CONTENTS

IMS 2005	-iii
CONTENTS	
ORGANIZATION AND STAFF	
COUNCIL	
BUILDINGS AND CAMPUS	
RESEARCH ACTIVITIES I	17
Department of Theoretical Studies I-A Theoretical Study and Design of Functional Molecular Systems: New Bonding, Structures, and	ı
Reactions	17
I-A-1 Counterion-Driven Spontaneous Polymerization of the Linear C ₆₀ ⁿ⁻ Chains in the fcc Fullerides and Its Magic Number Behavior	17
I-A-2 Amphoteric and Controllable Doping of Carbon Nanotubes by Encapsulation	1/
of Organic and Organometallic Molecules	17
I-A-3 Electronic Excited States and Stabilities of Fullerenes: Isomers of C ₇₈ and Mg@C ₇₂	17
I-A-4 1,6,7-Trigermabicyclo[4.1.0]hept-3-en-7-yl: The Isolable Bicyclic Germyl Radical	17
I-A-5 Isolation of a Se-Nitrososelenol: A New Class of Reactive Nitrogen Species	
Relevant to Protein Se-Nitrosation	18
I-A-6 A New Approach to Simulate the Depolymerization Process of a Two-Dimensional Hexagonal C ₆₀ Polymer	1.0
of a Two-Dimensional Hexagonal C_{60} PolymerI-A-7 Chemical Reactivity and Redox Property of $Sc_3@C_{82}$	18
I-A-7 Cheffical Reactivity and Redox Property of Sc ₃ @C ₈₂	10 18
I-A-9 Dispersion of Single-Walled Carbon Nanotube Bundles in Nonaqueous Solution	18
I-A-10 Regioselective Carbon–Carbon Bond Cleavage of an Open-Cage Diketone Derivative	10
of [60]Fullerene by Reaction with Aromatic Hydrazones	19
I-A-11 Gibbs Energy-Based Treatment of Metallofullerenes: Ca@C ₇₂ , Ca@C ₇₄ , Ca@C ₈₂ ,	1,
and La@C $_{82}$	19
I-A-12 Chemical Reactivities of the Cation and Anion of M@C ₈₂ (M = Y, La, and Ce)	19
I-A-13 Systematic Studies on Redox Behavior of Homonuclear Double-Bond Compounds	
of Heavier Group 15 Elements	19
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	19
I-A-15 Adsorption Configuration of NH 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)	20
I-A-18 Synthesis and Characterization of Stable Hypervalent Carbon Compounds (10-C-5) Bearing a 2,6-Bis(p-substituted phenyloxymethyl)benzene Ligand	20
I-A-19 Practical Performance Assessment of Accompanying Coordinate Expansion Recurrence	20
Relation Algorithm for Computation of Electron Repulsion Integrals	20
I-A-20 2D NMR Characterization of the La@C ₈₂ Anion	20
I-A-21 Open-Cage Fullerene Derivatives Suitable for the Encapsulation of a Hydrogen Molecule	-21
I-A-22 Computed Structure and Energetics of La@C ₆₀	21
I-A-23 Metallic Phase in the Metal-Intercalated Higher Fullerene Rb _{8.8(7)} C ₈₄	21
I-A-24 Interplay of Single-Wall Carbon Nanotubes and Encapsulated La@C ₈₂ , La ₂ @C ₈₀ ,	
and $Sc_3N@C_{80}$	
I-A-25 Structural Evolution of [2+1] Cycloaddition Derivatives of Single-Wall Carbon Nanotuber	s:
From Open Structure to Closed Three-Membered Ring Structure	22
with Increasing Tube Diameter	22
I-A-26 Missing Metallofullerene La@ C_{74} I-A-27 Chemical Reactivity of S $c_3N@C_{80}$ and La $_2@C_{80}$	
I-A-27 Chemical Reactivity of Sc ₃ N@C ₈₀ and La ₂ @C ₈₀	42
Carbon Nanotubes	??
I-A-29 Encapsulation of La@C ₈₂ and La 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	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-3 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 Development of Simulation Algorithms for Complex Systems	25
I-C-1 Liquid-Gas Phase Transitions Studied by Multibaric-Multithermal	
Monte Carlo Simulations	25
I-D Other Results on Molecular Simulations	25
I-D-1 Comparisons between a Molecular Dynamics and Hydrodynamics Treatment	
of Non-Stationary Thermal Processes in a Liquid	25
I-E Applications of the Zhu-Nakamura Theory to Nonadiabatic Chemical Dynamics	26
I-E-1 Nonadiabatic Transition and Chemical Dynamics: Multi-Dimensional	
Tunneling Theory and Applications of the Zhu-Nakamura Theory	26
I-E-2 Electron Transfer Rate to Cover the Whole Range from Adiabatic to Nonadiabatic Regime	
Based on the Zhu-Nakamura Theory	
I-E-3 Semiclassical Theory of Electron Transfer Beyond the Perturbation Theory	26
I-E-4 Generalized Trajectory Surface Hopping Approach	26
I-E-5 Semiclassical Theory of Thermal Rate Constant for Multi-Surface Processes	26
I-F Theory of Nonadiabatic Transition	27
I-F-1 Rabi Dynamics of Coupled Atomic and Molecular Bose-Einstein Condensates	27
I-F-2 A Basic Two-State Model for Bosonic Field Theories with a Cubic Nonlinearity	27
I-F-3 Incorporation of Nonadiabatic Transition into Wave Packet Dynamics	27
I-G Theory of Multi-Dimensional Tunneling	27
I-G-1 Instanton Theory for the Tunneling Splitting of Low Vibrationally Excited States	27
I-G-2 Effect of Out-Of Plane Vibration on the Hydrogen Atom Transfer Reaction	
in Malonaldehyde	27
I-G-3 Ground State and Vibrationally Assisted Tunneling in the Formic Acid Dimer	28
I-H Laser Control of Molecular Processes	28
I-H-1 Laser Control of Electronic Transitions of Wave Packet	
by Using Quadratically Chirped Pulses	28
I-H-2 Semiclassical Guided Optimal Control of Molecular Dynamics	28
I-I Development of New Molecular Functions	29
I-I-1 A Theoretical Study of Cyclohexadiene/ Hexatriene Photochemical Interconversion:	
Miltireference Configuration Interaction Potential Energy Surfaces and Transition Probabilities	es
for the Radiationless Decays	29
I-I-2 Reaction Dynamics of Cyclohexadiene/Hexatriene Ultrafast Photoisomerization	
through Conical Intersections	29
I-I-3 Encapsulation of Hydrogen Atoms by Fullerenes and Carbon Nanotubes	
with the Use of Nonadiabatic Transition	29
I-J Theoretical Studies of Electron Dynamics in Molecular Systems	30
I-J-1 High-Order Harmonic Generation from Silver Clusters:	
Laser-Frequency Dependence and the Screening Effect of d Electrons	30
I-J-2 Multiple Ionization of a Silver Diatomic Molecule in an Intense Laser Field	
I-K Electronic Structures and Photochemical Properties of Nanometer-Sized Metal Clusters	
I-K-1 Electronic Structure and Photochemical Properties of a Monolayer-Protected Gold Cluster	
I-K-2 Glutathione-Protected Gold Clusters Revisited: Bridging the Gap between Gold(I)-Thiolat	
Complexes and Thiolate-Protected Gold Nanocrystals	31
I-K-3 Gold-Thiolate Nanoring: Electronic Structure and Photochemical Properties	31
I-L Electronic Structure of a Molecule in Solution	
I-L-1 Electronic Structure Calculation of a Solvated Macro Molecule by Using Three-Dimension	
Reference Interaction Site Model Combined with Ab Initio Molecular Orbital Theory	32
I-L-2 New Theoretical Approach for the Diastereoselectivity of H/D Exchange Reaction	
on Methyl 3-Fluorobutanoate Anion	32
I-M Solvation Thermodynamics of Protein and Related Molecules	33
I-M-1 Hydrophobic Effects on Partial Molar Volume	33
I-M-2 Partial Molar Volume of Proteins Studied by the 3D-RISM Theory	33
I-M-3 Theoretical Study of Volume Changes Associated with the Helix-Coil Transition	
of an Alanine-Rich Peptide in Aqueous Solution	33
I-M-4 Combination of the Replica-Exchange Monte Carlo Method and the Reference Interaction	l
Site Model Theory for Simulating a Peptide Molecule in Aqueous Solution	34
I-M-5 Water Molecules in a Protein Cavity Detected by a Statistical-Mechanical Theory	34

