalmers and P. R. Griffiths Eds., John Wiley & Sons; West Sussex, **1**, 666 (2002).

H. HAMAGUCHI and K. IWATA, "Physics and Chemistry of S_1 *trans*-Stilbene in Solution as Studied by Time-Resolved Raman Spectroscopy," *Bull. Chem. Soc. Jpn.* **75**, 883 (2002).

H. KATAURA, T. KODAMA, K. KIKUCHI, H. HIRAHARA, S. IJIMA, S. SUZUKI, W. KRÄTSCHMER and Y. ACHIBA, "Optical Properties of Fullerene-Peapods," in *Nanonetwork Materials: Fullerenes, Nanotubes, and Related Systems*, S. Saito, T. Ando, Y. Iwasa, K. Kikuchi, M. Kobayashi and Y. Saito, Eds., American Institute of Physics Conference Proceedings; Melville, N. Y., **590**, 165 (2001).

K. SUEKI, K. AKIYAMA, C. KURATA, K. OOGAMA, Y. L. ZHAO, M. KATADA, S. ENOMOTO, S. AMBE, F. AMBE, H. NAKAHARA and K. KIKUCHI, "Behaviors of Metals in Production of Nanonetwork Materials Investigated by Radiochemical Technique," in *Nanonetwork Materials: Fullerenes, Nanotubes, and Related Systems*, S. Saito, T. Ando, Y. Iwasa, K. Kikuchi, M. Kobayashi and Y. Saito, Eds., American Institute of Physics Conference Proceedings; Melville, N. Y., **590**, 313 (2001).

T. ISHII, R. KANEHAMA, N. AIZAWA, M. YAMASHITA, H. MATSUZAKA, H. MIYASAKA, T. KODAMA, K. KIKUCHI, I. IKEMOTO, Y. IWASA and M. SHIRO, "Synthesis and Crystal Structure of Cocrystallite with Silver Octaethylporphyrin and C_{70} ," in *Nanonetwork Materials: Fullerenes, Nanotubes, and Related Systems*, S. Saito, T. Ando, Y. Iwasa, K. Kikuchi, M. Kobayashi and Y. Saito, Eds., American Institute of Physics Conference Proceedings; Melville, N. Y., **590**, 409 (2001).

K. AKIYAMA, K. SUEKI, Y. L. ZHAO, H. HABA, K. TSUKADA, T. KODAMA, K. KIKUCHI, T. OHTSUKI, Y. NAGAME, H. NAKAHARA and M. KATADA, "Characterization of Actinide Metallofullerenes," in *Nanonetwork Materials: Fullerenes, Nanotubes, and Related Systems*, S. Saito, T. Ando, Y. Iwasa, K. Kikuchi, M. Kobayashi and Y. Saito, Eds., American Institute of Physics Conference Proceedings; Melville, N. Y., **590**, 437 (2001).

M. CHIKAMATSU, K. KIKUCHI, T. KODAMA, H. NISHIKAWA, I. IKEMOTO, N. YOSHIMOTO, T. HANADA, Y. YOSHICA, N. TANIGAKI and K. YASE, "Out-of-Plane and In-Plane Structure of the Cast Films of Long Alkyl Chain-Linked C_{60} via Phenyl Ring," in *Nanonetwork Materials: Fullerenes, Nanotubes, and Related Systems*, S. Saito, T. Ando, Y. Iwasa, K. Kikuchi, M. Kobayashi and Y. Saito, Eds., American Institute of Physics Conference Proceedings; Melville, N. Y., **590**, 455 (2001).

K. KIKUCHI, K. SAKAGUCHI, N. OZAWA, T. KODAMA, H. NISHIKAWA, I. IKEMOTO, K. KOHDATE, D. MATSUMURA, T. YOKOYAMA and T. OHTA, "Valence Change of Tm Atom in Metallofullerene," in *Nanonetwork Materials: Fullerenes, Nanotubes, and Related Systems*, S. Saito, T. Ando, Y. Iwasa, K. Kikuchi, M. Kobayashi and Y. Saito, Eds., American Institute of Physics Conference Proceedings; Melville, N. Y., **590**, 473 (2001).

Coordination Chemistry Laboratories

Y. UOZUMI, K. SHIBATOMI, "Preparation of Optically Active Phosphines as Catalysts for Asymmetric Synthesis," *Jpn. Kokai Tokkyo Koho* **7** (2001).

Y. UOZUMI, "Palladium Catalysis in Water," in *My Favorite Organic Synthesis*, The Society of Synthetic Organic Chemistry; Japan, 242 (2002).

Y. UOZUMI, "Combinatorial Approaches towards Organic Synthetic Catalysts," *J. Soc. Synth. Org.* **60**, 434 (2002).

Y. UOZUMI and T. HAYASHI, "Solid-Phase Palladium Catalysis for High-Throughput Organic Synthesis," in *Combinatorial Chemistry-A Practical Handbook*, R. Hanco, P. Göltz and K. C. Nicolaou, Eds., Wiley-VCH; Weinheim, Germany (2002).

