CONTENTS

Department of Theoretical Studies
I-A  Theoretical Study and Design of Functional Molecular Systems: New Bonding, Structures, and Reactions
I-A-1  Counterion-Driven Spontaneous Polymerization of the Linear C_{60}^{-}\textsuperscript{n} Chains in the fcc Fullerides and Its Magic Number Behavior
I-A-2  Amphoteric and Controllable Doping of Carbon Nanotubes by Encapsulation
I-A-3  Electronic Excited States and Stabilities of Fullerences: Isomers of C_{78} and Mg@C_{72}
I-A-4  1,6,7-Trigemabicyclo[4.1.0]hept-3-en-7-yl: The Isolable Bicyclic Germyl Radical
I-A-5  Isolation of a Se-Nitrososelenol: A New Class of Reactive Nitrogen Species Relevant to Protein Se-Nitrosation
I-A-6  A New Approach to Simulate the Depolymerization Process of a Two-Dimensional Hexagonal C_{60} Polymer
I-A-7  Chemical Reactivity and Redox Property of Sc\textsubscript{3}N@C_{80}
I-A-9  Dispersion of Single-Walled Carbon Nanotube Bundles in Nonaqueous Solution
I-A-10  Regioselective Carbon–Carbon Bond Cleavage of an Open-Cage Diketone Derivative of [60]Fullerene by Reaction with Aromatic Hydrazones
I-A-11  Gibbs Energy-Based Treatment of Metallofullerenes: Ca@C_{72}, Ca@C_{74}, Ca@C_{82}, and La@C_{82}
I-A-12  Chemical Reactivities of the Cation and Anion of M@C_{82} (M = Y, La, and Ce)
I-A-14  Syntheses and Structures of Hypervalent Pentacoordinate Carbon and Boron Compounds Bearing an Anthracene Skeleton—Elucidation of Hypervalent Interaction Based on X-Ray Analysis and DFT Calculation
I-A-15  Adsorption Configuration of NH\textsubscript{3} on Single-Wall Carbon Nanotubes
I-A-16  Structural Characterization of Y@C_{82}
I-A-17  Synthesis and Characterization of Exohedrally Silylated M@C_{82} (M = Y and La)
I-A-18  Synthesis and Characterization of Stable Hypervalent Carbon Compounds (10-C-5) Bearing a 2,6-Bis(p-substituted phenyloxymethyl)benzene Ligand
I-A-19  Practical Performance Assessment of Accompanying Coordinate Expansion Recurrence
I-A-20  2D NMR Characterization of the La@C_{82} Anion
I-A-21  Open-Cage Fullerene Derivatives Suitable for the Encapsulation of a Hydrogen Molecule
I-A-22  Computed Structure and Energetics of La@C_{60}
I-A-23  Metallic Phase in the Metal-Intercalated Higher Fullerene Rb_{8.8(7)}C_{84}
I-A-24  Interplay of Single-Wall Carbon Nanotubes and Encapsulated La@C_{82}, La\textsubscript{2}@C_{80}, and Sc\textsubscript{3}N@C_{80}
I-A-26  Missing Metallofullerene La@C_{74}
I-A-27  Chemical Reactivity of Sc\textsubscript{3}N@C_{80} and La\textsubscript{2}@C_{80}
I-A-28  Large-Scale Separation of Metallic and Semiconducting Single-Walled Carbon Nanotubes
I-A-29  Encapsulation of La@C_{82} and La\textsubscript{2}@C_{80} inside Single-Walled Boron Nitride Nanotubes
I-B  Prediction of Protein Tertiary Structures and Protein Folding Problem
I-B-1  Classification and Prediction of Low-Energy Membrane Protein Helix Configurations by Replica-Exchange Monte Carlo Method
Contents

I-M  Solvation Thermodynamics of Protein and Related Molecules ------------------------------------------33
I-L  Electronic Structure of a Molecule in Solution --------------------------------------------------------------32
I-K  Electronic Structures and Photochemical Properties of Nanometer-Sized Metal Clusters --------30
I-J  Theoretical Studies of Electron Dynamics in Molecular Systems ----------------------------------------30
I-I  Development of New Molecular Functions --------------------------------------------------------------------29
I-G  Theory of Multi-Dimensional Tunneling ---------------------------------------------------------------------27
I-F  Theory of Nonadiabatic Transition -----------------------------------------------------------------------------27
I-E  Applications of the Zhu-Nakamura Theory to Nonadiabatic Chemical Dynamics 26
I-D  Other Results on Molecular Simulations  ---------------------------------------------------------------------25
I-C  Development of Simulation Algorithms for Complex Systems -------------------------------------------25
I-B  Combination of the Replica-Exchange Monte Carlo Method and the Reference Interaction Site Model Theory for Simulating a Peptide Molecule in Aqueous Solution 24
I-A  Multi-Overlap Molecular Dynamics Methods for Biomolecular Systems 24
I-B-4  Secondary-Structure Preferences of Force Fields for Proteins Evaluated by Generalized-Ensemble Simulations 24
I-C-5  Water Molecules in a Protein Cavity Detected by a Statistical-Mechanical Theory 34
I-C-3  Theoretical Study of Volume Changes Associated with the Helix-Coil Transition 33
I-C-2  Partial Molar Volume of Proteins Studied by the 3D-RISM Theory 33
I-C-1  Hydrophobic Effects on Partial Molar Volume 33
I-L-1  Electronic Structure Calculation of a Solvated Macro Molecule by Using Three-Dimensional Ab Initio Molecular Orbital Theory 32
I-K-3  Gold-Thiolate Nanoring: Electronic Structure and Photochemical Properties 31
I-K-2  Glutathione-Protected Gold Clusters Revisited: Bridging the Gap between Gold(I)-Thiolate Complexes and Thiolate-Protected Gold Nanocrystals 31
I-K-1  Electronic Structure and Photochemical Properties of a Monolayer-Protected Gold Cluster 30
I-F-3  Incorporation of Nonadiabatic Transition into Wave Packet Dynamics 27
I-F-2  A Basic Two-State Model for Bosonic Field Theories with a Cubic Nonlinearity 27
I-F-1  Rabi Dynamics of Coupled Atomic and Molecular Bose-Einstein Condensates 27
I-E-5  Semiclassical Theory of Thermal Rate Constant for Multi-Surface Processes 26
I-E-4  Generalized Trajectory Surface Hopping Approach 26
I-E-3  Semiclassical Theory of Electron Transfer Beyond the Perturbation Theory 26
I-E-2  Electron Transfer Rate to Cover the Whole Range from Adiabatic to Nonadiabatic Regime Based on the Zhu-Nakamura Theory 26
I-E-1  Nonadiabatic Transition and Chemical Dynamics: Multi-Dimensional Tunneling Theory and Applications of the Zhu-Nakamura Theory 26
I-D-1  Comparisons between a New Dynamics and Hydrodynamics Treatment of Non-Stationary Thermal Processes in a Liquid 25
I-C-4  Development of Simulation Algorithms for Complex Systems 25
I-B-3  Multi-Overlap Molecular Dynamics Methods for Biomolecular Systems 24
I-B-2  Combination of the Replica-Exchange Monte Carlo Method and the Reference Interaction Site Model Theory for Simulating a Peptide Molecule in Aqueous Solution 24
I-B-1  Secondary-Structure Preferences of Force Fields for Proteins Evaluated by Generalized-Ensemble Simulations 24
I-A-4  Molecular Simulations 23
I-A-3  Development of Simulation Algorithms for Complex Systems 23
I 554
I-N  Collective Density Fluctuations in Polar Liquids and Their Response to Ion Dynamics ..........34
  I-N-1  Site-Site Memory Equation Approach in Study of Density/Pressure Dependence of Translational Diffusion Coefficient and Rotational Relaxation Time of Polar Molecular Solutions: Acetonitrile in Water, Methanol in Water, and Methanol in Acetonitrile ..........35
  I-N-2  Theoretical Study on the Dynamic Properties of Compressed Water and Water-Hydrophobic Solute Mixtures ..........................................................35
  I-N-3  Solvation Dynamics in Water Investigated by RISM/Mode-Coupling Theory ..........35
I-O  Statistical Mechanics of Interfacial Fluids ..............................................................36
  I-O-1  A Molecular Theory of Liquid Interfaces .............................................................36
I-P  Photoinduced Phase Transitions in Molecular Materials ..........................................37
  I-P-1  Photoinduced Dynamics and Nonequilibrium Characteristics in Quasi-One-Dimensional Electron Systems: Mott Insulators vs. Band Insulators ..................................37
  I-P-2  Optical Responses of Photoexcited States in the One-Dimensional Ionic Hubbard Model ..........................................................37
  I-P-3  Quantum Ising Model Coupled with Conducting Electrons ..................................37
  I-P-4  Photoinduced Metallic Properties of One-Dimensional Strongly Correlated Electron Systems ..........................................................37
  I-P-5  Interchain-Coupling Effects on Photoinduced Neutral-Ionic Transition Dynamics in Mixed-Stack Charge-Transfer Complexes ..................................................38
  I-P-6  Theory of Photoinduced Phase Transitions ..........................................................38
I-Q  Collective Transport through Metal-Insulator Interfaces ........................................38
  I-Q-1  Mechanism of Ambipolar Field-Effect Carrier Injections in One-Dimensional Mott Insulators ..........................................................38
I-R  Strongly Correlated Electron Systems with Frustrations ........................................39
  I-R-1  Frustration-Induced η Inversion in the $S = 1/2$ Bond-Alternating Spin Chain ..........39
  I-R-2  Field-Induced Phase Transitions and Long-Range Orders in the $S = 1/2$ Bond-Alternating Chain with Frustrating Interaction ............................................39
  I-R-3  Field-Induced Incommensurate Order in Frustrated Spin Chain ................................39
  I-R-4  Phase Diagram of the Excitonic Insulator ............................................................39
  I-R-5  Effective Interaction between the Intermembrane Kagome Lattices in Na$_x$CoO$_2$ ..........39
  I-R-6  Magnetism in Strongly Correlated and Frustrated Systems ..................................40
I-S  Theory and Applications of Relativistic Quantum-Chemical Methods to Molecular Properties of Compounds Containing Heavy Elements .....................................................41
  I-S-1  Theoretical Studies on Circular Dichroism Spectra of Linear and Cyclic Dichalcogenide Compounds (Chalcogen = S, Se, Te) by the SAC and SAC-CI Methods ..................41
  I-S-2  Theoretical Studies on Magnetic Circular Dichroism by the Finite Perturbation Method with Relativistic Corrections ............................................................42
  I-S-3  $^{13}$C NMR Chemical Shifts of Small Molecules Interacting with Metal Complexes in Heme Proteins and Metal Enzymes ..........................................................42
I-T  Polyamorphism in Molecular Liquids ........................................................................43
  I-T-1  Construction of an Interaction-Site Model for Molecular Systems .........................43
I-U  Nonlinear Processes Induced by Ultrafast Laser Pulses ...........................................44
  I-U-1  Few-Cycle Effects in the Low Intensity Regime ....................................................44
I-V  Control of Photoionization Processes Using Lasers ...................................................44
  I-V-1  Control of the Spin-Polarization of Photoelectrons/Photoions Using Short Laser Pulses ..........44
  I-V-2  Control of Photoelectron Angular Distributions Using a Dressing Laser ..................44
I-W  Theoretical Studies on Dynamical Foundation of Chemical Reactions and Proteins ..........46
  I-W-1  Phase Space Reaction Network on Multibasin Energy Landscapes ................................46
  I-W-2  A Construction of Multidimensional Free Energy Landscape from an Ensemble of Single Molecule Time Series .................................................................46
  I-W-3  A New Technique to Differentiate the Origin of Observed non-Brownian Dynamics in the Principal Component Space .................................................................46
  I-W-4  Polypeptide in Water on the Lagrange Picture in Fluid Dynamics ..........................47