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 Molecula	ar
Solutions: Acetonitrile in Water, Methanol in Water, and Methanol in Acetonitrile	
I-N-2 Theoretical Study on the Dynamic Properties of Compressed Water and Water-Hydro	
Solute Mixtures	
I-N-3 Solvation Dynamics in Water Investigated by RISM/Mode-Coupling Theory	25
I-O Statistical Mechanics of Interfacial Fluids	30
I-O-1 A Molecular Theory of Liquid Interfaces	36
I-P Photoinduced Phase Transitions in Molecular Materials	
I-P-1 Photoinduced Dynamics and Nonequilibrium Characteristics in Quasi-One-Dimension	nal
Electron Systems: Mott Insulators vs. Band Insulators	37
I-P-2 Optical Responses of Photoexcited States in the One-Dimensional Ionic Hubbard Mo	del37
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	30
I-R Strongly Correlated Electron Systems with Frustrations	30
I-R-1 Frustration-Induced η Inversion in the $S = 1/2$ Bond-Alternating Spin Chain	30
I-R-2 Field-Induced Phase Transitions and Long-Range Orders	20
in the $S = 1/2$ Spin Bond-Alternating Chain with Frustrating Interaction	39
I-R-3 Field-Induced Incommensurate Order in Frustrated Spin Chain	
I-R-4 Phase Diagram of the Excitonic Insulator	39
I-R-5 Effective Interaction between the Interpenetrating Kagome Lattices in Na_xCoO_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 Prope	rties
of Compounds Containing Heavy Elements	41
I-S-1 Theoretical Studies on Circular Dichroism Spectra of Linear and Cyclic Dichalcogeni	.de
Compouns (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 Metho	od .
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 Pulse	es44
I-V-2 Control of Photoelectron Angular Distributions Using a Dressing Laser	
I-W Theoretical Studies on Dynamical Foundation of Chemical Reactions and Proteins	46
I-W-1 Phase Space Reaction Network on Multibasin Energy Landscapes	
I-W-2 A Construction of Multidimensional Free Energy Landscape from an Ensemble of Si	
Molecule Time Series	ingle
Molecule Time Series	40
I-W-3 A New Technique to Differentiate the Origin of Observed non-Brownian Dynamics	1.0
in the Principal Component Space	46
I-W-4 Polypeptide in Water on the Lagrange Picture in Fluid Dynamics	47
TARGET A CONTENT OF THE CONTENT OF T	40
SEARCH ACTIVITIES II	49
epartment of Molecular Structure	
$\hat{\Pi} ext{-} ext{A}\;\; ext{Development of Dynamic Near-Field Spectroscopy and Application to Nanometric System$	ems49
II-A-1 Morphological and Spectroscopic Properties of Thin Films of Self-Assembling Amp	hiphilic
Porphyrins on Hydrophilic Surface as Revealed by Scanning Near-Field Optical Microsoft	
II-A-2 Scanning Near-Field Optical Microscopic Study of Porphyrin Nanowire	
II-A-3 Imaging of Plasmon Modes in Gold Nanorods	
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	50
by Near-Field Spectroscopy	51
5 y 1 tour 1 lord 5 poetroscopy	51

	II-A-7 Ultrafast Near-Field Imaging of Single Gold Nanorods and Nanoplates	-51
	Nanoparticles	-52
П-В 5	Spectroscopic Studies on Atoms and Ions in Liquid Helium	-53
	II-B-1 Laser Spectroscopic Studies of Mg Atoms in Pressurized Liquid Helium	-53
II-C	Magnetic Structures of Magnetic Thin Films Studied by Using a Depth-Resolved XMCD	
Te	chnique	-54
	II-C-1 Direct Observation of an Oscillatory Behavior in the Surface Magnetization	~ .
	of Fe Thin Films Grown on a Ni/Cu(100) Film	-54
	II-C-2 Spin Reorientation Transition of Ni/Cu(100) and CO/Ni/Cu(100): Separation of the Surface and Bulk Components of the X-Ray Magnetic Circular Dichroism Spectrum	51
II-D	Structure and Function of Metalloproteins and Its Molecular Design	
п-р ,	II-D-1 L358P Mutation on P450cam Simulates Structural Changes upon Putidaredoxin Binding.	-50
	The Structural Changes Trigger Electron Transfer to Oxy-P450cam from Electron Donors	-56
	II-D-2 Structural Diversities of Active Site in Clinical Azole Bound Forms	
	between Sterol 14α-demethylases (CYP51) from Human and Mycobacterium tuberculosis	-56
	II-D-3 Two Heme Binding Sites Are Involved in the Regulated Degradation of the Bacterial Iron	
	Response Regulator (Irr) Protein	-57
	II-D-4 Involvement of Heme Regulatory Motif in Heme-Mediated Ubiquitination and Degradation	i ~7
пт.	of IRP2Structure and Energy Changes during Protein Reaction Dynamics	-57 -5 0
н-е з	II-E-1 Hydrogen Bonding Dynamics During Protein Folding of Reduced Cytochrome c :	-50
	Temperature and Denaturant Concentration Dependence	-58
	II-E-2 Conformational Dynamics of Phototropin 2 LOV2 Domain with the Linker	50
	upon Photoexcitation	-58
II-F	Controllable Magnetic Properties of Ultrathin Magnetic Films	
Us	ing Surface Chemical Techniques	-59
	II-F-1 MOKE and XMCD Study on K Adsorption on Fe Ultrathin Films on Cu(001)	-59
	II-F-2 Spin Reorientation Transition in Ag-Covered Co Films Grown on Vicinal Cu(001) Surface	~ 0
	Studied by Means of XMCD	-60
	II-F-4 Direct Observation of Biquadratic Exchange Interaction in Fe/Ni/Cu(001)	-00
	by Using MSHG	-61
II-G	Local Structures of Molecular-Based Magnetic Materials	01
Stı	udied by X-Ray Absorption Fine Structure Spectroscopy	-62
	II-G-1 Molecular Structure of Single-Molecule Magnet Mn ₁₁ Cr, Mn ₁₁ Cr ⁻ and Mn ₁₀ Fe ₂	-62
	II-G-2 Photoinduced Phase Transition of CuMo Cyanides Studied by XAFS Spectroscopy	-63
II-H	Development of Fluorescent and Bioluminescent Proteins	
for	Imaging Intracellular Molecular Dynamics	-64
	II-H-1 Quantitative Determination of Protein Nuclear Transport Induced by Phosphorylation or by Proteolysis	61
	II-H-2 A Stress Indicator for Noninvasively Imaging Endogenous Corticosterone in Living Mice	-04 -64
	11-11-2 A Sitess indicator for Norminasively imaging Endogenous Corticosterone in Living whee	-04
RESEAR	RCH ACTIVITIES III	65
	tment of Electronic Structure	
	Synthesis and Characterization of Exotic Molecule Based Nano-Crystals of Metal Acetylides:	
To	ward Carbon Encapsulated Metal Dot Array, Metal Nano-Networks and Metal-Carbon	
ну	Wirid Systems	
	III-A-2 Photochemical Conversion of (Cu ⁺ C≡C ⁻ -t-Butyl) ₂₄ Cluster Molecules to Cu Metallic	-03
	Nano-Sheets Embedded in Polymer Nano-Film	-66
	III-A-3 Guest Controlled Magnetism of CoC ₂ Nanoparticles	-66
	III-A-4 Formation of Carbon-Encapsulated Metallic Nano-Particles from Metal Acetylides	
	by Electron Beam Irradiation	-67
	III-A-5 Reexamination of the Structures and Energies of Li ₂ C ₂ and Li ₄ C ₄	-67
III-B	Ultrafast Dynamics and Scanning Tunneling Microscopy	-68
	III-B-1 Excited-State Double-Proton Transfer in the 7-Azaindole Dimer in Gas Phase 3.	
	Reaction Mechanism Studied by Picosecond Time-Resolved REMPI Spectroscopy	-68
	III-B-2 Ultrafast Excited-State Dynamics in Photochromic <i>N</i> -Salicylideneaniline Studied by Femtosecond Time-Resolved REMPI Spectroscopy	-6º
	III-B-3 Orientation of Nitrous Oxide on Palladium(1 1 0) by STM	-68
III-C	Spectroscopic and Dynamical Studies of Molecular Cluster Ions	-69
~	III-C-1 Infrared Photodissociation Spectra and Solvation Structure of $Mg^+(CH_3OH)_n$ ($n = 1-4$)	-69

