

REVIEW ARTICLES AND TEXTBOOKS

Department of Theoretical Studies

- S. ABE and Y. OKAMOTO**, Eds., *Lecture Notes in Physics: Nonextensive Statistical Mechanics and Its Applications*, Springer-Verlag, pp. 1–277 (2001).
- Y. OKAMOTO**, “Monte Carlo Simulated Annealing in Protein Folding,” in *Encyclopedia of Optimization Vol. III*, C. A. Floudas and P. M. Pardalos, Eds., Kluwer Academic, pp. 425–439 (2001).
- U. H. E. HANSMANN and Y. OKAMOTO**, “Protein Folding: Generalized-Ensemble Algorithms in Protein Folding,” in *Encyclopedia of Optimization Vol. IV*, C. A. Floudas and P. M. Pardalos Eds., Kluwer Academic, pp. 392–401 (2001).
- A. MITSUTAKE, Y. SUGITA and Y. OKAMOTO**, “Generalized-Ensemble Algorithms for Molecular Simulations of Biopolymers,” *Biopolymers (Pept. Sci.)* **60**, 96–123 (2001).
- Y. OKAMOTO**, “Simulations for Tertiary Structure Prediction,” in *New Developments in Genome Informatics: From the Viewpoint of Biophysics*, (in Japanese) *Biophysics* **40**, 308–309 (2000).
- Y. SUGITA and A. KITAO**, “Theoretical Studies on Formation of Tertiary Structure of Protein,” (in Japanese) *Biophysics* **40**, 368–373 (2000).
- M. KINOSHITA, Y. OKAMOTO and F. HIRATA**, “Solvent Effects on Formation of Tertiary Structure of Protein,” (in Japanese) *Biophysics* **40**, 374–378 (2000).
- Y. OKAMOTO**, “Post-Genome Analyses by Computer Simulations,” in *Genome, Life, and Computer*, (in Japanese) *Computer Today* **101**, 26–30 (2001).
- Y. OKAMOTO**, “How Far Can Computational Chemistry Approach the Full Understanding of Biological Phenomena,” in *Challenges in Theoretical Chemistry and Computational Chemistry*, (in Japanese) *Chemistry in the 21st Century* **9**, Chemical Society of Japan, pp. 65–70 (2001).
- M. KINOSHITA, Y. OKAMOTO and F. HIRATA**, “Theoretical Analysis of Peptide Conformations in Water and in Alcohol,” (in Japanese) *Protein, Nucleic Acid and Enzyme* **46**, May, pp. 713–718 (2001).
- Y. SUGITA, A. MITSUTAKE and Y. OKAMOTO**, “Protein Folding Simulations by Generalized-Ensemble Algorithms,” (in Japanese) *Butsuri* **56**, 591–599 (2001).
- Y. OKAMOTO**, “Biomolecular Simulations in the Post Genome Era,” in *New Frontiers of Genome Science*, (in Japanese) *Mathematical Sciences* **458**, 36–43 (2001).
- K. MITSUKE and H. NAKAMURA**, “Photo-Dynamics and Reaction Dynamics of Molecules (Satellite of XXI-ICPEAC),” *Comm. Atom. & Molec. Phys. Comm. Modern Phys.* **2**, Part D, 75 (2000).
- C. ZHU, Y. TERANISHI and H. NAKAMURA**, “Nonadiabatic Transitions due to Curve Crossings: Complete Solutions of the Landau-Zener-Stueckelberg Curve Crossing Problems and Their Applications,” *Adv. Chem. Phys.* **117**, 127 (2001).
- Y. TERANISHI, K. NAGAYA and H. NAKAMURA**, “New Way of Controlling Molecular Processes by Lasers,” in *Quantum Control of Molecular Reaction Dynamics*, R. J. Gordon and Y. Fujimura, Eds., World Scientific, **14**, 215 (2001).
- S. SAITO and K. UMEMOTO**, “Electronic Structure of Body-Centered Lattice Fullerides,” in *Electronic Properties of Novel Materials—Molecular Nanostuructures*, H. Kuzmany *et al.*, Eds., American Institute of Physics Conference Proceedings, **544**, 14 (2000).
- S. SAITO**, “Electronic Properties of Nanotube Based Materials,” in *Tours Symposium on Nuclear Physics IV*, A. Arnould *et al.*, Eds., American Institute of Physics Conference Proceedings, **561**, 214 (2000).
- M. KINOSHITA, Y. OKAMOTO and F. HIRATA**, “Solvent Effects on Formation of Tertiary Structure of Protein,” *Seibutsu Butsuri* (in Japanese) **40**, 374 (2000).
- M. KINOSHITA, Y. OKAMOTO and F. HIRATA**, “Theoretical Analysis of Peptide Conformations in Water and in Alcohol,” *Tanpakusitsu Kakusan Kouso* (in Japanese) **46**, 713 (2001).
- F. HIRATA, H. SATO, S. TEN-NO and S. KATO**, “The RISM-SCF/MCSCF Approach for the Chemical Processes in Solutions,” in *Computational Biochemistry and Biophysics*, O. M. Becker, A. D. MacKerell, Jr., B. Roux and M. Watanabe, Eds., Marcel Dekker Inc.; New York, pp. 417–439 (2001).
- H. SATO**, “Theory for Solvent Effects: A combination of Electronic Structure Theory and Liquid Theory—Quantum Mechanics, Statistical Mechanics and Acid-Base—,” *Kagaku to Kogyo (Chemistry and Chemical Industry)* (in Japanese) **54-2**, pp. 119–123 (2001).
- M. KUWABARA and K. YONEMITSU**, “Charge Ordering and Optical Conductivity of MMX Chains,” in *Physics in Local Lattice Distortions*, H. Oyanagi and A. Bianconi, Eds., American Institute of Physics; Melville, N.Y., 465 (2001).