RESEARCH ACTIVITIES II .................................................................49

Department of Molecular Structure
II-A  Development of Dynamic Near-Field Spectroscopy and Application to Nanometric Systems ....49
  II-A-2  Scanning Near-Field Optical Microscopic Study of Porphyrin Nanowire ..................49
  II-A-3  Imaging of Plasmon Modes in Gold Nanorods .......................................................50
  II-A-4  Near-Field Two-Photon Induced Photoluminescence from Single Gold Nanorods ..........50
  II-A-5  Dispersion Relation of Plasmon Modes in the Gold Nanorods ..................................50
  II-A-6  Imaging and Dispersion Relations of Surface Plasmon Modes in Silver Nanorods by Near-Field Spectroscopy .................................................................51
RESEARCH ACTIVITIES III

Department of Electronic Structure

III-A Synthesis and Characterization of Exotic Molecule Based Nano-Crystals of Metal Acetylides: Toward Carbon Encapsulated Metal Dot Array, Metal Nano-Networks and Metal-Carbon

Hybrid Systems

III-A-1 Self-Assembled Nanowire Synthesis of Highly-Anisotropic Copper Acetylide Molecules
III-A-2 Photochemical Conversion of \( \text{Cu}^+ \text{C} = \text{C} \text{-} \text{Butyl} )_{24} \) Cluster Molecules to Cu Metallic Nano-Sheets Embedded in Polymer Nano-Film
III-A-3 Guest Controlled Magnetism of CoC₂ Nanoparticles
III-A-4 Formation of Carbon-Encapsulated Metallic Nano-Particles from Metal Acetylides by Electron Beam Irradiation
III-A-5 Reexamination of the Structures and Energies of \( \text{Li}_2 \text{C}_2 \) and \( \text{Li}_4 \text{C}_4 \)

III-B Ultrafast Dynamics and Scanning Tunneling Microscopy

III-B-1 Excited-State Double-Proton Transfer in the 7-Aza-indole Dimer in Gas Phase 3. Reaction Mechanism Studied by Picosecond Time-Resolved REMPI Spectroscopy
III-B-2 Ultrafast Excited-State Dynamics in Photochromic \( \text{N-Salicylideneaniline} \)

Studyed by Femtosecond Time-Resolved REMPI Spectroscopy
III-B-3 Orientation of Nitrous Oxide on Palladium(1 1 0) by STM

III-C Spectroscopic and Dynamical Studies of Molecular Cluster Ions

III-C-1 Infrared Photodissociation Spectra and Solvation Structure of \( \text{Mg}^+(\text{CH}_3\text{OH})_n (n = 1-4) \)
III-D Development of High-Precision Coherent Control and Its Application

III-D-1 Space- and Time-Resolved Observation of Molecular Wave-Packet Interference on Femtosecond and Picometric Scales

III-D-2 Real-Time Observation of Phase-Controlled Molecular Wave-Packet Interference

III-D-3 Development of Quantum Gate Operations with Vibrational Eigenstates of Molecules

III-E Quantum-State Manipulation of Molecular Motions

III-E-1 Femtosecond Random-Phase Interferometry of Jet-Cooled Polyatomic Molecules

III-E-2 Wavepacket Observation of Methyl Internal Rotation in o-Fluorotoluene

III-E-3 Construction of an Experimental Apparatus for Nonadiabatic Quantum-State Manipulation of Molecular Motions

III-E-4 Development of High-Resolution Coherent Pulsed Laser

III-E-5 Laser Spectroscopy of the van der Waals Vibrations of Benzene-Water

III-F Photophysics and Photochemistry of Aromatic Molecules in the Condensed Phase

III-F-1 Excited-State Dynamics of 4-Thiothymidine with UVA Light Irradiation

III-F-2 Photochemical Reaction Dynamics of o-Quinones

III-F-3 Evidence of Phenoxy methyl Radical Formation in Laser Photolysis of Anisole in Solution