	III-C-2 Infrared Photodissociation Spectroscopy of $Mg^+(NH_3)_n$ ($n = 3-6$):	
	Direct Coordination or Solvation through Hydrogen Bonding	69
	III-C-3 Electronic Spectra of Jet-Cooled 3-Methyl-7-Azaindole Dimer. Symmetry of the Lowest	
	Excited Electronic State and Double-Proton Transfer	69
	III-C-4 Structures of $[(CO_2)_n(H_2O)_m]^ (n = 1-4, m = 1, 2)$ Cluster Anions.	
	I. Infrared Photodissociation Spectroscopy	70
III-D	Development of High-Precision Coherent Control and Its Application	71
	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	71
III-E	Quantum-State Manipulation of Molecular Motions	72
	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	75
	III-F-1 Excited-State Dynamics of 4-Thiothymidine with UVA Light Irradiation	
	III-F-2 Photochemical Reaction Dynamics of <i>o</i> -Quinones	75
	III-F-3 Evidence of Phenoxymethyl Radical Formation in Laser Photolysis of Anisole in Solution	
	of Anisole in Solution	76
	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	76
	III-G-1 Spectroscopy and Relaxation Dynamics of Photoexcited Anisole	
	and Anisole-d ₃ Molecules in a Supersonic Jet	.77
	III-G-2 Internal Rotational Motion of the Chloromethyl Group	
	of the Jet-Cooled Benzyl Chloride Molecule	77
	III-G-3 Molecular Structure and Excited State Dynamics of Jet-Cooled <i>o</i> -, <i>m</i> - and <i>p</i> -Fluoroanisole	
	of Jet-Cooled <i>o</i> -, <i>m</i> - and <i>p</i> -Fluoroanisole	77
	III-G-4 Evidence for a Non-Planar Conformer and Conformational Isomerization	
	of <i>ο</i> -Fluoroanisole in a Low-Temperature Ar Matrix	.77
*** **	III-G-5 Molecular Structure and Puckering Vibration of 1-Aminoindan in a Supersonic Jet	78
III-H	Photochemical Reactions in Microreactors	
	III-H-1 Application of Microfabricated Reactors for Asymmetric Photoreaction	78
	III-H-2 Photocatalytic Reaction in Microfabricated Reactors	78
111-1	In-Situ Observation of Surface Reactions by Variable Temperature Scanning Tunneling	
M	icroscopy	80
	III-I-1 In-Situ Observation of CO Oxidation on Ag(110)(2×1)-O	00
	by Scanning Tunneling Microscopy: Structural Fluctuation and Catalytic Activity	
	III-I-2 Propagation of Reaction Front in the Disproportionate Reaction of H ₂ O on Ag(110)(5×1)-C	
	Surface: Role of Hydrogen Bonding Interaction	80
DECEAL	RCH ACTIVITIES IV	01
RESEAR	CHACIIVIIIESIV)1
Donor	tment of Melecular Assemblies	
Depar	tment of Molecular Assemblies	0.1
IV-A	Optical Study of Charge Ordering States in Organic Conductors	81
	IV-A-1 Examination of the Charge-Sensitive Vibrational Modes in ET Molecule	81
	IV-A-2 Infrared and Raman Studies of θ -(BEDT-TTF) ₂ CsZn(SCN) ₄ :	0.1
	Comparison with the Frozen State of θ -(BEDT-TTF) ₂ RbZn(SCN) ₄	81
	IV-A-3 Robust Superconducting State in the Low-Quasiparticle-Density Organic Metals	
	β "-(BEDT-TTF) ₄ [(H ₃ O) M (C ₂ O ₄) ₃]· Y :	0.2
	Superconductivity due to Proximity to a Charge-Ordered State	82
	IV-A-4 Influence of the Cooling Rate on Low-Temperature Raman and Infrared-Reflection Spectr	
	of Partially Deuterated κ-(BEDT-TTF) ₂ Cu(N(CN) ₂)Br	82
	IV-A-5 Optical Second Harmonic Generation in a Charge-Ordered Organic Conductor	0.5
	α-(BEDT-TTF) ₂ I ₃	83
	IV-A-6 Correlation between Structural Instabilities and Raman Shift and Width	00
	in β -(ET) ₂ I ₃ and κ -(ET) ₂ Cu[N(CN) ₂]I	83
	IV-A-7 Inhomogeneous Charge Distribution in (EDO-TTF) ₂ X (X = ReO ₄ and GaCl ₄)	
	IV-A-8 Re-Examination of the Site Charge Difference in TEA(TCNQ) ₂	84

	IV-A-9 Spectroscopic Evidence for the Monovalent-to-Divalent Phase Transition	
	of Biferrocenium (F ₁ TCNQ) ₃	-84
	IV-A-10 Phase Separation in the Monovalent-to-Divalent Phase Transition	
	of Biferrocenium-(F ₁ TCNQ) ₃	-85
IV-B	Magnetic Resonance Studies for Molecular-Based Conductors	-86
	IV-B-1 Charge Disproportionation in (TMTTF) ₂ SCN Observed by ¹³ C NMR	-86
	IV-B-2 Redistribution of Electronic Charges in the Spin-Peierls State in (TMTTF) ₂ AsF ₆	
	Observed by ¹³ C NMR	-86
	IV-B-3 Deuteration Effect and Possible Origin of the Charge-Ordering Transition of (TMTTF) ₂ X	
	IV-B-4 Redistribution of Electronic Charge in (TMTTF) ₂ ReO ₄ : ¹³ C NMR Investigation	-87
	IV-B-5 Spin Structure of Organic Conductors (TMTTF) ₂ X	-87
	IV-B-6 Multi-Frequency ESR Measurements for (TMTTF) ₂ X	-88
	IV-B-7 Extremely Slow Charge Fluctuations in the Metallic State of the Two-Dimensional	
	$Molecular\ Conductor\ \theta - (BEDT-TTF)_2RbZn(SCN)_4\$	-88
	IV-B-8 Sliding Spin-Density Wave of (TMTSF) ₂ PF ₆ Studied with Narrow-Band Noise	-88
IV-C	Synchrotron X-Ray Diffraction Experiments and MEM Analyses for Single Crystals	
of	Organic Conductors	
	IV-C-1 Low-Temperature Charge-Ordering State of (TMTTF) ₂ PF 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 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	
	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,	
	Co ₃ (HCOO) ₆ , and Its N ₂ Sorption Characteristic	-92
	IV-E-4 Superconductivity and Voltex Phases in the Two-Dimensional Organic Conductor	
	λ -(BETS) ₂ Fe _x Ga _{1-x} Cl ₄ (x = 0.45)	-92
	IV-E-5 Constant Resistivity State in the Field-Induced Organic Superconductor,	
	λ -(BETS) ₂ Fe _x Ga _{1-x} Cl ₄	-93
	IV-E-6 (Tetrathiafulvalene)[Fe ^{III} (C ₂ O ₄)Cl ₂]: An Organic-Inorganic Hybrid Exhibiting Canted Antiferromagnetism	
	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 Ab Initio Electronic Structure Calculation of Single-Component Molecular Conductor	
	Au(tmdt) ₂ (Tmdt = Trimethylenetetrathiafulvalenedithiolate)	-95
	IV-E-10 The Light-Induced Excited Spin State Trapping Effect on Ni(dmit) ₂ Salt	
	with an Fe(III) Spin-Crossover Cation: [Fe(qsal) ₂][Ni(dmit) ₂]·2CH ₃ CN	-95
	IV-E-11 Synergic Behavior between Spin and Conducting Property in Ni(dmit) ₂ Salt	
		-96
	IV-E-12 Synthesis and Molecular Structure of a Novel PROXYL-Fused π-Electron Donor,	
	PROXYL-ET-STF	
IV-F	Electronic and Magnetic Properties of π -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 d-Electron-Induced Negative Magnetroresistance of π -d Interaction System	
	Including Brominated-TTF Donor	-98
	IV-F-4 Electronic and Mgnetic Properties of π - d Interaction System (EDTDM) ₂ FeBr ₄	
	IV-F-5 Observation of Zigzag- and Armchair-Edges of Graphite	-99
IV-G	Progress of Conjugated Phenomena Coupled with Spin and Photon	
fo	r Assembled Hetero-Molecular System1	00
	IV-G-1 Reversible Photomagnetism in a Cobalt Layered Compound	
	Coupled with Photo-Chromic Diarylethene	00
IV-H	Molecular Crystals toward Nano-Devices by Use of d-π Interaction, Crystal Designing	
an	d Optical Doping	
	IV-H-1 Light-Induced Transformation of Molecular Materials into Devices	
	IV-H-2 Molecular Conductors Containing Photoreactive Species	01
	IV-H-3 A New Optical Doping Method toward Molecular Electronics	02
	IV-H-4 Photochemical Method of Device Fabrication Starting from Molecular Crystals	02
	IV-H-5 Photochemical Control of Dark Conductivity	
	—A New Approach to Devices Based on Molecular Crystals	02
	IV-H-6 Molecular Unit Based on Metal Phthalocyanine; Designed for Molecular Electronics1	02

