21COE:
"First Symposium of Fukui Institute for Fundamental Chemistry, Kyoto University"
November 19, 2003 in Fukui Institute for Fundamental Chemistry, Kyoto University

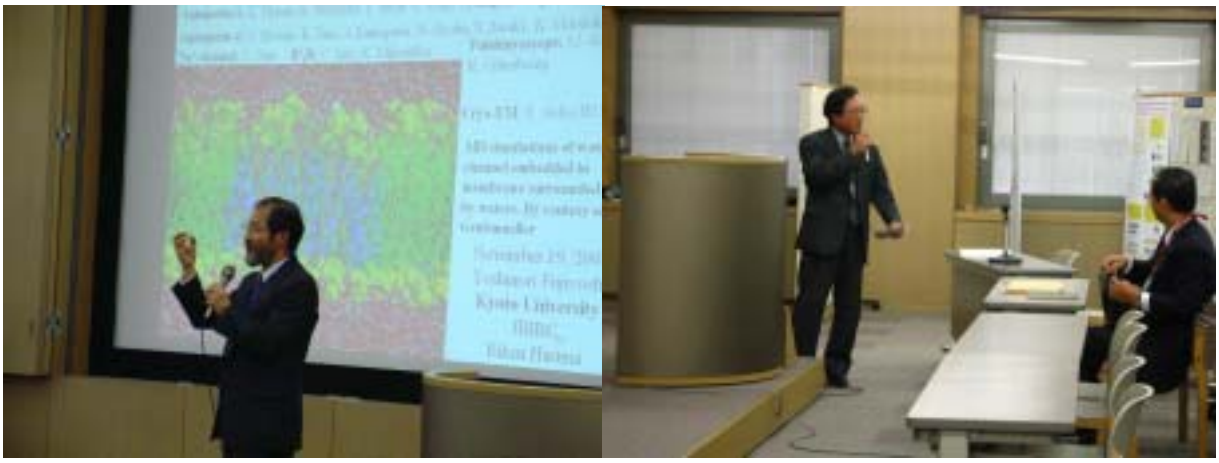
Host: H. Nakatsuji (Dept. Synthetic Chemistry and Biological Chemistry, Grad. Sch. Eng.)
K. Hirao (Dept. Material Chemistry, Grad. Sch. Eng.)

Invited speakers:
Professor Yuan T. Lee (Academia Sinica, Taipei)
Professor Yoshinori Fujiyoshi (Division of Biological Science, Grad. Sch. Sci. Kyoto University)
Professor Shigeki Kato (Division of Chemistry, Grad. Sch. Sci. Kyoto University)

First Symposium of Fukui Institute for Fundamental Chemistry, Kyoto University was held on November 19, 2003. After opening address by Prof. Isao Morishima, three lectures were presented by invited speakers.

Prof. Yuan T. Lee gave a lecture entitled "40 Years of Dynamics of Chemical Reactions -- Personal Perspective --". He talked about his research on the chemical reaction dynamics with which he was awarded the Nobel Prize. His talk began from the motivation to study of reaction dynamics and the background of those days. He explained the design of the molecular beam experiment and the experimental equipments with some important results including interesting episodes in that time. He also presented his recent studies on the reaction dynamics of complex molecules like benzene with using the cross beam experiment. His lecture again showed us the strong impact of the molecular beam experiment as the analytical tools of the chemical reaction; his effort and success greatly encouraged the young researchers.

Prof. Yoshinori Fujiyoshi gave a lecture entitled “Structure and Function of Water and Ion Channels in Our Body“. The structure and gating mechanism of water channel in the membrane protein, aquaporins (AQP) were presented. The role of the AQP in vision and the function of water molecules were studied in terms of the dipole interaction and hydrogen bond. The role of acetylcholine receptor (ACh) in moving muscle and its alkali ion channel were also presented. The structural change by ACh binding in protein has the gating mechanism of sodium ion channel. His attempt to elucidate the mechanism in life by chemistry and molecular biology stimulated the interest of many searchers in wide research fields.