III-F-4 Production and Excited State Dynamics of the Photorearranged Isomer of Benzyl Chloride and Its Methyl Derivatives Studied by Stepwise Two-Color Laser Excitation Techniques

III-G Spectroscopy and Excited State Dynamics of Jet-Cooled Aromatic Molecules

III-G-1 Spectroscopy and Relaxation Dynamics of Photoexcited Anisole and Anisole-d3 Molecules in a Supersonic Jet

III-G-2 Internal Rotational Motion of the Chloromethyl Group of the Jet-Cooled Benzyl Chloride Molecule

III-G-3 Molecular Structure and Excited State Dynamics of Jet-Cooled o-, m-, and p-Fluoroanisole

III-G-4 Evidence for a Non-Planar Conformer and Conformational Isomerization of o-Fluoroanisole in a Low-Temperature Ar Matrix

III-G-5 Molecular Structure and Puckering Vibration of 1-Aminoindan in a Supersonic Jet

III-H Photochemical Reactions in Microreactors

III-H-1 Application of Microfabricated Reactors for Asymmetric Photoreaction

III-H-2 Photocatalytic Reaction in Microfabricated Reactors

III-I In-Situ Observation of Surface Reactions by Variable Temperature Scanning Tunneling Microscopy

III-I-1 In-Situ Observation of CO Oxidation on Ag(110)(2×1)-O by Scanning Tunneling Microscopy: Structural Fluctuation and Catalytic Activity

III-I-2 Propagation of Reaction Front in the Disproportionate Reaction of H2O on Ag(110)(5×1)-O Surface: Role of Hydrogen Bonding Interaction

RESEARCH ACTIVITIES IV

Department of Molecular Assemblies

IV-A Optical Study of Charge Ordering States in Organic Conductors

IV-A-1 Examination of the Charge-Sensitive Vibrational Modes in ET Molecule

IV-A-2 Infrared and Raman Studies of θ-(BEDT-TTF)2Cu[N(CN)2]Br

IV-A-3 Robust Superconducting State in the Low-Quasiparticle-Density Organic Metals

IV-A-4 Influence of the Cooling Rate on Low-Temperature Raman and Infrared-Reflection Spectra of Partially Deuterated κ-(BEDT-TTF)2Cu(N(CN)2)Br

IV-A-5 Optical Second Harmonic Generation in a Charge-Ordered Organic Conductor

IV-A-6 Correlation between Structural Instabilities and Raman Shift and Width in β-(BEDT-TTF)2Br and κ-(BEDT-TTF)2Cu[N(CN)2]I

IV-A-7 Inhomogeneous Charge Distribution in (EDO-TTF)2X (X = ReO4 and GaCl4)

IV-A-8 Re-Examination of the Site Charge Difference in TEA(TCNQ)2
IV-A 9  Spectroscopic Evidence for the Monovalent-to-Divalent Phase Transition of Biferrocenium (F\textsubscript{3}TTCNQ\textsubscript{3}) .......................... 82
IV-A 10  Phase Separation in the Monovalent-to-Divalent Phase Transition of Biferrocenium-F\textsubscript{3}TTCNQ\textsubscript{3} .................................................. 83
IV-B  Magnetic Resonance Studies for Molecular-Based Conductors .................................. 86
IV-B 1  Charge Disproportionation in (TMTTF)\textsubscript{2}SCN Observed by \textsuperscript{13}C NMR .................. 86
IV-B 2  Redistribution of Electronic Charges in the Spin-Peierls State in (TMTTF)\textsubscript{2}AsF\textsubscript{5} Observed by \textsuperscript{13}C NMR ........................................ 86
IV-B 3  Deuteration Effect and Possible Origin of the Charge-Ordering Transition of (TMTTF)\textsubscript{2}X .......................................................... 87
IV-B 4  Redistribution of Electronic Charge in (TMTTF)\textsubscript{2}ReO\textsubscript{4}; \textsuperscript{13}C NMR Investigation .................. 87
IV-B 5  Spin Structure of Organic Conductors (TMTTF)\textsubscript{2}X ................................................. 88
IV-B 6  Multi-Frequency ESR Measurements for (TMTTF)\textsubscript{2}X .............................................. 88
IV-B 7  Extremely Slow Charge Fluctuations in the Metallic State of the Two-Dimensional Molecular Conductor \(\theta\)(BEDT-TTF)\textsubscript{2}RbZn(SCN)\textsubscript{4} .......................... 88
IV-B 8  Sliding Spin-Density Wave of (TMTSF)\textsubscript{2}PF\textsubscript{6} Studied with Narrow-Band Noise ......... 88

IV-C  Synchrotron X-Ray Diffraction Experiments and MEM Analyses for Single Crystals of Organic Conductors ........................................... 88
IV-C 1  Low-Temperature Charge-Ordering State of (TMTTF)\textsubscript{2}PF\textsubscript{6} .............................. 89
IV-D  EPR Study toward Molecular Biology as Microscopic and Selective Probes Measurements 89
IV-D 1  First Detection of the Multiline Signal from the S\textsubscript{2}-State Manganese Cluster of Photosystem II by Single-Crystal W-Band EPR Spectroscopy ..................... 90
IV-E  Development of Multi-Functional Molecular Systems ................................................. 91
IV-E 1  Dielectric Properties of Porous Molecular Crystals Containing Polar Molecules .......... 91
IV-E 2  Giant Dielectric Constants of Porous Molecular Crystal with Guest Water Cluster ... 91
IV-E 3  Synthesis and Characterization of a Porous Magnetic Diamond Framework Compound, \(\pi\)-(BETS)\textsubscript{2}Fe\textsubscript{3}(HCOO)\textsubscript{6}, and Its N\textsubscript{2} Sorption Characteristic ........................................... 92
IV-E 4  Superconductivity and Voltex Phases in the Two-Dimensional Organic Conductor \(\lambda\)-(BETS)\textsubscript{2}Fe\textsubscript{3}Ga\textsubscript{1–x}Cl\textsubscript{4} (x = 0.45) ..................... 92
IV-E 5  Constant Resistivity State in the Field-Induced Organic Superconductor, \(\lambda\)-(BETS)\textsubscript{2}Fe\textsubscript{3}Ga\textsubscript{1–x}Cl\textsubscript{4} .......................................................... 93
IV-E 6  (Tetrathiafulvalene)[Fe\textsuperscript{III} (C\textsubscript{2}O\textsubscript{4})Cl\textsubscript{2}]: An Organic-Inorganic Hybrid Exhibiting Canted Antiferromagnetism .............................................. 93
IV-E 7  Development of Single-Component Molecular Metals .............................................. 94
IV-E 8  Crystal Structures and Physical Properties of Single-Component Molecular Conductors Consisting of Nickel and Gold Complexes with Bis(trifluoromethyl)tetrathiafulvalenedithiolate Ligands ......................................................... 94
IV-E 9  \textit{Ab Initio} Electronic Structure Calculation of Single-Component Molecular Conductor Au(tmdt)\textsubscript{2} (Tmdt = Trimethylene-tetrathiafulvalenedithiolate) .................... 95
IV-E 10  The Light-Induced Excited Spin State Trapping Effect on Ni(dmit)\textsubscript{2} Salt with an Fe(III) Spin-Crossover Cation: [Fe(qsal)\textsubscript{2}][Ni(dmit)\textsubscript{2}][2CH\textsubscript{3}CN .......... 95
IV-E 11  Synergetic Behavior between Spin and Conducting Property in Ni(dmit)\textsubscript{2} Salt with Fe(III) Spin-Crossover Cation .................................. 96
IV-E 12  Synthesis and Molecular Structure of a Novel PROXYL-Fused \(\pi\)-Electron Donor, PROXYL-ET-STF ......................................................... 96
IV-F  Electronic and Magnetic Properties of \(\pi\)-Electron-Based Molecular Systems ................. 98
IV-F 1  Metal-Insulator Transition in Iodinated Amorphous Conducting Carbon Films ............ 98
IV-F 2  Magnetic Resonance Study of Nanodiamonds ......................................................... 98
IV-F 3  \(\delta\)-Electron-Induced Negative Magnetoresistance of \(\pi\)-d Interaction System Including Brominated-TTF Donor ..................................... 98
IV-F 4  Electronic and Magnetic Properties of \(\pi\)-d Interaction System (EDTDM)\textsubscript{2}FeBr\textsubscript{4} ......................................................... 99
IV-F 5  Observation of Zigzag- and Armchair-Edges of Graphite .......................................... 99