IV-H-7 Anisotropic Giant Magnetoresistance Originating from the π -d Interaction	
in a Molecule	
IV-H-8 Phthalocyanine-Pphthalocyanine Salt Crystal: A Unique Assembly Design	
IV-H-9 Physical Properties of Electrically Conducting and Stable Molecular Neutral Radical Conducting and Stable Molecular Radical Conducting and Stable Radical Conducting and Stab	al
Solid [Co(2,3-Nc)(CN) ₂]CH ₃ CN (2,3-Nc = 2,3-Naphthalocyanine)	103
in a One-dimensional Conductor, $TPP[Co(Pc)(CN)_2]_2$	104
IV-H-11 Structural, Electrical and Magnetic Properties of α -(ET) ₇ [MnCl ₄] ₂ ·(1,1,2-C ₂ H ₃ Cl ₅	10 4
(ET = bis(ethylenedithio)tetrathiafulvalene)	
IV-H-12 New Binuclear Copper Complexes [(9S3)Cu(CN)Cu(9S3)] X_n	
$(X = BF_4, n = 1; X = TCNQ, n = 2)$ (9S3 = 1,4,7-trithiacyclononane):	
Syntheses, Crystal Structures and Magnetic Properties	104
IV-H-13 Crystal Design of Cation-Radical Salts Based on the Supramolecular Self-Organiz	zing
Arrangement of Mellitate Anions	105
IV-H-14 A Helical π -Radical Cation Column in the Double Helix of Mellitate Anions	105
IV-H-15 Network Formation of Mellitate Anions ($[C_6(COO)_6H_{6-n}]^{n-}$) in the Salts	100
with Piperidinium Derivatives and <i>ο</i> -Phenylenediammonium	100 107
IV-I Charge and Spin Dynamics of Organic Conductors	107 107
IV-I-2 Coherent-Incoherent Crossover Behavior of Electron on κ-(BEDT-TTF) ₂ Ag(CN) ₂ -I	
IV-I-3 Charge Ordering State on (BEDT-TTF) ₃ Cl ₂ ·2H ₂ O	
RESEARCH ACTIVITIES V	109
Description of a Chamber of Malacalan Calaca	
Department of Applied Molecular Science	
V-A Molecular Design and Functions of Photoactive	100
and Spin-Active Supramolecular Assemblies	
V-A-1 Molecular Design of Light-Harvesting Americae V-B Bioinorganic Chemistry and Structural Biology of Heme Proteins	109 110
V-B-1 Proton Transfer at Helium Temperatures during Dioxygen Activation	110
by Heme Monooxygenases	110
V-B-2 Roles of Distal Asp in Heme Oxygenase from Corynebacterium diphtheriae, HmuO	
A Water-Driven Oxygen Activation Mechanism	110
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	on110
V-C Pro-Oxidants-Induced Iron Release from the Fe-S Cluster of Mitochondrial Aconitase	
and Its Prevention by Flataxin	111
V-C-1 Reversible Redox-Dependent Modulation of Mitochondrial Aconitase and Proteolytic Activity during <i>In Vivo</i> Cardiac Ischemia/Reperfusion	111
V-D Quantum Emissions from Solid in Femtosecond Intense Laser Field and Its Application	111
to Dynamic Imaging	
V-D-1 Picosecond Time-Resolved X-Ray Diffraction from a Laser-Shocked Germanium C	
over Hugoniot Elastic Limit	112
V-D-2 Enhanced Generation of Fast Protons from a Polymer-Coated Metal Foil	
by a Femtosecond Intense Laser Field	112
V-D-3 Electron Imaging of Charge Separated Field on a Copper Film Induced	
by Femtoseond Laser Irradiation	112
RESEARCH ACTIVITIES VI	113
RESEARCH ACTIVITIES VI	113
Department of Vacuum UV Photoscience	
VI-A Electronic Structure and Decay Mechanism of Inner-Shell Excited Molecules	113
VI-A-1 Development of a Transmission-Grating Spectrometer for Soft-X-Ray Emission St	
VI-A-2 Application of R Matrix/MQDT Method to both Valence and Core Excitations in N	VO113
VI-B Soft X-Ray Photoelectron-Photoabsorption Spectroscopy and Electronic Structure	
of Molecular Solids and Clusters	114
VI-B-1 Photoionization of Small Krypton Clusters in the Kr 3d Regime:	114
Evidence for Site-Specific Photoemission	114 ands
—Molecular Alignment through Vibronic Coupling	
VI-C Ultrafast Dynamics of Molecules in Intense Laser Fields	114 115
VI-C-1 Probing the Ultrafast Nuclear Motion in CS_2^{2+} in Intense Laser Fields	 115
VI-C-2 Concerted and Sequential Coulomb Explosion Processes of N ₂ O in Intense Laser F	
by Coincidence Momentum Imaging	

VI-C-3 Development of an Intense	Sub-10fs Laser Source
with a Hollow Fiber/Chirped Min	rror Compressor11
VI-D Synchrotron Radiation Stimulated	Surface Reaction and Nanoscience11
VI-D-1 Synchrotron Radiation Indu	ced Si–H Dissociation on H-Si(111)–1×1 Surfaces
Studied by In-Situ Monitoring in	the Undulator-STM System11
VI-D-2 Giant Vesicle Fusion on the	Microelectrodes Fabricated by Femto-Second Laser Ablation
Followed by Synchrotron Radiat	ion Etching11
	ration Spectroscopy11
VI-E-1 Orientation of Avidin Molecular	cules Immobilized
on the COOH-Modified SiO ₂ /Si(100) Surface11
VI-E-2 Hydrogen-Atom-Induced O	xidation Reaction on Water-Terminated Si Surface,
	retical Study11
	f Bio-Functional Materials on Silicon Surfaces11
VI-F-1 Fabrication of Avidin Single	Molecular Layer on Silicon Oxide Surfaces and Formation
	ranes11
	s on OH-Density-Controlled Silicon Dioxide Surfaces11
	mation by the Vesicle Fusion Induced by the Vesicle-Surface
Electrostatic Attractive Interaction	on12
VI-F-4 The Current Noise Characte	ristic of a Single Ion Channel12
VI-F-5 A New Type of Fluorescence	e Recovery After Photobleaching Apparatus
	ments of UV Lamp and 560 nm Laser12
VI-G Photoionization and Photodissocia	tion Dynamics
Studied by Electron and Fluorescence	e Spectroscopy12
VI-G-1 Photofragmentation Mechan	isms of H ₂ O Studied by Ultraviolet Dispersed Spectroscopy -12
VI-H Extreme UV Photoionization Stud	ies of Fullerenes by Using a Grazing-Incidence
Windocaromator and High-Temperat	ure Mass Spectrometer12
	Cross Section of C ₆₀ in the Extreme Ultraviolet12 n Valence Ionization12
VI-H-3 Photofragmentation of C_{60} VI-H-3 Photofragmentation of C_{60}	
Statistical Analysis on the Annea	rance Energies of C_{60-2n}^{z+} $(n \ge 1, z = 1-3)$ 12
VI-H-4 Fragmentation Mechanism	of Highly Excited C_{70} Cations in the Extreme Ultraviolet12
VI-H-5 $4d \rightarrow 4f$ Dipole Resonance	of the Metal Atom
Encapsulated in a Fullerene Cage	e: Ce@C ₈₂ 12
VI-H-6 Photoion Yield Curves of D	y@C ₈₂ in the Vacuum UV Region12
VI-H-7 $4d$ – $4f$ Dipole Resonance of	the Pr Atom in an Endohedral Metallofullerene, $Pr@C_{82}$ 12
VI-I Kinetic Energy Analysis of the Frag	gment ions Produced from Fullerenes12
VI–I–1 Development of the Photofr	agment Imaging Apparatus
to Measure Scattering Distribution	ons of the C_{60-2n}^{z+} and C_{70-2n}^{z+} Fragments
Produced by Dissociative Photoi	onization of C_{60} and C_{70} 12
	100
RESEARCH ACTIVITIES VII	129
Department of Computational	Molocular Science
Department of Computational I	of Systems in Condensed Phase12
	ational Relaxation Mechanism in Condensed Phase
	ssical Molecular Dynamics: I. A Test of IBC Model Solute in Nonpolar Solvent at High Density12
	ational Relaxation Mechanism in Condensed Phase
	ssical Molecular Dynamics: II. Non-Collisional Mechanism
for the Relayation of a Polar Sol	ite in Supercritical Water12
	ssical Complex Systems13
	Dynamics Study of Dynamic Structure Factor and Dispersion
	quid and Supercritical Water13
VII-C Development of Simulation Algor	ithms for Quantum Many-Body Systems13
	onyl Sulfide Molecules in Superfluid Helium Clusters:
A Path Integral Hybrid Monte Co	arlo Study13
	ation Spectroscopy13
VII-D-1 Improved Computation of	Sum Frequency Generation Spectrum of Water Surface13
VII-E Theory of Mass Transfer Kinetics	at Liquid-Vapor Interfaces13
VII-E-1 Mass Accommodation Coe	fficient of Water13
	Structure and Dynamics of Electronically Excited States -13
VII-F-1 Encapsulation of Hydrogen	Atoms by Fullerenes and Carbon Nanotubes
with the Use of Nonadiabatic Tra	ansition13
VII-F-2 Ab Initio Calculated Struct	ures of Conformers for 1,3-Dimethoxy-p-tert-Butylcalix[4]
Crown-5-Ether Complexed with	Potassium Cation13