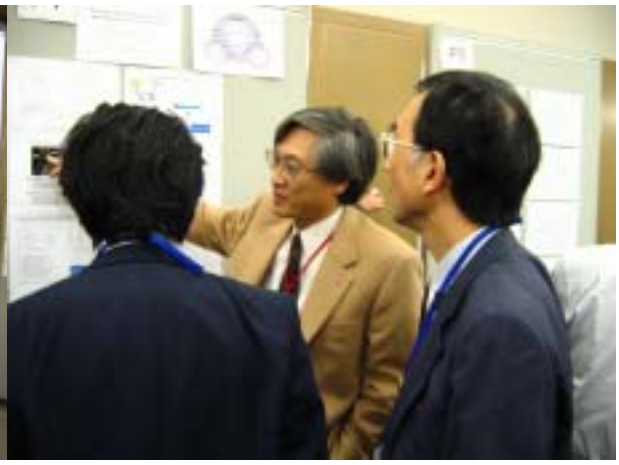


Prof. Shigeki Kato gave a lecture entitled “Theoretical Study of Chemical Reactions in Gas and Liquid Phases“. The theoretical studies on the mode selective chemical reactions of some small molecules in gas phase were presented. Reaction mechanisms in the electronic and vibronic excited states were studied in high accuracy. The chemical reactions in liquid phase were studied by the RISM theory and QM/MM method. The n-π* and π- π* excitations of carbonyl compounds were precisely studied with considering the freedom of solvent. The reaction path of enzyme was calculated by the QM/MM method and its free energy profile was presented. His talk explained the modern theoretical approach in the chemical reaction and showed the increasing importance of the theoretical study in the chemical reaction.

The poster presentations were multidisciplinary and cover broad area of science; sixty seven posters in the various field of science, namely, Material Chemistry, Polymer Chemistry, Physical Chemistry, Quantum Chemistry, Theoretical Chemistry, Biological Chemistry, Biology, Biophysics, and Physics, etc. were presented and the contributions are not only from Kyoto University, but also from Osaka City University and Osaka University etc. All the presentations were scientifically high level and the session was very successful for providing the opportunity to exchange ideas and to interact with each other among the different research field. Actually, the discussions were very active and many participants enjoyed their discussions. This interaction will contribute to the fresh activation of the research field and development of the collaborations among the different research area. This session also enabled the discussions of many young scientists in the different research fields and it was significant for the interchange of their research. The poster session program is given in the followings.







Poster Session Program

1**. ONIOM Method: Theory and Application**
Toshiaki Matsubara
Fukui Institute for Fundamental Chemistry, Kyoto University

2. **Photoactivation of Bacteriorhodopsin Studied by an Ab Initio Quantum Mechanical/ Molecular Mechanical Molecular Dynamics Simulation**
Shigehiko Hayashi[1], Emad Tajkhorshid[2], and Klaus Schulten[2]
[1]*Fukui Institute for Fundamental Chemistry, Kyoto University, and PREST-JST*
[2]*Beckman Institute, University of Illinois at Urbana-Champaign*

3. **Core Ionization Spectra and Doublet Radical Excited States by Open-Shell SAC/SAC-CI Method**
Yuhki Ohtsuka[1] and Hiroshi Nakatsuji[1,2]
[1]*Fukui Institute for Fundamental Chemistry, Kyoto University*
[2]*Department of Synthetic Chemistry and Biological Chemistry, Graduate School of Engineering, Kyoto University*

4. **Hydrogen Atom Production from the Photolysis of Water Ice Particles**
Masahiro Kawasaki
Department of Molecular Engineering, Graduate School of Engineering, Kyoto University

5. **Development and Application of a Flow-NMR Probe for Observing Organic Reactions in Sub- and Supercritical Water**

M. Mukaide, Y. Urasaki, F. Amita, H. Oka, O. Kajimoto, K. Takegoshi, and T. Terao
Department of Chemistry, Graduate School of Science, Kyoto University

6. **Nuclear Spin Conversion of Methane in Quantum Crystals**
Yuuki Miyamoto, Mizuho Fushitani, Daisuke Ando, and Takamasa Momose
Department of Chemistry, Graduate School of Science, Kyoto University

7. **Softening of Small Clusters in Superfluid He Droplets**
Susumu Kuma, Takamasa Momose, Michael Slipchenko, and Andrey Vilesov
Department of Chemistry, Graduate School of Science, Kyoto University, and Department of Chemistry, The University of Southern California

8. **Study of Electron Effective Mass of Cluster Materials Defined by KP Perturbation Theory on Molecular Orbitals**
Jun Yasui[1], Takumi Tomita[2], Kazuyoshi Yamashita[2], and Yoshinori Hayafuji[2]
[1]*TOYOBO Research Center Co., Ltd.*
[2]*School of Science & Technology, Kwansei Gakuin University*