IV-G  Progress of Conjugated Phenomena Coupled with Spin and Photon for Assembled Hetero-Molecular System ........................................ 100
IV-G 1  Reversible Photomagnetism in a Cobalt Layered Compound Coupled with Photo-Chromatic Diarylethene ............................................ 100
IV-H  Molecular Crystals toward Nano-Devices by Use of \(d\)-\(\pi\) Interaction, Crystal Designing and Optical Doping ......................................................... 101
IV-H 1  Light-Induced Transformation of Molecular Materials into Devices .......................... 101
IV-H 2  Molecular Condutors Containing Photoactive Species .............................................. 101
IV-H 3  A New Optical Doping Method toward Molecular Electronics .................................. 102
IV-H 4  Photochemical Method of Device Fabrication Starting from Molecular Crystals .... 102
IV-H 5  Photochemical Control of Dark Conductivity —— A New Approach to Devices Based on Molecular Crystals .............................. 102
IV-H 6  Molecular Unit Based on Metal Phthalocyanine; Designed for Molecular Electronics 102
Department of Applied Molecular Science

V-A Molecular Design and Functions of Photoactive and Spin-Active Supramolecular Assemblies

V-A-1 Molecular Design of Light-Harvesting Antennae

V-B Bioinorganic Chemistry and Structural Biology of Heme Proteins

V-B-1 Proton Transfer at Helium Temperatures during Dioxygen Activation by Heme Monooxygenases

V-B-2 Roles of Distal Asp in Heme Oxygenase from Corynebacterium diphtheriae, HmuO: A Water-Driven Oxygen Activation Mechanism

V-B-3 O$_2$- and H$_2$O$_2$-Dependent Verdoheme Degradation by Heme Oxygenase: Reaction Mechanisms and Potential Physiological Roles of the Dual Pathway Degradation

V-C Pro-Oxidants-Induced Iron Release from the Fe-S Cluster of Mitochondrial Aconitase and its Prevention by Flataxin

V-C-1 Reversible Redox-Dependent Modulation of Mitochondrial Aconitase and Proteolytic Activity during In Vivo Cardiac Ischemia/Reperfusion

V-D Quantum Emissions from Solid in Femtosecond Intense Laser Field and Its Application to Dynamic Imaging

V-D-1 Picosecond Time-Resolved X-Ray Diffraction from a Laser-Shocked Germanium Crystal over Hugoniot Elastic Limit

V-D-2 Enhanced Generation of Fast Protons from a Polymer-Coated Metal Foil by a Femtosecond Intense Laser Field

V-D-3 Electron Imaging of Charge Separated Field on a Copper Film Induced by Femtosecond Laser Irradiation

Department of Vacuum UV Photoscience

VI-A Electronic Structure and Decay Mechanism of Inner-Shell Excited Molecules


VI-A-2 Application of R Matrix/MQDT Method to both Valence and Core Excitations in NO

VI-B Soft X-Ray Photoelectron-Photoabsorption Spectroscopy and Electronic Structure of Molecular Solids and Clusters

VI-B-1 Photonization of Small Krypton Clusters in the Kr 3d Regime: Evidence for Site-Specific Photoemission

VI-B-2 Core Excitation in O$_3$ Localized to One of Two Symmetry-Equivalent Chemical Bonds: Molecular Alignment through Vibrionic Coupling

VI-C Ultrafast Dynamics of Molecules in Intense Laser Fields

VI-C-1 Probing the Ultrafast Nuclear Motion in CS$_2$$_{2+}$ in Intense Laser Fields

VI-C-2 Concerted and Sequential Coulomb Explosion Processes of N$_2$O in Intense Laser Fields by Coincidence Momentum Imaging
Contents

VI-C-3 Development of an Intense Sub-10fs Laser Source with a Hollow Fiber/Chirped Mirror Compressor .................................................................115
VI-D Synchrotron Radiation Stimulated Surface Reaction and Nanoscience .................................................................117
VI-D-1 Synchrotron Radiation Induced Si–H Dissociation on H-Si(111)–1x1 Surfaces Studied by In-Situ Monitoring in the Undulator-STM System .................................................................117
VI-D-2 Giant Vesicle Fusion on the Microelectrodes Fabricated by Femtosecond Laser Ablation Followed by Synchrotron Radiation Etching .................................................................117
VI-E Noble Semiconductor Surface Vibration Spectroscopy .................................................................118
VI-E-1 Orientation of Avidin Molecules Immobilized on the COOH-Modified SiO2/Si(100) Surface .................................................................118
VI-E-2 Hydrogen-Atom-Induced Oxidation Reaction on Water-Terminated Si Surface, 2H+H2O/Si(100)–(2x1): A Theoretical Study .................................................................118
VI-F Integration and Characterization of Bio-Functional Materials on Silicon Surfaces .................................................................119
VI-F-1 Fabrication of Avidin Single Molecule Layer on Silicon Oxide Surfaces and Formation of Tethered Lipid Bilayer Membranes .................................................................119
VI-F-2 Deposition of Lipid Bilayers on OH-Density-Controlled Silicon Dioxide Surfaces .................................................................119
VI-F-3 Supported Lipid Bilayer Formation by the Vesicle Fusion Induced by the Vesicle-Surface Electrostatic Attractive Interaction .................................................................120
VI-F-4 The Current Noise Characteristic of a Single Ion Channel .................................................................120
VI-F-5 A New Type of Fluorescence Recovery After Photobleaching Apparatus Using both Illumination Arrangements of UV Lamp and 560 nm Laser .................................................................121
VI-G Photoionization and Photodissociation Dynamics
Studied by Electron and Fluorescence Spectroscopy .................................................................122
VI-G-1 Photofragmentation Mechanisms of H2O Studied by Ultraviolet Dispersed Spectroscopy .................................................................122
VI-H Extreme UV Photoionization Studies of Fullerenes by Using a Grazing-Incidence Monochromator and Low-Temperature Mass Spectrometer .................................................................122
VI-H-1 Absolute Photoabsorption Cross Section of C60 in the Extreme Ultraviolet .................................................................123
VI-H-2 Photofragmentation of C60 in Valence Ionization .................................................................123
VI-H-3 Photofragmentation of C60 in the Extreme Ultraviolet:
Statistical Analysis on the Appearance Energies of C60-2n+n+ (n ≥ 1, z = 1–3) .................................................................124
VI-H-4 Fragmentation Mechanism of Highly Excited C70 Cations in the Extreme Ultraviolet .................................................................124
VI-H-5 4d → 4f Dipole Resonance of the Metal Atom Encapsulated in a Fullerene Cage: Ce@C82 .................................................................124
VI-H-6 Photoion Yield Curves of Dy@C82 in the Vacuum UV Region .................................................................125
VI-H-7 4d–4f Dipole Resonance of the Pr Atom in an Endohedral Metallofullerene, Pr@C82 .................................................................125
VI-I Kinetic Energy Analysis of the Fragment ions Produced from Fullerenes .................................................................126
VI-I-1 Development of the Photofragment Imaging Apparatus
to Measure Scattering Distributions of the C60-2n+n+ and C70-2n+n+ Fragments
Produced by Dissociative Photoionization of C60 and C70 .................................................................126