N. TOKITOH, "New Aspects in the Chemistry of Silaaromatic Compounds," *Organometallic News* (in Japanese) **6** (2002).

K. ONITSUKA, F. TAKEI and S. TAKAHASHI, "Syntheses and Properties of Helical Chiral Polyisocyanides," *Kobunshi Kako* (in Japanese) **50**, 122 (2001).

F. TAKEI, K. ONITSUKA and S. TAKAHASHI, "Screw-Sense-Selective Polymerization of Isocyanides," *Jasco Report* (in Japanese) **43**, 47 (2001).

S. TAKAHASHI and K. ONITSUKA, "Precise Synthesis of Organometallic Macromolecules," *Kagaku Kogyo* (in Japanese) **52**, 919 (2001).

K. ONITSUKA and S. TAKAHASHI, "Precise Synthesis of Helical Chiral Polymers Catalyzed by Transition Metal Complexes," *Syokubai* (in Japanese) **44**, 334 (2002).

Laser Research Center for Molecular Science

Z. LIU, N. SARUKURA and M. A. DUBINSKII, "All-Solid-State, Short-Pulse, Tunable, Ultraviolet Laser Sources Based on Ce^{3+} Activated Fluoride Crystals," in *Ultraviolet Spectroscopy and UV Lasers*, P. Misra and M. A. Dubinskii, Eds., Marcel Dekker; New York (2002).

I. SHOJI, T. TAIRA and A. IKESUE, "Ceramic Lasers," *The Transactions of the Institute of Electronics, Information and Communication Engineers C* **J84-C**, 918 (2001).

T. TAIRA, et al., "Optical Society in Future," *CD-ROM, Kagaku* (in Japanese) **31**, (2002).

A. IKESUE, T. TAIRA and K. YOSHIDA, "The Fabrication of Nd:YAG Ceramics with Extremely Low Optical Scattering and the Development of High Performance Ceramic Laser," *Fine Ceramics Report* (in Japanese) **20**, 192 (2002).

Research Center for Molecular-scale Nanoscience

H. TADA and S. TANAKA, "Electrical Measurement in Molecular-Scale," in *Molecular Nanotechnology* (in Japanese), K. Matsushige and K. Tanaka, Eds., Kagaku Dojin; Kyoto (2002).

Y. NEGISHI and T. TSUKUDA, "Synthesis and Mass Spectroscopic Characterization of Metal Clusters," *Aerosol Kenkyu* (in Japanese) **17**, 9 (2002).

M. KOMIYAMA, *Handbook of Interfaces*, Y. Iwasawa, Y. Umezawa, T. Sawada and K. Tsujii, Eds., NTS; Tokyo (2001).

N. UENO, K. K. OKUDAIRA, Y. AZUMA, S. KERA and S. HASEGAWA, "Studies of Organic Thin Films and Interfaces by Various Electron Spectroscopies: Molecular Orientation, Electronic States and Reactions," in *Conjugated Polymer and Molecular Interfaces: Science and Technology for Photonic and Optoelectronic Applications*, Salaneck, Seki, Kahn and Pireaux, Eds., Marcel Dekker Inc; NY, **6** 153 (2001).

Y. KUBOZONO, "Preparation of Fullerene-Based Hybrid Materials," *Kagaku Kogyo* **53**, 13 (2002).

Computer Center

T. SUZUKI and S. NANBU, "Non-Adiabatic Bending Dissociation of OCS Induced by Orbital Unlocking," in *Symposium Series No. 828/Low-Lying Potential Energy Surfaces*, American Chemical Society Books (2002).

Center for Integrative Bioscience

Y. WATANABE, "Constriction of Heme Enzymes: Four Approaches," *Curr. Opin. Chem. Biol.* **6**, 208 (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).

Y. WATANABE, "Two-Electron Oxidized Derivatives of Fe(III) Porphyrins," *J. Biol. Inorg. Chem.* **6**, 846 (2001).

S. AONO, "Gene Regulation by CO: Structure and Function of the CO-Sensing Transcriptional Regulator CoxA," *Kagaku to Seibutsu* (in Japanese) **40**, 206 (2002).

S. AONO, "CO Receptor System in a Microorganism," *Igaku no Ayumi* (in Japanese) **201**, 533 (2002).

H. FUJII, "Electronic Structure and Reactivity of High-Valent Oxo Iron Porphyrins," *Coord. Chem. Rev.* **226**, 51 (2002).

H. FUJII, "Oxygen Activation Mechanism of Heme Oxygenase," *Chemical Industry* (in Japanese) **53**, 18 (2002).

T. KITAGAWA and S. HIROTA, "Raman Spectroscopy of Proteins," in *The Handbook of Vibrational Spectroscopy*, J. M., Chalmers and P. R. Griffiths, Eds., John Wiley & Sons; Chichester (2002).

Y. MIZUTANI and T. KITAGAWA, "Vibrational Energy Relaxation of Metalloporphyrins in a Condensed Phase Probed by Time-Resolved Resonance Raman Spectroscopy," *Bull. Chem. Soc. Jpn.* **75**, 623 (2002).

Y. MIZUTANI, K. YAMAMOTO and T. KITAGAWA, "Studies on Dynamics of Protein Folding/Unfolding by Using the Laser-Induced Temperature Jump Technique," *Tanpakusitsu Kakusan Kouso* (in Japanese) **47**, 670 (2002).