9. **Influence of Hydrogen Incorporation on the Compressional Mechanism of Mg_2SiO_4**
Tomoyuki Yamamoto[1], David A. Yuen[2], Isao Tanaka[3], Hirohiko Adachi[3], and Kazuyuki Hirao[1,4]
[1]*Fukui Institute for Fundamental Chemistry, Kyoto University*
[2]*Department of Geology and Geophysics, University of Minnesota*
[3]*Department of Materials Science and Engineering, Graduate School of Engineering, Kyoto University*
[4]*Department of Material Chemistry, Graduate School of Engineering, Kyoto University*

10. **Optical Spectra and EPR Parameters of Rare-Earth Ions in LaF_3 Crystal**
M.G. Brik[1], I. Tanaka[2], K. Ogasawara[3], T. Ishii[4], H. Adachi[2], and K. Hirao[1,5]
[1]*Fukui Institute for Fundamental Chemistry, Kyoto University*
[2]*Department of Materials Science and Engineering, Graduate School of Engineering, Kyoto University*
[3]*School of Science and Technology, Kwansei Gakuin University*
[4]*The Institute of Laser-Physics, University of Hamburg*
[5]*Department of Material Chemistry, Graduate School of Engineering, Kyoto University*

11. **Proton Conduction in $CsHSO_4$ by First-Principle Calculations**
Xuezhi Ke[1], Isao Tanaka[2], Hirohiko Adachi[2], and Kazuyuki Hirao[1,3]
[1]*Fukui Institute for Fundamental Chemistry, Kyoto University*
[2]*Department of Materials Science and Engineering, Graduate School of Engineering, Kyoto University*
[3]*Department of Material Chemistry, Graduate School of Engineering, Kyoto University*

12. **Thermodynamics of SnO_2 Surfaces by First Principles Calculations**
Wolfgang Bergermayer[1], Isao Tanaka[2], Hirohiko Adachi[2], and Kazuyuki Hirao[1,3]
[1]*Fukui Institute for Fundamental Chemistry, Kyoto University*
[2]*Department of Materials Science and Engineering, Graduate School of Engineering, Kyoto University*
[3]*Department of Material Chemistry, Graduate School of Engineering, Kyoto University*

13. **Synthesis of Novel Bowl-Shaped Neutral Radicals and Characterization of their Spin**

Density Distributions by ESR/ENDOR/TRIPLE Measurements

Shinsuke Nishida[1], Yasushi Morita[1,3], Kozo Fukui[3], Tadahiro Kobayashi[1], Kazunobu Sato[2], Daisuke Shiomi[2], Takeji Takui[2], and Kazuhiro Nakasuji[1]
[1]*Graduate School of Science, Osaka University*
[2]*Graduate School of Science, Osaka City University*
[3]*PRESTO-JST*

14. **Fine-Structure ESR Spectra of the Ground-State Triplet Diradical Composed of Different Kind of Organic Radicals**

Kozo Fukui[1], Yasushi Morita[1,2], Junya Kawai[2], Shigeaki Nakazawa[4], Kazunobu Sato[3], Daisuke Shiomi[3], Takeji Takui[3], and Kazuhiro Nakasuji[2]
[1]*PRESTO-JST*
[2]*Graduate School of Science, Osaka University*
[3]*Graduate School of Science, Osaka City University*
[4]*RIKEN-PDC*

15. **Ab Initio and DFT Calculations for Molecular Geometries and Electronic Structures of Halogen-Substituted Alkylcarbenes**

Kenji Sugisaki, Kazuo Toyota, Kazunobu Sato, Daisuke Shiomi, and Takeji Takui
Departments of Chemistry and Materials Science, Graduate School of Science, Osaka City University

16. **Electronic and Molecular Structures of Calix[4]arene-Based Nitroxide Radicals as Studied by CW and Pulsed ESR Spectroscopy**

Takatoshi Sawai, Kazunobu Sato, Daisuke Shiomi, Q. Wang, J. –S. Wang, Y. Li, G. –S. Wu, and Takeji Takui
Departments of Chemistry and Materials Science, Graduate School of Science, Osaka City University and Department of Chemistry, Tsinghua University, China

17. **Ab Initio Calculation of Zero Field Splitting Tensor**

Kazuo Toyota, Kazunobu Sato, Daisuke Shiomi, and Takeji Takui
Departments of Chemistry and Materials Science, Graduate School of Science, Osaka City University

18. **Spin Structures of Highly Delocalized High-Spin Organic Molecules as Studied by Multi-Electron Reduced Density Matrix Approach**