	Probabilities for the $\tilde{A}^2A_1-\tilde{X}^2B_1$ System of H_2O^+ and D_2O^+
	Factors Based on Global Potential Energy Surfaces132
VII-F-4 Analysis of the Ultravi	ed Nitrous Oxide Specie Using 3D Wavepacket Propagation132
VII-F-5 Theoretical Study of the	
for the H Atom-Induced Wa	ter-Terminated Si Surface $2H+H_2O/Si(100)-(2\times1)$ 133
RESEARCH ACTIVITIES VI	II135
Coordination Chemistry Lal	
VIII-A Reduction of CO ₂ and Oxida	ation of Organic Molecules Aiming at Energy Conversion
	lectricity135
VIII-A-1 Redox Behavior of N	ew Ru-Dioxolene-Ammine Complexes and Catalytic Activity
VIII A 2 Equilibrium of Low	dation of Alcohol under Mild Conditions135
Controlled by the Depart Ab	and High-Spin States of Ni(II) Complexes
VIII A 2 A Platinum Puthaniu	ility of the Bidentate Ligands135 m Dinuclear Complex Bridged by Bis(terpyridyl)xanthene136
	High-Valent Rhenium Complex on an Indium-Doped Tin-Oxide
	tic Activity of a <i>trans</i> -Dioxorhenium(V) Complex
in Electrochemical Oxidatio	n of Alcohols136
	and Electrochemical Properties of Ruthenium(II) Complexes
Bearing 2.6-Bis(2-naphthyri	dyl)pyridine136
VIII-A-6 Synthesis, Structures	and Electrochemical Properties of Ruthenium (II) Complexes
Bearing Bidentate 1,8-Naph	
and Terpyridine Analogous	(N,N,C)-Tridentate Ligands136
VIII-A-7 Synthesis and Electro	schemical Properties of Bis(bipyridine)ruthenium(II) Complexes
	dinylidene Ligands Induced by Cyclometalation of N'-Methylated
Bipyridinium Analogs	137
VIII-A-8 Electronic Structural	Changes Between Nickel(II)-Semiquinonato
	states Driven by Chemical and Physical Perturbation137
	Structures of $[W(3,6-Dichloro-1,2-Benzenedithiolate)_3]^{n-}$ $(n=1,2)$
on the Oxidation Number an	Benzenedithiolate) ₃] ²⁻ : Dependence of the Coordination Geometry
in Trigonal Prismatic and O	ctahedral Structures137
	n(VI) and Mono-oxo-Molybdenum(IV) Complexes
	c Dithiolene Ligands: New Models with Weakened Mo=O Bond
Characters for the Arsenite (Oxidase Active Site137
VIII-A-11 Electrochemical Hyd	drogenation of $[Ru(bpv)_2(napv-kN)(CO)]^{2+}$:
Inhibition of Reductive Ru–	CO Bond Cleavage by a Ruthenacycle138
VIII-A-12 Stabilization and De	estabilization of the Ru–CO Bond
	-onato (bpyO)-Localized Redox Reaction
	PF ₆)138
VIII-B Coordination Chemistry of S	Sterically Hindered Ligands and Multidentate Ligands,
and Activation of Small Molecule	28
VIII-B-1 Synthesis of a vanadi	ium(III) Tris(arylthiolato) Complex and Its Reactions with Azide
of an Azo N-N Pond	ation of a Sulfenamide Complex <i>via</i> Cleavage139
	um Complexes of Preorganized Tripodal Triaryloxide Ligands139
	of the Homo- and Heterometallic Clusters141
	² -Diamido/ η^6 -Naphthalene Complex Featuring a Coordinatively
	asic (η ⁵ -C ₅ Me ₅)Ru Diamide Fragment141
VIII-C-2 Dinuclear Ruthenium	(II) Catecholato and 2,3-Naphthalenediolato Complexes
Featuring κ^2 -Diaryloxo/ η^6 -A	Arene Coordination Mode141
VIII-D Modification of Myoglobin b	y Replacing the Native Heme with Metalloporphyrinoids143
VIII-D-1 Ligand Binding Prope	erties of Myoglobin Reconstituted with Iron Porphycene:
Unusual O ₂ Binding Selective	vity against CO Binding143
VIII-D-2 Unusual Ligand Disc	rimination by a Myoglobin Reconstituted with a Hydrophobic
	143
	xidase Activity of Myoglobin Reconstituted with Iron Porphycene:
	te to the Reaction of Ferric Myoglobin with Hydrogen Peroxide143
VIII-D-4 Preparation and O ₂ B	inding Study of Myoglobin Having a Cobalt Porphycene144

VIII-	E Synthesis of Transition Metal Complexes Containing a Novel Metal-Silicon	
an	d Metal-Gallium Bonding	145
	VIII-E-1 Synthesis of a Cofacial Schiff-Base Dimanganese(III) Complex	
	for Asymmetric Catalytic Oxidation of Sulfides	145
	VIII-E-2 Synthesis and Structure of a Base-Stabilized Silyl(silylene)tantalum Complex	145
	VIII-E-3 Synthesis and Structures of the First Titanium(IV) Complexes	
	with Cyclic Tetrasiloxide Ligands: Incomplete and Complete Cage Titanosiloxanes	145
VIII-	F Syntheses, Structures, and Reactivities of Multinuclear Transition Metal Complexes	
wi	th $ {O}$ - and N -Donor Ligands	147
	VIII-F-1 A Cyanamido-Bridged Diiridium Complex:	
	A Reactive Building Block for Polynuclear Cyanamido Complexes	147
	VIII-F-2 Synthesis, Structures, and Solution Behavior of Di- and Trinuclear	
	Titanium(IV)-Cyclophosphato Complexes	147
VIII-	G Organometallic Chemistry: Synthesis, Characterization, and Catalysts	148
	VIII-G-1 Living Polymerization of 1-Hexene Catalyzed by Half-Metallocene Dimethyl	
	Complexes of Hafnium with Bidentate N-Substituted Iminometylpyrrolyl Ligands	148
	VIII-G-2 Unique Preferential Conformation and Movement of Ru(acac) ₂ Fragment(s)	
	Coordinated in an η^4 -s-trans Fashion to All Diene Unit(s) of α , ω -Diphenylpolyenes	148
	VIII-G-3 A Topological Isomer of Ferrocene: Theoretical Approach	1.10
	for Transition Metal Complexes with Conjugated All Trans Cyclodecapentaene	148
VIII-	H Development of Metal-Conjugated Multi-Electron Redox Systems	4 = 0
in	Metal-Dixolene Complexes and Activation of Water Ligand	150
	VIII-H-1 Synthesis of a Ru-OH ₂ Complex Bearing a Ferrocene-Attached Catecholato Ligand	4.50
	and Its Spontaneous Proton Release	150
DECEAL	RCH ACTIVITIES IX	151
RESEAR	CH ACTIVITIES IX	191
Dagaa	uch Conton for Molocular Scale Nanagaianae	
	rch Center for Molecular-Scale Nanoscience	151
IX-A	Nano-Science and Nano-Technology toward Molecular Scale Electronics	
	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	150
	Exhibiting Photoresponsive Properties	152
	IX-A-4 Simple Preparation Method for Supramolecular Porphyrin Arrays on Mica Using Air/Water Interface	150
	IX-A-5 Novel Photochemical Synthesis of Pentacene and Its Derivatives	
		132
	IX-A-6 Porphyrin Molecules Working as Nanodevice on Single-Walled Carbon Nanotube Wiring	152
	IX-A-7 Electronic Properties of Single-Walled Carbon Nanotube/Porphyrin Polymer Complex	133
	Measured by Point-Contact Current Imaging Atomic Force Microscopy	152
		133
	IX-A-8 Preparation of Very Reactive Thiol-Protected Gold Nanoparticles: Revisiting the Brust-Schiffrin Method	153
IV D	Development of Organic Semiconductors for Molecular Thin-Film Devices	
IA-D	IV D 1 Organia Thin Film Transistors with High Floatron Mobility	
	Based on Perfluoropentacene	155
	IX-B-2 Organic Light-Emitting Diodes Using Multifunctional Phosphorescent	133
	with Iridium-Complex Core and Charge-Transporting Dendrons	155
IV-C	Field-Effect Transistors with Organic Semiconductors	155 15 6
IX-C	IX-C-1 Preparation of Organic Light-Emitting Field-Effect Transistors	150
	with Asymmetric Electrodes	156
	IX-C-2 Field-Effect Transistors Based on Single-Crystalline Wires	150
	of Bis-(1, 2, 5-Thiadiazolo)-p-Quinobis(1, 3-Dithiole)	156
IV-D	Molecular Assemblies on Silicon Surfaces via Silicon–Carbon Covalent Bonds	150 157
IA-D	IX-D-1 Characterization of Molecular Assemblies on Silicon Surfaces	137
	by Attenuated Total Reflectance Infrared Spectroscopy	157
IV-F	Low Temperature Scanning Tunneling Microscopy and Spectroscopy of Organic Molecules	157
	Metal Surfaces	
OI	IX-E-1 Scanning Tunneling Microscopy and Spectroscopy of Phthalocyanine Molecules	13/
	on Metal Surfaces	157
IV E	Ratchet Motions of a Droplet Caused by Electrochemical Reaction of Monolayers	13/ 150
17-1	IX-F-1 Electrochemically Generated Wetting Gradient and Its Application	130
	for the Transport of Droplets	159
	IX-F-2 Transport of a Droplet by Directional Deformations with Asymmetric Electrode	150
	11.1.2 Transport of a Diopict by Directional Deformations with Asymmetric Electione	-133