RESEARCH ACTIVITIES VII .................................................................129

Department of Computational Molecular Science

VII-A Computer Simulation of Quantum Systems in Condensed Phase .................................................................129
VII-A-1 A Study of Molecular Vibrational Relaxation Mechanism in Condensed Phase Based upon Mixed Quantum-Classical Molecular Dynamics: I. A Test of IBC Model for the Relaxation of a Nonpolar Solute in Nonpolar Solvent at High Density .................................................................129
VII-A-2 A Study of Molecular Vibrational Relaxation Mechanism in Condensed Phase Based upon Mixed Quantum-Classical Molecular Dynamics: II. Non-Collisional Mechanism for the Relaxation of a Polar Solute in Supercritical Water .................................................................129

VII-B Molecular Dynamics Study of Classical Complex Systems .................................................................130
VII-B-1 A Large-Scale Molecular Dynamics Study of Dynamic Structure Factor and Dispersion Relation of Acoustic Mode in Liquid and Supercritical Water .................................................................130

VII-C Development of Simulation Algorithms for Quantum Many-Body Systems .................................................................130
VII-C-1 Quantum Rotation of Carbonyl Sulfide Molecules in Superfluid Helium Clusters:
A Path Integral Hybrid Monte Carlo Study .................................................................130

VII-D Theory of Sum Frequency Generation Spectroscopy .................................................................131
VII-D-1 Improved Computation of Sum Frequency Generation Spectrum of Water Surface .................................................................131

VII-E Theory of Mass Transfer Kinetics at Liquid-Vapor Interfaces .................................................................131
VII-E-1 Mass Accommodation Coefficient of Water .................................................................131

VII-F Theoretical Studies on Electronic Structure and Dynamics of Electronically Excited States .................................................................132
VII-F-1 Encapsulation of Hydrogen Atoms by Fullerenes and Carbon Nanotubes with the Use of Nonadiabatic Transition .................................................................132
RESEARCH ACTIVITIES VIII  ------------------------------135

Coordination Chemistry Laboratories

VIII-A  Reduction of CO₂ and Oxidation of Organic Molecules Aiming at Energy Conversion between Chemical Energy and Electricity ........................................135
  VIII-A-1  Redox Behavior of New Ru-Dioxolene-Ammine Complexes and Catalytic Activity toward Electrochemical Oxidation of Alcohol under Mild Conditions 135
  VIII-A-2  Equilibrium of Low- and High-Spin States of Ni(II) Complexes Controlled by the Donor Ability of the Bidentate Ligands 136
  VIII-A-3  A Platinum-Ruthenium Dinuclear Complex Bridged by Bis(terpyridyl)xanthene 136
  VIII-A-5  Synthesis, Chemical- and Electrochemical Properties of Ruthenium(II) Complexes Bearing 2,6-Bis(2-naphthyridyl)pyridine 137
  VIII-A-7  Synthesis and Electrochemical Properties of Bis(bipyridine)ruthenium(II) Complexes Bearing Pyridinyl- and Pyridinylidene Ligands Induced by Cyclometalation of N'-Methylated Bipyridinium Analog 138
  VIII-A-8  Electronic Structural Changes Between Nickel(II)-Semiquinonato and Nickel(II)-Catecholato states Driven by Chemical and Physical Perturbation 138
  VIII-A-9  Synthesis and Crystal Structures of [W(3,6-Dichloro-1,2-Benzene-dithiolato)₃]^{n+} \quad (n = 1, 2) and [Mo(3,6-Dichloro-1,2-Benzene-dithiolato)₃]^{2-}: Dependence of the Coordination Geometry on the Oxidation Number and Counter-Cation in Trigonal-Prismatic and Octahedral Structures 139
  VIII-A-10  Dioxo-Molybdenum(VI) and Mono-oxo-Molybdenum(IV) Complexes Supported by New Aliphatic Dithiolene Ligands: New Models with Weakened Mo=O Bond Characters for the Arsenite Oxidase Active Site 139
  VIII-A-11  Electrochemical Hydrogenation of [Ru(bpy)(bpyO)(CO)]^{2+}: Inhibition of Reductive Ru–CO Bond Cleavage by a Ruthenacycle 139
  VIII-A-12  Stabilization and Destabilization of the Ru–CO Bond During the 2,2'-Bipyridin-6-onato (bpyO)-Localized Redox Reaction of [Ru(terpy)(bpyO)(CO)](PF₆)₃ 139

VIII-B  Coordination Chemistry of Sterically Hindered Ligands and Multidentate Ligands, and Activation of Small Molecules ........................................139
  VIII-B-1  Synthesis of a Vanadium(III) Tris(aryliothiolato) Complex and Its Reactions with Azide and Azo Compounds: Formation of a Sulfenamide Complex via Cleavage of an Azido N=N Bond 139
  VIII-B-2  Titanium and Zirconium Complexes of Preorganized Triposda Triaryloxide Ligands 139

VIII-C  Preparation and Properties of the Homo- and Heterometallic Clusters ........................................141
  VIII-C-1  A Dinuclear Ru(II) k₂-Diamido/η⁶-Naphthalene Complex Featuring a Coordinatively Unsatuated Yet Highly p-Basic (η³-C₅Mes)Ru Diamide Fragment 141
  VIII-C-2  Dinuclear Ruthenium(II) Catecholato and 2,3-Naphthalenediolato Complexes Featuring k²-Diarylloxo/η⁶-Arene Coordination Mode 141

VIII-D  Modification of Myoglobin by Replacing the Native Heme with Metalloporphyrinoids ........................................143
  VIII-D-1  Ligand Binding Properties of Myoglobin Reconstituted with Iron Porphycene: Unusual O₂ Binding Selectivity against CO Binding 143
  VIII-D-2  Unusual Ligand Discrimination by a Myoglobin Reconstituted with a Hydrophobic Domain-Linked Heme 143
  VIII-D-3  Enhancement of Peroxidase Activity of Myoglobin Reconstituted with Iron Porphycene: Compound III Formation due to the Reaction of Ferric Myoglobin with Hydrogen Peroxide 143
  VIII-D-4  Preparation and O₂ Binding Study of Myoglobin Having a Cobalt Porphycene 144
IX-B  Development of Organic Semiconductor Devices for Molecular Thin-Film Devices 155
IX-B-1  Organic Thin-Film Transistors with High Electron Mobility
IX-B-2  Organic Light-Emitting Diodes Using Multifunctional Phosphorescent Iridium-Complex Core and Charge-Transporting Dendrons

IX-C  Field-Effect Transistors with Organic Semiconductors 156
IX-C-1  Preparation of Organic Light-Emitting Field-Effect Transistors
IX-C-2  Field-Effect Transistors Based on Single-Crystalline Wires
IX-D  Molecular Assemblies on Silicon Surfaces via Silicon–Carbon Covalent Bonds 157
IX-D-1  Characterization of Molecular Assemblies on Silicon Surfaces
IX-E  Low Temperature Scanning Tunneling Microscopy and Spectroscopy of Organic Molecules on Metal Surfaces 157
IX-E-1  Scanning Tunneling Microscopy and Spectroscopy of Phthalocyanine Molecules on Metal Surfaces
IX-F  Ratchet Motions of a Droplet Caused by Electrochemical Reaction of Monolayers 158
IX-F-1  Electrochemically Generated Wetting Gradient and Its Application for the Transport of Droplets
IX-F-2  Transport of a Droplet by Directional Deformations with Asymmetric Electrode