Department of Molecular Structure

- Y. MAEDA, T. WAKAHARA, T. AKASAKA, M. FUJITSUKA, O. ITO, K. KOBAYASHI and S. NAGASE**, "Metal-free Bis-silylation and Bis-germiration: C₆₀-Sensitized Reaction of Unsaturated Compounds with disilirane and digermirane," *Recent Research Developments in Organic Chemistry* **5**, 151–163 (2001).
- T. KATO, T. AKASAKA, K. TASHIRO and T. AIDA**, "An Inclusion Complex of a cyclic Dimer of Metallocporphyrin with La@C₈₂," in *Recent Advances in the Chemistry and Physics of Fullerenes*, P. V. Kamat, D. M. Guldi and K. M. Kadish, Eds., The Electrochemical Society; Pennington, NJ (2001).
- T. AKASAKA, T. WAKAHARA, M. KONDO, S. SHIRAKURA, Y. MAEDA, S. NAGASE, K. KOBAYASHI, M. WAELCHLI, K. YAMAMOTO, T. KATO, M. KAKO, Y. NAKADAIRA, X. GAO, E. V. CAEMELBECKE and K. M. KADISH**, "Chemistry of Endohedral Metallofullerenes: Structural Determination of the La@C₈₂ Isomer," in *Recent Advances in the Chemistry and Physics of Fullerenes*, P. V. Kamat, D. M. Guldi and K. M. Kadish, Eds., The Electrochemical Society; Pennington, NJ (2001).
- T. WAKAHARA, T. AKASAKA, K. KOBAYASHI and S. NAGASE**, "Recent Advances in Chemistry of Endohedral Metallofullerenes," *Kagaku* **56**, 60–61 (2001).
- T. AKASAKA, T. WAKAHARA, S. NAGASE and K. KOBAYASHI**, "Silylfullerenes," *J. Syn. Org. Chem. Japan* **58**, 1066–1076 (2000).
- M. FUJITSUKA, O. ITO, K. YAMAMOTO and T. AKASAKA**, "Photophysical and Photochemical Properties of Higher Fullerenes," *Recent Research Developments in Physical Chemistry* **4**, 135–148 (2000).

S. OKUBO, T. KATO, M. INAKUMA and H. SHINOHARA, "Spin Dynamics of ESR-active Lanthanum Endohedral Fullerenes," in *Proceedings of the Symposium on Chemistry and Physics of Fullerenes and Carbon Nanomaterials* **10**, P. V. Kamat, D. M. Guldi and K. M. Kadish, Eds., The Electrochemical Society, Inc.; Pennington, pp. 291–297 (2000).

Department of Electronic Structure

- Y. UOZUMI and T. TSUKUDA**, "Preparations and New Functions of Metal Nanoparticles," *Kagaku* (in Japanese) **56**, 68 (2001).

- T. SUZUKI and B. J. WHITAKER**, "Non-adiabatic dynamics effects in Chemistry revealed by time-resolved charged particle imaging," *Int. Rev. Phys. Chem.* **20**, 313 (2001).
- T. SUZUKI**, "Non-adiabatic bending dissociation of OCS," in *ACS symposium series, American Chemical Society*, K. Dyall and M. Hoffmann, Eds. (2001).