Kazunobu Sato, Kazuo Toyota, Daisuke Shiomi, and Takeji Takui
Departments of Chemistry and Materials Science, Graduate School of Science, Osaka City University

19. **Solution-Phase ESR Spectra and Solid-State Magnetic Properties of a Model System Single-Component Organic Molecule-Based Ferrimagnetics**

Kensuke Maekawa, Tomoaki Ise, Daisuke Shiomi, Kazunobu Sato, and Takeji Takui
Departments of Materials Science and Chemistry, Graduate School of Science, Osaka City University; PRESTO-JST

20. **Selectivity of Ferrimagnetic and Diamagnetic Ground States for a Novel Organic Heterospin Chain**

Yuki Kanzaki, Tomoaki Ise, Daisuke Shiomi, Kazunobu Sato, and Takeji Takui

Departments of Materials Science and Chemistry, Graduate School of Science, Osaka City University; PRESTO-JST

21. **Electronic States of Dioxins as Studied by the SAC-CI Method**
Teruaki Koto, Kazuo Toyota, Kazunobu Sato, Daisuke Shiomi, and Takeji Takui
Departments of Chemistry and Materials Science, Graduate School of Science, Osaka City University

22. **Organic Triradicals Based on Nitronyl Nitroxide and TEMPO Radical Components as Models for Single-Component Organic Molecule-Based Ferrimagnetics**
Chika Kaneda, Tomoaki Ise, Daisuke Shiomi, Kazunobu Sato, and Takeji Takui
Departments of Materials Science and Chemistry, Graduate School of Science, Osaka City University; PRESTO-JST

23. **The Absolute Signs of the Fine Structure Parameters of the Exited Triplet States and Polyanionic High-Spin States of Fullerene C_{60} and C_{70}**
Nobuyuki Mori, Kozo Fukui, Shigeaki Nakazawa, Kazuo Toyota, Kazunobu Sato, Daisuke Shiomi, and Takeji Takui
Departments of Chemistry and Materials Science, Graduate School of Science, Osaka City University

24. **Pseudo Jahn-Teller Distortion of Co(II)octaethylporphyrin as Studied by Single-Crystal ESR/ENDOR Spectroscopy**
Naoki Yokokura, Hideto Matsuoka, Kazunobu Sato, Daisuke Shiomi, Kazuo Toyota, D. Dolphin, the late C. A. McDowell, and Takeji Takui
Departments of Chemistry and Materials Science, Graduate School of Science, Osaka City University and Department of Chemistry, University of British Columbia

25. **Imino- and Nitronyl-Nitroxide Biradicals as Building Blocks for Organic Supramolecular Ferrimagnets**
Kenicni Hayakawa, Tomoaki Ise, Daisuke Shiomi, Kazunobu Sato, and Takeji Takui
Departments of Materials Science and Chemistry, Graduate School of Science, Osaka City University; PRESTO-JST

26. **Thermal Analysis of Cooperative Adsorption on Co(II) Porous Coordination Polymers**
Kazuhiro Uemura and Susumu Kitagawa
Department of Synthetic Chemistry & Biological Chemistry, Graduate School of Engineering, Kyoto University

27. **Direct Growth of Crystals with Macroscopic Superlattice Morphologies**
Shigeyuki Masaoka and Susumu Kitagawa
Department of Synthetic Chemistry & Biological Chemistry, Graduate School of Engineering, Kyoto University

28. **Electronic Structure and Vibronic Interaction of M@C_{74}**
Ken Tokunaga, Tohru Sato, and Hiroshi Imahori
Department of Molecular Engineering, Graduate School of Engineering, Kyoto University

29. **Three-Dimensional Assemblies of Porphyrin-Modified Gold Nanoclusters on ITO Electrode for Efficient Light Energy Conversion System**
Atsushi Fujimoto, Tomoo Sato, Yukie Mori, Yoshihiro Matano, and Hiroshi Imahori

Department of Molecular Engineering, Graduate School of Engineering, Kyoto University

30. **Folding Kinetics of Single-Chain Monellin Examined by Time-Resolved Spectroscopies**

Tetsunari Kimura[1], Satoshi Takahashi[1,2], Suguru Konno[3], Koichiro Ishimori[1], and Isao Morishima[1,4]
[1]*Department of Molecular Engineering, Graduate School of Engineering, Kyoto University*
[2]*Institute for Protein Research, Osaka University*
[3]*Fukui Medical University*
[4]*Fukui Institute for Fundamental Chemistry, Kyoto University*