 RESEARCH ACTIVITIES IX ........................................... 151

IX-A  Photo Precursor for Pentacene 151
IX-A-1  Photo Precursor for Pentacene
IX-A-2  Synthesis and Self-Assembly of Novel Porphyrin Molecular Wires 151
IX-A-3  Molecular Junctions Composed of Oligothiophene Dithiol Bridged Gold Nanoparticles Exhibiting Photosensitive Properties 152
IX-A-4  Simple Preparation Method for Supramolecular Porphyrin Arrays on Mica Using Air/Water Interface 152
IX-A-5  Novel Photochemical Synthesis of Pentacene and Its Derivatives 152
IX-A-6  Porphyrin Molecules Working as Nanodevice on Single-Walled Carbon Nanotube Wiring 153
IX-A-7  Electronic Properties of Single-Walled Carbon Nanotube/Porphyrin Polymer Complex Measured by Point-Contact Current Imaging Atomic Force Microscopy 153
IX-A-8  Preparation of Very Reactive Thiol-Protected Gold Nanoparticles: Revisiting the Brust-Schiffrin Method 153
IX-B-1  Organic Thin-Film Transistors with High Electron Mobility Based on Perfluoropentacene 155
IX-C  Field-Effect Transistors with Organic Semiconductors 156
IX-C-1  Preparation of Organic Light-Emitting Field-Effect Transistors
IX-C-2  Field-Effect Transistors Based on Single-Crystalline Wires of Bis-(1, 2, 5-Thiadiazolo)-p-Quinobis(1, 3-Dithiole) 156
IX-D  Molecular Assemblies on Silicon Surfaces via Silicon–Carbon Covalent Bonds 157
IX-D-1  Characterization of Molecular Assemblies on Silicon Surfaces by Attenuated Total Reflectance Infrared Spectroscopy 157
IX-E  Low Temperature Scanning Tunneling Microscopy and Spectroscopy of Organic Molecules on Metal Surfaces 157
IX-E-1  Scanning Tunneling Microscopy and Spectroscopy of Phthalocyanine Molecules on Metal Surfaces 157
IX-F  Ratchet Motions of a Droplet Caused by Electrochemical Reaction of Monolayers 158
IX-F-1  Electrochemically Generated Wetting Gradient and Its Application for the Transport of Droplets 158
IX-F-2  Transport of a Droplet by Directional Deformations with Asymmetric Electrode 159
| IX-G | Development of Multi-Function Integrated Macromolecules and Their Organization on Substrate Surfaces for Planar Molecular-Scale Electronics Circuits | 160 |
| IX-G-1 | Step-Wised Synthesis of Multifunctional Molecular Wires for Planar Metal-Molecule-Metal Junctions | 160 |
| IX-H | Heterogeneous Aquacatalysis | 161 |
| IX-H-1 | PS-PEG Resin-Supported Palladium-MOP Complexes. Application in Asymmetric π-Allylic Reduction | 161 |
| IX-H-2 | Hydrogenation and Dehalogenation under Aqueous Conditions with an Amphiphilic Polymeric-Supported Nanopalladium Catalyst | 161 |
| IX-H-3 | Cycloisomerization of 1,6-Enynes: Asymmetric Multi-Step Preparation of a Hydrindane Framework in Water with Polymeric Catalysts | 161 |
| IX-H-4 | Controlled Monoarylation of Dibromoarenes in Water with a Polymeric Palladium Catalyst | 161 |
| IX-I | Development of New Nanomaterials as Components in Advanced Molecular Systems | 162 |
| IX-I-1 | Gold Nanoparticles Stabilized by Tripod Thioether Oligomers: Synthesis and Molecular Dynamics Studies | 162 |
| IX-J | Designing Artificial Photosynthesis at Molecular Dimensions | 162 |
| IX-J-1 | Electrochemical Properties of Ferrocene-Dendrimer-Porphyrins | 163 |
| IX-K | Development of New Metal Complexes as Redox Catalysts | 163 |
| IX-K-1 | Synthesis, Structure and Electrochemistry of New Cobalt Complexes with Cyclopentadienyl and Bidentate Ligands | 164 |
| IX-L | Photochemistry on Well-Defined Surfaces | 165 |
| IX-L-1 | Photochemistry of Cyclohexane on Cu(111) | 165 |
| IX-M | Ultrafast Dynamics at Well-Defined Surfaces | 165 |
| IX-M-1 | Femtosecond Wavepacket Dynamics of Cs Adsorbates on Pt(111): Coverage and Temperature Dependences | 165 |
| IX-M-2 | Mode Selective Excitation of Coherent Surface Phonons on Alkali-Covered Metal Surfaces | 166 |
| IX-M-3 | Excitation Mechanism of Coherent Surface Phonons on Alkali-Metal Covered Surfaces | 166 |
| IX-N | Multiphoton Photoelectron Spectroscopy of Electronic States of Nano-Structured Materials on Surfaces | 166 |
| IX-N-1 | The Electronic Structure and Femtosecond Electron Transfer Dynamics at Noble Metal/iris-(8-hydroxyquinoline) Aluminum Interfaces | 166 |
| IX-O | Chemistry of One-Dimensional Nano-Surface Compounds Studied by Scanning Tunneling Microscopy | 167 |
| IX-O-1 | In-Situ Observation of CO Oxidation on Ag(110)(2x1)-O by Scanning Tunneling Microscopy: Structural Fluctuation and Catalytic Activity | 167 |
| IX-P | Structures, Stabilities and Physicochemical Properties of Organometallic Hybrid Clusters | 168 |
| IX-P-1 | Glutathione-Protected Gold Clusters Revisited: Bridging the Gap between Gold(I)-Thiolate Complexes and Thiolate-Protected Gold Nanocrystals | 168 |
| IX-P-2 | Large-Scale Synthesis of Thiolated Au25 Clusters via Ligand Exchange Reactions of Phosphine-Stabilized Au11 Clusters | 168 |
| IX-P-3 | Subnanometer-Sized Gold Clusters with Dual Molecular Receptors: Synthesis and Assembly in One-Dimensional Arrangements | 169 |
| IX-P-4 | Size-Specific Catalytic Activity of Polymer-Stabilized Gold Nanoclusters for Aerobic Alcohol Oxidation in Water | 169 |
| IX-P-5 | Fabrication of Two dimensional Arrays of Size-Selected Gold Clusters | 169 |
| IX-Q | Structural Analyses of Biological Macromolecules by Ultra-High Field NMR Spectroscopy | 170 |
| IX-Q-1 | Ultra-High Field NMR Study of Carbohydrate-Protein Interactions | 170 |
| IX-Q-2 | Ultra-High Field NMR Study of Glycoproteins | 170 |
| IX-R | Electronic Structure and Collision Dynamics of Atoms and Molecules Studied by Electron Impact at Large Momentum Transfer | 172 |
| IX-R-1 | Development and Use of a Multichannel (e,2e) Spectrometer for Electron Momentum Densities of Molecules | 172 |
| IX-R-2 | Observation of Molecular Frame (e,2e) Cross Section Using an Electron-Electron-Fragment Ion Triple Coincidence Apparatus | 172 |
| IX-R-3 | (e,3e) Collisions on Mg in the Impulsive Regime Studied by Second Born Approximation | 172 |
| IX-R-4 | Electron Momentum Spectroscopy of Valence Satellites of Neon | 172 |
| IX-R-5 | Theoretical Fine Spectroscopy with Symmetry-Adapted-Cluster Configuration-Interaction Method: Outer- and Inner-Valence Ionization Spectra of Furan, Pyrrole, and Thiophene | 173 |
| IX-R-6 | Observation of a Molecular Frame (e,2e) Cross Section: An (e,2e+M) Triple Coincidence Study on H2 | 173 |
| IX-R-7 | (e,2e) and (e,3–1e) Studies on Double Processes of He at Large Momentum Transfer | 173 |
UVSOR Facility

IX-U Development of the UVSOR Light Source
IX-U-1 Successful Commissioning of New RF Cavity
IX-U-2 Ion Trapping Phenomena at UVSOR-II