- T. YAMASE**, "Molecular Aspect of Energy Transfer from Tb³⁺ to Eu³⁺ in Polyoxometalate Lattices: An Approach for Molecular Design of Rare-Earth Metal-oxide Phosphors," in *Polyoxometallates: From Topology to Industrial Applications*, M. T. Pope and A. Müller, Eds., Kluwer Academic Publishers, pp. 187–203 (2001).

Department of Molecular Assemblies

- K. YAKUSHI**, "Reflection spectroscopic study of organic conductors," *Bull. Chem. Soc. Jpn.* **73**, 2643 (2000).
- K. YAKUSHI, M. SIMONYAN and Y. DING**, "Spectroscopic Studies of Solid Phthalocyanines and Their Charge-Transfer Salts," *J. Porphyrins Phthalocyanines* **5**, 13 (2001).

- H. KOBAYASHI, A. KOBAYASHI and P. CASSOUX**, "BETS as a Source of Molecular Magnetic Superconductors (BETS = bis(ethylenedithio)tetraselenafulvalene)," *Chem. Soc. Rev.* **29**, 325 (2000).

- R. KATO**, "Conductive Copper Salts of 2,5-Disubstituted N,N'-Dicyanobenzoquinonediimines (DCNQIs): Structural and Physical Properties," *Bull. Chem. Soc. Jpn.* **73**, 515 (2000).

- T. OGAWA**, "Structural Chemistry of Organobismuth Compounds," in *Organobismuth Chemistry*, H. Suzuki, Ed., Elsevier Science S.A.; Lausanne (2001).

Department of Applied Molecular Science

- M. K. KABIR, N. MIYAZAKI, S. KAWATA, K. ADACHI, H. KUMAGAI, K. INOUE, S. KITAGAWA, K. IIJIMA and M. KATADA**, "Novel Layered Structures Constructed from Iron-chloranilate Compounds," *Coord. Chem. Rev.* **198**, 157 (2000).

- H. MASUDA, H. KITAMURA, K. JITSKUWA and H. EINAGA**, "Unique Inorganic-Organic Hybrid Systems Self-Organized by Triply-Hydrogen Bonding Interaction and Their Functions," in *Precision Polymers and Nano-Organized Systems*, Kodansha Scientific, pp. 239–242 (2000).

Department of Vacuum UV Photoscience

N. KOSUGI, "Highly bright synchrotron radiation gives a new horizon to resonant photoelectron spectroscopy," (in Japanese) *KAGAKU (CHEMISTRY)* **56**, 60–61 (2001).

M. KOMIYAMA and T. SHIMAGUCHI, "Recent Applications of Atomic Force Microscopy to the Study of Pyridine-Base Molecules Adsorbed on the (010) Surfaces of Heulandite and Stilbite Crystals," in *Natural Zeolites for the Third Millennium*, C. Colella and F. A. Mumpton, Eds., De Frede Editore; Naples, pp. 315–320 (2000).

M. KOMIYAMA, "AFM Observations of Adsorbed Molecular Structure on Zeolite (010) Surface," (in Japanese) *Hyomen Kagaku (J. Surf. Sci. Soc. Jpn.)* **21**, 576–583 (2000).

M. NAGAI, A. ONAKA, M. KOMIYAMA, K. DOMEN and T. FUJITA, "Catalyst Study for the 21st Century," (in Japanese) *Shokubai (Catalyst and Catalysis)* **42**, 546–551 (2000).

M. KOMIYAMA, "Shokubai-no-Jiten (Encyclopaedia of Catalysis)," (in Japanese) M. Misonou, Y. Ono and Y. Morooka Eds., Asakura; Tokyo (2000).

I. H. SUZUKI, N. SAITO, S. NAGAOKA, T. IBUKI, Y. SHIMIZU, Y. TAMENORI, H. OHASHI, Y. SENBA and H. OHASHI, "Observation of Resonant Auger Electron Emission Following Photoexcitation of the Kr 2p Electron to the 5s Orbital," *Atomic Collision Res. Jpn.* **26**, 69 (2000).

Coordination Chemistry Laboratories

I. TANIGUCHI, "Bioelectrochemistry" in *Denki-kagaku Binran* (in Japanese), Electrochem. Soc. Jpn., Ed., Maruzen; Tokyo (2000).

I. TANIGUCHI, "Chemically Modified Electrode" and "Photovolatge" in *Shokubai-Jiten*, (in Japanese), Y. Ono, M. Misonoo and Y. Morooka, Eds., Asakura-shoten; Tokyo (2000).