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	1.61
Polymer-Supported Nanopalladium Catalyst	-101
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	-101 . -162
IX-I-1 Gold Nanoparticles Stabilized by Tripod Thioether Oligomers:	-102
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	
IX-N-1 The Electronic Structure and Femtosecond Electron Transfer Dynamics at Noble Metal/tris-(8-hydroxyquinoline) Aluminum Interfaces	
at Noble Metal/tris-(8-hydroxyquinoline) Aluminum Interfaces	-166
IX-O Chemistry of One-Dimensional Nano-Surface Compounds	1.0
Studied by Scanning Tunneling Microscopy	-167
IX-O-1 In-Situ Observation of CO Oxidation on Ag(110)(2×1)-O by Scanning Tunneling	1.77
Microscopy: Structural Fluctuation and Catalytic Activity	-10/
IX-P Structures, Stabilities and Physicochemical Properties of Organometallic Hybrid Clusters - IX-P-1 Glutathione-Protected Gold Clusters Revisited: Bridging the Gap	-100
between Gold(I)-Thiolate Complexes and Thiolate-Protected Gold Nanocrystals	168
IX-P-2 Large-Scale Synthesis of Thiolated Au ₂₅ Clusters <i>via</i> Ligand Exchange Reactions	-100
of Phosphine-Stabilized Au ₁₁ Clusters	168
IX-P-3 Subnanometer-Sized Gold Clusters with Dual Molecular Receptors:	100
Synthesis and Assembly in One-Dimensional Arrangements	-169
IX-P-4 Size-Specific Catalytic Activity of Polymer-Stabilized Gold Nanoclusters	10)
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	
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
TYPO (O) O III ' N ' I I I I I D '	
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	
IX-R-6 Observation of a Molecular Frame $(e,2e)$ Cross Section: An $(e,2e+M)$ Triple Coincidence	e 170
Study on H_2	172
1A-R-1 (e,2e) and (e,3-1e) studies on Double Processes of He at Large Momentum Transfer	-1/3

	IX-R-8 Electron Momentum Spectroscopy of the HOMO of Acetone	173
	IV D O (2 1) D · · · · · · · · · · · · · · · · · ·	
	The Plane-Wave Second Born Approximation	-174
	IX-R-10 Binary (e,2e) Study on Xe: Momentum Profile for the 4d Orbital Revisited	-174
	IX-R-11 Binary (e,2e) Study on Inner Shell Orbitals of Ar and Xe	
	IX-R-12 Construction of a New $(e,2e+M)$ Apparatus for Complete Imaging	
	of Molecular Orbitals	174
IX-S	Electronic Structure and Collision Dynamics of Atoms and Molecules	
St	udied by Photon Impact	
	IX-S-1 Inner-Shell Photoelectron Angular Distributions from Fixed-in-Space OCS Molecules	175
	IX-S-2 Coincidence Velocity Imaging Apparatus for the Study of Angular Correlations	177
	between Photoelectrons and Photofragments	-175
	IX-S-3 Non-Dipole Effects in the Angular Distribution of Photoelectrons from the K-Shell of N ₂ Molecule	175
	IX-S-4 Direct Observation of a Symmetry Lowering in Core-Electron Ionization	-1/3
	for Highly Symmetric Molecules	175
IX-T	Study of Electronic Structure of Organic Thin Film and Organic/Inorganic Interface	
1/1-1	IX-T-1 Deep Insight into a Valence Hole in Organic Semiconductors:	-170
	High-Resolution Ultraviolet Photoemission Study	176
	IX-T-2 UPS Fine Structures of Highest Occupied Band	
	in Vanadyl-Phthalocyanine Ultrathin Film	-176
	IX-T-3 Fine Structure of the Highest Occupied Band in OTi-Phthalocyanine Monolayer	
	IX-T-4 Hole/Vibration Coupling of the Highest Occupied Band in Pentacene Thin Film	176
	IX-T-5 Quantitative Analysis of Photoelectron Angular Distribution of a Single Domain Organic	2
	Monolayer Film: NTCDA on GeS(001)	177
	IX-T-6 UPS Study of VUV-Photodegradation of Polytetrafluoroethylene (PTFE) Ultrathin Film	
	by Using Synchrotron Radiation	177
	IX-T-7 Site-Specific Ion Desorption of Fluorinated Phthalocyanine Studied with Electron-Ion	177
	Coincidence Spectroscopy	1//
	of C ₆₀ -Functionalized 11-Amino-1-Undecane Thiol Self-Assembled Monolayer:	
	of C ₆₀ -1 unctionalized 11-Annio-1-Ordecane Thorsen-Assembled Worldayer.	
	Molecular Orientation and Evidence for C_{co} Aggregation	177
	Molecular Orientation and Evidence for C ₆₀ Aggregation	177
UVSO		177
UVSO IX-U	R Facility	
UVSO IX-U	R Facility Development of the UVSOR Light Source	-179
IX-U	PR Facility Development of the UVSOR Light Source	179 179 179
IX-U	PR Facility Development of the UVSOR Light Source	179 179 179 179
IX-U	Processor of the UVSOR Light Source	179 179 179 179
IX-U	Development of the UVSOR Light Source	179 179 179 179 -179
IX-U	Processor of the UVSOR Light Source	179 179 179 179 179
IX-U	Pevelopment of the UVSOR Light Source	179 179 179 179 179 180
IX-U	Development of the UVSOR Light Source	179 179 179 179 179 180
IX-U	Pevelopment of the UVSOR Light Source	179 179 179 179 179 180 180
IX-U	Development of the UVSOR Light Source	179 179 179 179 179 180 180
IX-U	Development of the UVSOR Light Source	179 179 179 179 179 180 180
IX-U	Development of the UVSOR Light Source	179 179 179 179 180 180 180
IX-U	Pevelopment of the UVSOR Light Source	179 179 179 179 180 180 180
IX-U	Pevelopment of the UVSOR Light Source	179 179 179 179 180 180 180 180
IX-U	Pevelopment of the UVSOR Light Source	179 179 179 179 180 180 180 180
IX-U	Pevelopment of the UVSOR Light Source IX-U-1 Successful Commissioning of New RF Cavity IX-U-2 Ion Trapping Phenomena at UVSOR-II 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 ⁻¹ np Resonance IX-V-4 Coincidence Auger Spectroscopy IX-V-5 Collision Dynamics of the Kr ⁸⁺ + N ₂ 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-Eu ₈ Ga ₁₆ Ge ₃₀ IX-V-8 Influence of Cage Distortions on the Electronic Structure and Optical Properties of Ba ₆ Ge ₂₅ IX-V-9 Indirect and Direct Energy Gaps in Kondo Semiconductor YbB ₁₂	179 179 179 179 180 180 180 180 181
IX-U	Pevelopment of the UVSOR Light Source IX-U-1 Successful Commissioning of New RF Cavity IX-U-2 Ion Trapping Phenomena at UVSOR-II 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 ⁻¹ np Resonance IX-V-4 Coincidence Auger Spectroscopy IX-V-5 Collision Dynamics of the Kr ⁸⁺ + N ₂ 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-Eu ₈ Ga ₁₆ Ge ₃₀ IX-V-8 Influence of Cage Distortions on the Electronic Structure and Optical Properties of Ba ₆ Ge ₂₅ IX-V-9 Indirect and Direct Energy Gaps in Kondo Semiconductor YbB ₁₂ IX-V-10 Kondo Ground States and Non-Fermi-Liquid Behavior in CeNi _{1-x} Co _x Ge ₂	179 179 179 179 180 180 180 180 181
IX-U	Pevelopment of the UVSOR Light Source IX-U-1 Successful Commissioning of New RF Cavity IX-U-2 Ion Trapping Phenomena at UVSOR-II 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 ⁻¹ np Resonance IX-V-4 Coincidence Auger Spectroscopy IX-V-5 Collision Dynamics of the Kr ⁸⁺ + N ₂ 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-Eu ₈ Ga ₁₆ Ge ₃₀ IX-V-8 Influence of Cage Distortions on the Electronic Structure and Optical Properties of Ba ₆ Ge ₂₅ IX-V-9 Indirect and Direct Energy Gaps in Kondo Semiconductor YbB ₁₂ IX-V-10 Kondo Ground States and Non-Fermi-Liquid Behavior in CeNi _{1-x} Co _x Ge ₂ IX-V-11 Infrared Spectroscopy under Multiextreme Conditions: Direct Observation of Pseudogap Formation and Collapse in CeSb	179 179 179 179 180 180 180 181 181
IX-U	Pevelopment of the UVSOR Light Source IX-U-1 Successful Commissioning of New RF Cavity IX-U-2 Ion Trapping Phenomena at UVSOR-II 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 ⁻¹ np Resonance IX-V-4 Coincidence Auger Spectroscopy IX-V-5 Collision Dynamics of the Kr ⁸⁺ + N ₂ 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-Eu ₈ Ga ₁₆ Ge ₃₀ IX-V-8 Influence of Cage Distortions on the Electronic Structure and Optical Properties of Ba ₆ Ge ₂₅ IX-V-9 Indirect and Direct Energy Gaps in Kondo Semiconductor YbB ₁₂ IX-V-10 Kondo Ground States and Non-Fermi-Liquid Behavior in CeNi _{1-x} Co _x Ge ₂ IX-V-11 Infrared Spectroscopy under Multiextreme Conditions: Direct Observation of Pseudogap Formation and Collapse in CeSb IX-V-12 Infrared Study on CeSb under High Pressures	179 179 179 179 180 180 180 181 181 181
IX-U	Percentage of the UVSOR Light Source IX-U-1 Successful Commissioning of New RF Cavity IX-U-2 Ion Trapping Phenomena at UVSOR-II 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 ⁻¹ np Resonance IX-V-4 Coincidence Auger Spectroscopy IX-V-5 Collision Dynamics of the Kr ⁸⁺ + 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-Eu ₈ Ga ₁₆ Ge ₃₀ IX-V-8 Influence of Cage Distortions on the Electronic Structure and Optical Properties of Ba ₆ Ge ₂₅ IX-V-9 Indirect and Direct Energy Gaps in Kondo Semiconductor YbB ₁₂ IX-V-10 Kondo Ground States and Non-Fermi-Liquid Behavior in CeNi _{1-x} Co _x Ge ₂ IX-V-11 Infrared Spectroscopy under Multiextreme 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 Zr ₅₅ Al ₁₀ Cu ₃₀ Ni ₅	179 179 179 179 180 180 180 181 181 181
IX-U	Provelopment of the UVSOR Light Source IX-U-1 Successful Commissioning of New RF Cavity IX-U-2 Ion Trapping Phenomena at UVSOR-II 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 ⁻¹ np Resonance IX-V-4 Coincidence Auger Spectroscopy IX-V-5 Collision Dynamics of the Kr ⁸⁺ + N ₂ 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-Eu ₈ Ga ₁₆ Ge ₃₀ IX-V-8 Influence of Cage Distortions on the Electronic Structure and Optical Properties of Ba ₆ Ge ₂₅ IX-V-9 Indirect and Direct Energy Gaps in Kondo Semiconductor YbB ₁₂ IX-V-10 Kondo Ground States and Non-Fermi-Liquid Behavior in CeNi _{1-x} Co _x Ge ₂ IX-V-11 Infrared Spectroscopy under Multiextreme 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 Zr ₅₅ Al ₁₀ Cu ₃₀ Ni ₅ IX-V-14 Carrier-Induced Infrared Magnetic Circular Dichroism	179 179 179 179 179 180 180 180 181 181 181 181 182 182
IX-U	Development of the UVSOR Light Source	179 179 179 179 179 180 180 180 181 181 181 181 182 182
IX-U	Development of the UVSOR Light Source	179 179 179 179 179 180 180 180 181 181 181 181 182 182 182
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 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 ⁻¹ np Resonance IX-V-4 Coincidence Auger Spectroscopy IX-V-5 Collision Dynamics of the Kr ⁸⁺ + N ₂ 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-Eu ₈ Ga ₁₆ Ge ₃₀ IX-V-8 Influence of Cage Distortions on the Electronic Structure and Optical Properties of Ba ₆ Ge ₂₅ IX-V-9 Indirect and Direct Energy Gaps in Kondo Semiconductor YbB ₁₂ IX-V-10 Kondo Ground States and Non-Fermi-Liquid Behavior in CeNi _{1-x} Co _x Ge ₂ IX-V-11 Infrared Spectroscopy under Multiextreme 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 Zr ₅₅ Al ₁₀ Cu ₃₀ Ni ₅ IX-V-14 Carrier-Induced Infrared Magnetic Circular Dichroism in the Magnetoresistive Pyrochlore Tl ₂ Mn ₂ O ₇ IX-V-15 Magnetic Ordering in Frustrated Ce ₅ Ni ₂ Si ₃ IX-V-16 Features of Fluorescence Spectra of Polyethylene Terephthalate Films	179 179 179 179 179 180 180 180 181 181 181 181 182 182 182
IX-U	Development of the UVSOR Light Source	179 179 179 179 179 180 180 180 181 181 181 181 182 182 182
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 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 ⁻¹ np Resonance IX-V-4 Coincidence Auger Spectroscopy IX-V-5 Collision Dynamics of the Kr ⁸⁺ + N ₂ 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-Eu ₈ Ga ₁₆ Ge ₃₀ IX-V-8 Influence of Cage Distortions on the Electronic Structure and Optical Properties of Ba ₆ Ge ₂₅ IX-V-9 Indirect and Direct Energy Gaps in Kondo Semiconductor YbB ₁₂ IX-V-10 Kondo Ground States and Non-Fermi-Liquid Behavior in CeNi _{1-x} Co _x Ge ₂ IX-V-11 Infrared Spectroscopy under Multiextreme 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 Zr ₅₅ Al ₁₀ Cu ₃₀ Ni ₅ IX-V-14 Carrier-Induced Infrared Magnetic Circular Dichroism in the Magnetoresistive Pyrochlore Tl ₂ Mn ₂ O ₇ IX-V-15 Magnetic Ordering in Frustrated Ce ₅ Ni ₂ Si ₃ IX-V-16 Features of Fluorescence Spectra of Polyethylene Terephthalate Films	179179179179179180180180181181181181182182182183