IX-V Researches by the Use of UVSOR
IX-V-1 Development of Velocity Imaging Spectrometer for Observing Negative Fragment Ions
IX-V-2 Dynamics of Double Photoionization near the Ar 2p Threshold
Investigated by Threshold Electron-Auger Electron Coincidence Spectroscopy
IX-V-3 Origin of Threshold Electrons Produced in Decay of the Xe 4d 1hp Resonance
IX-V-4 Coincidence Auger Spectroscopy
IX-V-5 Collision Dynamics of the Kr 6s + N2 System
Studied by a Multi-Coincidence Technique
IX-V-6 Collision Dynamics of MCI-Molecule Systems
Studied by Multi-Coincidence Technique
IX-V-7 Optical Investigations of the Clathrate α-Eu4Ge16Ge30
IX-V-8 Influence of Cage Distortions on the Electronic Structure and Optical Properties
of Ba6Ge25
IX-V-9 Indirect and Direct Energy Gaps in Kondo Semiconductor YbB12
IX-V-10 Kondo Ground States and Non-Fermi-Liquid Behavior in CeNi1-xCoxGe2
IX-V-11 Infrared Spectroscopy under Multietreme Conditions:
Direct Observation of Pseudogap Formation and Collapse in CeSb
IX-V-12 Infrared Study on CeSb under High Pressures
IX-V-13 Electronic Structure of Bulk Metallic Glass Zr55Al10Cu30Ni5
IX-V-14 Carrier-Induced Infrared Magnetic Circular Dichroism
in the Magnetoresistive Pyrochlore Ti2Mn2O7
IX-V-15 Magnetic Ordering in Frustrated CeNi4S6C6
IX-V-16 Features of Fluorescence Spectra of Polyethylene Terephthalate Films
IX-V-17 Anomalous Magnetic Properties and Non-Fermi-Liquid Behavior in Single Crystals
of the Kondo Lattice CeNiGe2-xS1x
IX-V-18 Sub-Natural Linewidth Auger Electron Spectroscopy of the 2s Hole Decay in HCl
Laser Research Center for Molecular Science

IX-W  Developments and Researches of New Laser Materials
IX-W-1  Growth and Scintillation Properties of Yb Doped Aluminate, Vanadate and Silicate Single Crystals --------184
IX-W-2  Onset Detection of Solid-State Phase Transition in Estrogen-Like Chemical via Terahertz Transmission Spectroscopy 184
IX-W-3  Design Principle of Wide-Gap Fluoride Hetero-Structures for Deep Ultraviolet Optical Devices 184
IX-W-4  Terahertz Time-Domain Spectroscopy of Amino Acids and Polypeptides 184

IX-X  Development and Research of Advanced Tunable Solid State Lasers
IX-X-1  Spectroscopic Properties of Yb:GdVO₄ Single Crystal: Stark Levels, Selection Rules, and Polarized Cross Sections 186
IX-X-2  Spectroscopic Properties of All-Ceramic Composite with Layer-by-Layer of Nd:Y₃Al₅O₁₂ and Nd:Y₃ScAl₄O₁₂ 186
IX-X-3  Hybrid Process for Measurement of Spectroscopic Properties of Nd:GdVO₄ 187
IX-X-4  Absorption, Emission Spectrum Properties and Efficient Laser Performances of Yb:Y₃ScAl₄O₁₂ Ceramics 187
IX-X-5  Passive Mode Locking of a Mixed Garnet Yb:Y₃ScAl₄O₁₂ Ceramic Laser 187
IX-X-6  High-Power Operation of Diode Edge-Pumped, Glue-Bonded, Composite Yb:Y₃Al₅O₁₂ Microchip Laser with Ceramic, Undoped YAG Pump Light-Guide 187
IX-X-7  Continuous-Wave Deep Blue Generation in a Periodically Poled MgO:LiNbO₃ Crystal by Single-Pass Frequency Doubling of a 912-nm Nd:GdVO₄ Laser 188
IX-X-8  Continuous-Wave Ultraviolet Generation at 354-nm in a Periodically Poled MgO:LiNbO₃ by Frequency Tripling of a Diode End-Pumped Nd:GdVO₄ Microlaser 188
IX-X-9  High-Power Continuous-Wave Intracavity Frequency-Doubled Nd:GdVO₄-LBO Laser under Diode Pumping into the Emitting Level 188
IX-X-10  Deep Blue Generation at 456 nm in a Periodically Poled MgO:LiNbO₃ Ridge-Type Waveguide by Single-Pass Frequency Doubling of a Nd:GdVO₄ Micro-Laser 188
IX-X-11  Efficient 1.06 and 1.34-µm Laser Emission of Highly-Doped Nd:YAG under 885-nm Diode Pumping into the Emitting Level 188
IX-X-12  High-Power Multi-Pass Pumped Microchip Nd:GdVO₄ Laser 189
IX-X-13  Highly Efficient New Pumping Configuration for Microchip Solid State Laser 189
IX-X-14  High Energy Quasi-Phase-Matched Optical Parametric Oscillation in a 3-mm-Thick Periodically Poled MgO:LiNbO₃ Device 189

Equipment Development Center

IX-Y  Development of New Instruments and Experimental Devices
IX-Y-1  Development of a High-Precision Slit Blade for the Transmission-Grating Spectrometer 190
IX-Y-2  Manufacture of Glass Microreactor Chips 191
IX-Y-3  Micro Processing by a Femto-Second Laser 191
IX-Y-4  Development of Electrical Control System of Fluorescence Recovery after Photobleaching Apparatus Using Semiconductor Laser for Illumination 192

Safety Office

IX-Z  Development of Novel Heterocyclic Compounds and Their Molecular Assemblies for Advanced Materials
IX-Z-1  Molecular Arrangement in the Cocrystals of 1,1’3,3’-Tetramethyl-2,2’-bi-1H-imidazolium Bis(tetraphenylborate) with Ketone, Aldehyde, and Nitrile as Guest Molecules 193
IX-Z-2  Macrocyclic and Acyclic Bis(2,5-diphenyl-1,3,4-oxadiazole)s with Electron-Transporting and Hole-Blocking Ability in Organic Electro luminescent Devices 193
IX-Z-3  Synthesis, Characterization and FET Properties of Novel Dithazolylbenzothiadiazole Derivatives 193