I. TANIGUCHI, "Bioelectroanalytical Chemistry Using Functionalized Electrodes: Fundamentals and Applications," in *Proc. Workshop cum Seminar on Electroanalytical Chemistry and Allid Topics (ELAC-2000)*, S. K. Aggarwar, H. S. Sharma, N. Gopinath and D. S. C. Purushotham, Eds., BARC; Mumbai (2000).

R. OKAZAKI and N. TOKITO, "Heavy Ketones, the Heavier Element Congeners of a Ketone," *Acc. Chem. Res.* **33**, 625 (2000).

N. TOKITO and **R. OKAZAKI**, "Recent Topics in the Chemistry of Heavier Congeners of Carbenes," *Coord. Chem. Rev.* **210**, 251 (2000).

N. TOKITO, "New Aspects in the Chemistry of Low-Coordinated Inter-Element Compounds of Heavier Group 15 Elements," *J. Organomet. Chem.* **611**, 217 (2000).

N. TOKITO and **R. OKAZAKI**, "Recent Advances in the Chemistry of Group 14-Group 16 Double Bond Compounds," *Adv. Organomet. Chem.* **47**, 121 (2001).

I. HAMACHI, J. WATANABE, R. EBOSHI, T. HIRAOKA and S. SHINKAI, "Incorporation of Artificial Receptors into a Protein/Peptide Surface: A Strategy for On/Off Type of Switching of Semisynthetic Enzymes," *Biopolymers* **55**, 459 (2001).

K. ONITSUKA and S. TAKAHASHI, "Synthesis and catalysis of organotransition metal dendrimers," *Yuki Gosei Kagaku Kyokaishi (J. Synth. Org. Chem. Jpn.)* (in Japanese) **58**, 988 (2000).

Laser Research Center for Molecular Science

K. TOMINAGA, H. OHTAKE, N. SARUKURA, K. SAITOW, H. SASAKAWA, A. TAMURA, I. V. RUBTSOV and K. YOSHIHARA, "Spectroscopic Application of the THz Radiation Generated by Ultrashort Pulses—Static Far Infrared Absorption Measurement in Condensed Phases—," in *Advances in Multiphoton Process and Spectroscopy* **14**, S. H. Lin, A. A. Villaey and Y. Fujimura, Eds., World Scientific; Singapore (2001).

I. SHOJI and T. TAIRA, "Trend of Microchip laser development," *Optical Alliance* **12**, 19–24 (2001).

Center for Integrative Bioscience

Y. WATANABE, "Asymmetric Oxidation of Sulfides and olefins by Myoglobin Mutants," *Review on Heteroatom Chemistry* **22**, 135 (2001).

L. QUE, Jr. and Y. WATANABE, "Oxygenase Pathways: Oxo, Peroxo, and Superoxo," *Science* **292**, 651 (2001).

K. KINOSITA, Jr., R. YASUDA and H. NOJI, "F₁-ATPase: a Highly Efficient Rotary ATP Machine," *Essays Biochem.* **35**, 3 (2000).

K. KINOSITA, Jr., R. YASUDA, H. NOJI and K. ADACHI, "A Rotary Molecular Motor That Can Work at Near 100% Efficiency," *Phil. Trans. Roy. Soc. Lond. B.* **355**, 473 (2000).

R. YASUDA, H. NOJI, K. ADACHI, T. NISHIZAKA, Y. KATO-YAMADA, M. YOSHIDA and K. KINOSITA, Jr., "Rotation of ATP Synthase," in *Na/K-ATPase and Related ATPases*, K. Taniguchi and S. Kaya, Eds., Elsevier; Amsterdam (2000).

S. ISHIWATA, J. TADASHIGE, I. MASUI, T. NISHIZAKA and K. KINOSITA, Jr., "Microscopic Analysis of Polymerization and Fragmentation of Individual Actin Filaments," in *Results and Problems in Cell Differentiation, Vol. 32: Molecular Interactions of Actin*, C. dos Remedios, Ed., Springer-Verlag; Berlin (2001).

T. KITAGAWA, "Structures of reaction intermediates of cytochrome c oxidase probed by time-resolved vibrational spectroscopy," *J. Inorg. Biochem.* **82**, 9 (2000).

T. KITAGAWA, "Progress report on molecular biometallics (1996-2000), a project of the priority areas for research under the auspices of the Japanese government," *J. Biol. Inorg. Chem.* **5**, 410 (2000).