	ch Center for Molecular Science	
	nents and Researches of New Laser Materials	184
IX-W-1 (Growth and Scintillation Properties of Yb Doped Aluminate, Vanadate	
and Si	licate Single Crystals	184
IX-W-2 (Onset Detection of Solid-State Phase Transition in Estrogen-Like Chemical	
via Te	rahertz Transmission Spectroscopy	184
IX-W-3 I	Design Principle of Wide-Gap Fluoride Hetero-Structures	
for De	ep Ültraviolet Optical Devices	184
IX-W-4 7	Cerahertz Time-Domain Spectroscopy of Amino Acids and Polypeptides	184
IX-X Developm	ent and Research of Advanced Tunable Solid State Lasers	180
IX-X-1 S	pectroscopic Properties of Yb:GdVO ₄ Single Crystal: Stark Levels, Selection Rules,	
	larized Cross Sections	186
of Nd:	pectroscopic Properties of All-Ceramic Composite with Layer-by-Layer Y ₃ Al ₅ O ₁₂ and Nd:Y ₃ ScAl ₄ O ₁₂	186
IX-X-3 H	lybrid Process for Measurement of Spectroscopic Properties of Nd:GdVO ₄	187
IV-X-4 A	bsorption, Emission Spectrum Properties and Efficient Laser Performances	
of Yb:	Y ₃ ScAl ₄ O ₁₂ Ceramics	187
IX-X-5 P	assive Mode Locking of a Mixed Garnet Yb:Y ₃ ScAl ₄ O ₁₂ Ceramic Laser	187
IX-X-6 H	ligh-Power Operation of Diode Edge-Pumped, Glue-Bonded, Composite Yb:Y ₃ Al ₅ O ₁₂ chip Laser with Ceramic, Undoped YAG Pump Light-Guide	
	ontinuous-Wave Deep Blue Generation in a Periodically Poled MgO:LiNbO ₃ Crystal	
by Sin	gle-Pass Frequency Doubling of a 912-nm Nd:GdVO ₄ Laser	188
IX-X-8 C	ontinuous-Wave Ultraviolet Generation at 354-nm in a Periodically Poled MgO:LiNbO ₃ quency Tripling of a Diode End-Pumped Nd:GdVO ₄ Microlaser	
IX-X-9 H	ligh-Power Continuous-Wave Intracavity Frequency-Doubled Nd:GdVO ₄ -LBO Laser	
under	Diode Pumping into the Emitting Level	188
	Deep Blue Generation at 456 nm in a Periodically Poled MgO:LiNbO ₃ Ridge-Type	
	guide by Single-Pass Frequency Doubling of a Nd:GdVO ₄ 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:GdVO ₄ Laser	189
	Highly Efficient New Pumping Configuration for Microchip Solid State Laser	189
IX-X-14 Period	High Energy Quasi-Phase-Matched Optical Parametric Oscillation in a 3-mm-Thick ically Poled MgO:LiNbO ₃ Device	189
Equipment De	evelopment Center	
IX-Y Developm	ent of New Instruments and Experimental Devices	190
IX-Y-1 D	evelopment of a High-Precision Slit Blade for the Transmission-Grating Spectrometer -	190
IX-Y-2 M	Manufacture of Glass Microreactor Chips	191
IX-Y-3 N	ficro Processing by a Femto-Second Laser	191
	evelopment of Electrical Control System of Fluorescence Recovery after Photobleaching	
	atus Using Semiconductor Laser for Illumination	
Safety Office		
	ent of Novel Heterocyclic Compounds and Their Molecular Assemblies	
	d Materials	193
	Tolecular Arrangement in the Cocrystals of 1,1',3,3'-Tetramethyl-2,2'-bi-1 <i>H</i> -imidazolium	
Ris(tet	raphenylborate) with Ketone, Aldehyde, and Nitrile as Guest Molecules	193
	facrocyclic and Acyclic Bis(2,5-diphenyl-1,3,4-oxadiazole)s	.) -
	lectron-Transporting and Hole-Blocking Ability	
in Oro	anic Electroluminescent Devices	193
IX-7-3 S	ynthesis, Characterization and FET Properties of Novel Dithazolylbenzothiadiazole	. , .
	tives	193
KESEAKCH .	ACTIVITIES X	
Okazaki Insti	tute for Integrative Bioscience	
	ecule Physiology	195
X-A-1 O	ne Rotary Mechanism for F ₁ -ATPase over ATP Concentrations	107
from N	Millimolar down to Nanomolar	195
X-A-2 A	ΓP-Driven Stepwise Rotation of F ₀ F ₁ -ATP Synthase	195
X-A-3 A	ctivation of Pausing F ₁ Motor by External Force	172