RESEARCH ACTIVITIES X

Okazaki Institute for Integrative Bioscience

X-A  Single-Molecule Physiology
X-A-1  One Rotary Mechanism for F₁-ATPase over ATP Concentrations from Millimolar down to Nanomolar 195
X-A-2  ATP-Driven Stepwise Rotation of F₁,F₂-ATP Synthase 195
X-A-3  Activation of Pausing F₁ Motor by External Force 195
X-B Bioinorganic Chemistry of Heme-Based Sensor Proteins ..........................................................197
  X-B-1 Spectroscopic and Redox Properties of a CooA Homologue from Carboxydoterms hydrogenoformans ..........................................................197
  X-B-2 Oxygen Sensing Mechanism of HemAT from B. subtilis: A Resonance Raman Spectroscopic Study ..........................................................197
  X-B-3 Structure and Function of a Novel Redox Sensor DcrA Containing a C-Type Heme ............197
X-C Bioinorganic Chemistry of a Novel Heme Enzyme that Catalyzes the Dehydration Reaction --198
  X-C-1 Regulation of Aldoxime Dehydratase Activity by Redox-Dependent Change in the Coordination Structure of the Aldoxime-Heme Complex .........................................................198
X-D Reaction Mechanism of Metalloenzymes Related to Oxygen Activation ....................................199
  X-D-1 Oxidizing Intermediates from the Sterically Hindered Salen Iron Complexes Related to the Oxygen Activation by Nonheme Iron Enzymes ..................................................199
  X-D-2 Synthesis of Sterically Hindered Tris(4-imidazolyl)carbinol Ligands and their Copper(I) Complexes Related to Metalloenzymes ..........................................................199
  X-D-3 O2- and H2O2-Dependent Verdoxene Degradation by Heme Oxygenase: Reaction Mechanisms and Potential Physiological Roles of the Dual Pathway Degradation ........200
X-E Reaction Mechanism of Metalloenzymes related to Global Nitrogen Cycle ................................200
  X-E-1 Spectroscopic Characterization of Reaction Intermediates in a Model for Copper Nitrite Reductase ........................................................................200
X-F Biomolecular Science ..................................................................................................................202
  X-F-1 Resonance Raman Characterization of the P Intermediate in the Reaction of Bovine Cytochrome c Oxidase ........................................................................202
  X-F-2 Core Structure of Amyloid Fibril Proposed from IR-Microscope Linear Dichroism ............202
  X-F-3 Activation of Heme-Regulated Eukaryotic Initiation Factor 2 Alpha by Nitrile Oxide Is Induced by the Formation of a Five-Coordinate NO-Heme Complex: Optical Absorption, Electron Spin Resonance and Resonance Raman Spectral Studies ..................................................203
  X-F-4 Steric and Hydrogen-Bonding Effects on the Stability of Copper Complexes with Small Molecules .......................................................................................203
  X-F-5 Identification of Crucial Histidines Involved in Carbon-Nitrogen Triple Bond Synthesis by Aldoxime Dehydratase ..........................................................203
  X-F-6 Thermal Stability of Mononuclear Hydroperoxocopper(II) Species. Effects of Hydrogen Bonding and Hydrophobic Field ......................................................204
  X-F-7 Energy Funneling of IR Photons Captured by Dendritic Antennae and Acceptor Mode Specificity: Anti-Stokes Resonance Raman Studies on Iron(III) Porphyrin Complexes with a Poly(Aryl Ether) Dendrimer Framework ........................................................................204
  X-F-8 Structural Model of the Amyloid Fibril Formed by β2-Microglobulin #21-31 Fragment Based on Vibrational Spectroscopy .........................................................204
  X-F-9 Excited State Property of Hardly Photodissociable Heme-CO Adduct Studied by Time-Dependent Density Functional Theory .........................................................205
  X-F-10 Mechanism for Transduction of the Ligand-Binding Signal in Heme-Based Gas Sensory Proteins Revealed by Resonance Raman Spectroscopy ........................................205
  X-F-11 UV Resonance Raman Study of Model Complexes of the CuB Site of Cytochrome c Oxidase ........................................................................205
  X-F-12 Resonance Raman Investigation on the Specific Sensing Mechanism of a Target Molecule by Gas Sensory Proteins .................................................................206
  X-F-13 Communication Pathway between Heme and Protein in Myoglobin ................................206
  X-F-14 FT-IR Approaches on Amyloid Fibril Structure .................................................................206
  X-F-16 Axial Ligand Substituted Nonheme FeIV=O complexes: Observation of Near-UV LMCT Bands and Fe=O Raman Vibrations ........................................................................206
  X-F-17 Reversible O-O Bond Cleavage and Formation of a Peroxo Moiety of a Peroxocarbonate Ligand Mediated by an Iron(III) Complex ......................................................207
  X-F-19 Spectroscopic and Redox Properties of a CooA Homologue from Carboxydoterms hydrogenoformans ........................................................................207
  X-F-20 Structural Diversities of Active Site in Clinical Azole-Bound Forms between Sterol 14α-Demethylases (CYP51s) from Human and Mycobacterium tuberculosis ........208
  X-F-21 Stopped-Flow Spectrophotometric and Resonance Raman Analyses of Aldoxime Dehydratase Involved in Carbon-Nitrogen Triple Bond Synthesis .................................208
X-F-22  Synthesis, Characterization, and Thermal Stability of New Mononuclear Hydrogenperoxocopper(II) Complexes with N$_2$O-Type Tripodal Ligands
Bearing Hydrogen-Bonding Interaction Sites .............................................208
X-F-23  Spectroscopic Characterization of the Isolated Heme-Bound PAS-B Domain of Neuronal PAS Domain Protein 2 (NPAS2) Associated with Circadian Rhythms .............................................209
X-F-24  Covalent Cofactor Attachment to Proteins: Cytochrome c Biogenesis ......................................................209
X-F-25  Structure and Dioxygen-Reactivity of Copper(I) Complexes
Supported by Bis(6-methylpyridin-2-yl)methylamine Tridentate Ligands .............................................209
X-F-26  Resonance Raman and FT-IR Studies on Proximal and Distal Histidine Environment of Cytooglobin and Neuroglobin .............................................210
X-F-27  Dynamic Ligation Properties of the Escherichia coli Heme Chaperone CcmE to Non-Covalently Bound Heme ......................................................210

X-G  Collaborative Research with FANTOM Consortium .............................................211
X-G-1  The international Consortium, FANTOM*, Discovered UBL Domains
Interspersed over Mammalian Genomes .............................................211

RESEARCH FACILITIES .................................................................................213
Research Center for Molecular-scale Nanoscience .............................................213
UVSOR Facility ......................................................213
Laser Research Center for Molecular Science .............................................214
Equipment Development Center ......................................................214
Safety Office ......................................................214
Research Center for Computational Science .............................................214

SPECIAL RESEARCH PROJECTS .................................................................217
(a)  Chemical Reaction Dynamics .................................................................217
Folding Mechanism of Protein Molecules Studied by Generalized-Ensemble Algorithms .................................................................217
Electronic Structure and Decay Mechanism of Inner-Shell Excited Molecules .................................................................217
Computational Study of Quantum Dynamics of a Solute in Solution .................................................................217
Chemical Reactions at Surfaces and Nano-Structured Materials
 Studied by Spatio-Temporally Resolved Spectroscopy .................................................................218
Towards Complete Imaging of Molecular Orbital Patterns:
 Development of Molecular Frame ($\epsilon,2\epsilon$) Spectroscopy .................................................................218
(b)  Molecular Photophysics and Science .................................................................219
Theoretical Studies of Quantum Many-Particle Dynamics in Open Systems .................................................................219
Spatiotemporal Dynamics in Nanometric Molecular Assemblies by Near-Field Spectroscopy .................................................................219
Studies on Laser Cooling and Trapping of Metastable Helium Atoms
 and Laser Spectroscopic Studies of Atoms and Ions in Liquid Helium .................................................................219
Methods of Analysis for Protein Dynamics in Living Cells .................................................................219
Development of Attosecond Coherent Control and Its Application .................................................................220
Laser Manipulation of Molecular Motions and Its Application to Reaction Dynamics Studies .................................................................220
Probing Ultrafast Molecular Dynamics by Extremely Short Laser Pulses .................................................................220
Photoionization and Photodissociation of Fullerenes and Metal Encapsulated Fullerenes,
Their Mechanisms, Kinetics, and Dynamics .................................................................220
Theoretical Development of Interfacial Sum Frequency Generation Spectroscopy .................................................................221
Decay and Dissociation Dynamics of Core Excited Molecules .................................................................221
(c)  Novel Materials Science ........................................................................222
Quantum Chemistry Calculations of Large Molecular Systems .................................................................222
Theory for Equilibrium and Non-Equilibrium Properties of Low-Dimensional Molecular Materials
 with Strong Correlation .................................................................222
UHV Systems for MOKE, MSHG, XMCD and STM Measurements .................................................................222
Development and Characterization of Metal/Carbon Hybrid Nano-Systems .................................................................223
Charge ordering in Organic Conductors .................................................................223
Multi-Frequency and Pulsed ESR Investigation for Molecular-Based Materials .................................................................224
Broad-Line Solid State NMR Investigation of Molecular-Based Conductors .................................................................224
Synchrotron X-Ray Diffraction Experiments and MEM Analyses for Single Crystals
 of Organic Conductors .................................................................225
Development of New Functional Molecular Systems .................................................................225
Synthesis and Properties of Novel Chiral Organic-Inorganic Molecule-Based Magnets .................................................................225
Design and Functions of Novel Soft Nanomaterials Based on Molecular Programming .................................................................226
Giant Vesicle Fusion on Microelectrodes Fabricated by Femtosecond Laser Ablation
 Followed by Synchrotron Radiation Etching .................................................................226
Reduction of CO$_2$ and Oxidation of Organic Molecules Aiming at Reversible Conversion between Chemical and Electrical Energies .................................................................227

Annual Review 2005 xix