X-B	Bioinorganic Chemistry of Heme-Based Sensor Proteins	-197
	X-B-1 Spectroscopic and Redox Properties of a CooA Homologue	
	from Carboxydothermus 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	
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	100
	Related to the Oxygen Activation by Nonheme Iron Enzymes	-199
	X-D-2 Synthesis of Sterically Hidered Tris(4-imidazolyl)carbinol Ligands and their Copper(I)	100
	Complexes Related to Metalloenzymes	-199
	X-D-3 O ₂ - and H ₂ O ₂ -Dependent Verdoheme Degradation by Heme Oxygenase:	200
VE	Reaction Mechanisms and Potential Physiological Roles of the Dual Pathway Degradation	
A-E	Reaction Mechanism of Metalloenzymes related to Global Nitrogen Cycle	-200
	for Copper Nitrito Poduetose	200
VF	for Copper Nitrite ReductaseBiomolecular Science	-200 202
A-I	X-F-1 Resonance Raman Characterization of the P Intermediate in the Reaction of Bovine	-202
	Cytochrome c Oxidase	-202
	X-F-2 Core Structure of Amyloid Fibril Proposed from IR-Microscope Linear Dichroism	
	X-F-3 Activation of Heme-Regulated Eukaryotic Initiation Factor 2α Kinase (HRI) Activation	202
	by Nitric Oxide Is Induced by the Formation of a Five-Coordinate NO-Heme Complex:	
	Optical Absorption, Electron Spin Resonance and Resonance Raman Spectral Studies	-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	
	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 β ₂ -Microglobulin #21-31 Fragment	• • •
	Based on Vibrational Spectroscopy	-204
	X-F-9 Excited State Property of Hardly Photodissociable Heme-CO Adduct	205
	Studied by Time-Dependent Density Functional Theory	-205
	X-F-10 Mechanism for Transduction of the Ligand-Binding Signal in Heme-Based Gas Sensory	205
	Proteins Revealed by Resonance Raman SpectroscopyX-F-11 UV Resonance Raman Study of Model Complexes of the Cu _B Site	-203
	of Cytochrome c Oxidase	205
	X-F-12 Resonance Raman Investigation on the Specific Sensing Mechanism	-203
	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-15 Structural and Spectroscopic Characterization	200
	of (μ-Hydroxo or μ-Oxo)(μ-Peroxo)Diiron(III) Complexes: Models for Peroxo Intermediates	
	of Non-Heme Dilron Proteins Structural and Spectroscopic Characterization	
	of (μ-Hydroxo or μ-Oxo)(μ-Peroxo)Diiron	-206
	X-F-16 Axial Ligand Substituted Nonheme Fe ^{IV} =O complexes:	
	Observation of Near-UV LMCT Bands and Fe=O Raman Vibrations	
	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-18 Synthesis and Reactivity of a (μ-1,1-Hydroperoxo)(μ-Hydroxo)Dicopper(II) Complex:	• -
	Ligand Hydroxylation by a Bridging Hydroperoxo Ligand	-207
	X-F-19 Spectroscopic and Redox Properties of a CooA Homologue	20-
	from Carboxydothermus hydrogenoformans	-207
	X-F-20 Structural Diversities of Active Site in Clinical Azole-Bound Forms	200
	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
	of Algorithe Denythalase involved in Caroon-Minogen Triple Dond Symmesis	-208

X-F-22 Synthesis, Characterization, and Thermal Stability of New Mononuclear	
Hydrogenperoxocopper(II) Complexes with N ₃ O-Type Tripodal Ligands	
Bearing Hydrogen-Bonding Interaction Sites	208
X-F-23 Spectroscopic Characterization of the Isolated Heme-Bound PAS-B Domain of Neuro	nal
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-methyl)amine Tridentate Ligands	209
X-F-26 Resonance Raman and FT-IR Studies on Proximal and Distal Histidine Environment	
of Cytoglobin 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	212
RESEARCH FACILITIES	213
Research Center for Molecular-scale Nanoscience	213
UVSOR Facility	
Laser Research Center for Molecular Science	214
Equipment Development Center	214
Safety Office	214
Research Center for Computational Science	·Z14
SPECIAL RESEARCH PROJECTS	217
(a) Chemical Reaction Dynamics	⊿⊥ <i>1</i> 217
Folding Mechanism of Protein Molecules Studied by Generalized-Ensemble Algorithms	
Electronic Structure and Decay Mechanism of Inner-Shell Excited Molecules	
Computational Study of Quantum Dynamics of a Solute in Solution	217 217
Chemical Reactions at Surfaces and Nano-Structured Materials	217
Studied by Spatio-Temporally Resolved Spectroscopy	218
Towards Complete Imaging of Molecular Orbital Patterns:	210
Development of Molecular Frame $(e,2e)$ 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 -	
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	
Decay and Dissociation Dynamics of Core Excited Molecules	221
(c) Novel Materials Science	
Quantum Chemistry Calculations of Large Molecular Systems	
Theory for Equilibrium and Non-Equilibrium Properties of Low-Dimensional Molecular Mater	
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	
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	
Synthesis and Properties of Novel Chiral Organic-Inorganic Molecule-Based Magnets	
Design and Functions of Novel Soft Nanomaterials Based on Molecular Programming Giant Vesicle Fusion on Microelectrodes Fabricated by Femtosecond Laser Ablation	220
Followed by Synchrotron Radiation Etching	226
Reduction of CO ₂ and Oxidation of Organic Molecules Aiming at Reversible Conversion	220
between Chemical and Electrical Energies	227

(2) Research Symposia	235 236 236 237 241 245
(3) Cooperative Research	235 236 236 237
(3) Cooperative Research	235 236 236 237
(3) Cooperative Research	235 236 236
(3) Cooperative Research	235 236 236
(3) Cooperative Research(4) Use of Facility	235 236
(3) Cooperative Research	235
(2) Research Symposia	235
(A) D	
(1) Special Projects	233
JOINT STUDIES PROGRAMS	233
Molecular Science of Proteins Based on Vibrational Spectroscoy	
Molecular Mechanism of Metalloenzymes Related to Oxygen Activation and Denitrification Processes	231
Regulation of Biological Function by the Heme-Based Gas-Molecule Sensor Protein	
Development and Research of Advanced Tunable Solid State Lasers	
Developments and Researches of New Laser Materials	
Optical and Photoelectrical Studies on Fermiology of Strongly Correlated Electron S	
Structural Analyses of Multi-Domain Proteins by Use of Ultra-High Field NMR Spondagured at 920 MHz ¹ H Resonance FrequencyObservation of Intense Bursts of Terahertz Synchrotron Radiation at UVSOR-II	229
Tuning Catalytic Activities of Gold Clusters via Hybrization of Functional Molecule	
Synthesis of Buckybowls and Heterobuckybowls	229
as Basis of Chemical Energy Conversion Systems	229
Asymmetric Aquacatalysis with Polymeric Palladium Complexes	Complexes
Novel Pincer Complexes and Their Catalytic Properties	228
Tot organic Eight Emitting 2 to the	228
for Organic Light-Emitting Diodes	
Synthesis of Perfluorinated Fluorene Oligomers and Applications for Organic Light-Emitting Diodes	
Studies on Development of Molecules and the Device Fabrications for Molecular Scale Electronics	227

Abbreviations

IMS: Institute for Molecular Science SOKENDAI: The Graduate University for Advanced Studies