31. **Collapse and Search Dynamics of Apomyoglobin Folding Revealed by Submillisecond**
Observations of a-Helical Contents and Compactness

Takanori Uzawa[1], Shuji Akiyama[2], Tetsunari Kimura[1], Satoshi Takahashi[1], Koichiro Ishimori[1], Isao Morishima[1,3], and Tetsuro Fujisawa[2]
[1]*Department of Molecular Engineering, Graduate School of Engineering, Kyoto University*
[2]*RIKEN Harima Institute/SPring-8, Structural Biochemistry Laboratory*
[3]*Fukui Institute for Fundamental Chemistry, Kyoto University*

32. **The Observation of the Dioxygen Activation of Cytochrome b_0 from Escherichia Coli by Submillisecond-Resolved Freeze Quench EPR Spectroscopy**

Koji Matsuura[1], Shiro Yoshioka[1], Satoshi Takahashi[1], Koichiro Ishimori[1], Tatsushi Mogi[2], Hiroshi Hori[3], and Isao Morishima[1,4]
[1]*Department of Molecular Engineering, Graduate School of Engineering, Kyoto University*
[2]*Department of Biological Sciences, Graduate School of Science, University of Tokyo*
[3]*Division of Biophysical Engineering, Graduate School of Engineering Science, Osaka University*
[4]*Fukui Institute for Fundamental Chemistry, Kyoto University*

33. **Atomic Structure of Bacteriorhodopsin at pH 10.0 Revealed by Electron Crystallography**

Yifan Cheng[1], Yoshiaki Kimura[2], Yoshinori Fujiyoshi[3], Kaoru Mitsuoka[4]
[1]*Harvard Medical School*
[2]*BERI*
[3]*Graduate School of Science, Kyoto University*
[4]*LTM Center, Kyoto University*

34. **Amplification of Receptor Signalling by Ca^{2+} Entry-Mediated Translocation and Activation of PLC γ 2 in B Lymphocytes**

Motohiro Nishida, Kenji Sugimoto, Yuji Hara, Emiko Mori, Takashi Mori, Tomohiro Kurosaki, and Yasuo Mori
Laboratory of Molecular Biology, Department of Synthetic Chemistry and Biological Chemistry, Graduate School of Engineering, Kyoto University

35. **Cysteine Oxidation is Essential for TRPC5-Mediated Ca^{2+} Entry**

Takashi Yoshida, Motohiro Nishida, Yuji Hara, and Yasuo Mori
Laboratory of Molecular Biology, Department of Synthetic Chemistry and Biological Chemistry, Graduate School of Engineering, Kyoto University

36. **Corresponding States Theory of Structural Thermodynamics and Kinetics of**

Proteins
Kuo Kan Liang
AIST, Tsukuba Central 5

37. **Forward/Backward Motion of Oil Droplet Driven by Laser**
Sergei Rybalko and Nobuyuki Magome
Yoshikawa Laboratory, Department of Physics, Graduate School of Science, Kyoto University

38. **Controlling DNA Transcriptional Activity by Higher-Order Conformation Changes**
Francois Luckel
Yoshikawa Laboratory, Department of Physics, Graduate School of Science, Kyoto University

39. **Shear-Induced BCC-LAM and HEX-LAM Transitions in Block Copolymer Solutions**
Igor Rychkov
Yoshikawa Laboratory, Department of Physics, Graduate School of Science, Kyoto University

40. **Effect of Electrostatic Interaction and Translation of Counterions on Intramolecular Phase Segregation**
Takafumi Iwaki
Yoshikawa Laboratory, Department of Physics, Graduate School of Science, Kyoto University

41. **Expansion of Informational Space by the Evaluation of Surface Reaction Rate on Tin Dioxide Gas Sensors**
Tatsuya Ogawara
Yoshikawa Laboratory, Department of Physics, Graduate School of Science, Kyoto University

42. **Optical Trapping of a Water Droplet in Air: Experiment and Theory on the Trapping Efficiency**
Akihiro Isomura, Masahiro Kohira, and Nobuyuki Magome
Yoshikawa Laboratory, Department of Physics, Graduate School of Science, Kyoto University

43. **Theoretical Study of Hydrogen-Bonded Supramolecules and Molecular Networks**
Fumihiko Tanaka
Department of Polymer Chemistry, Graduate School of Engineering, Kyoto University

44. **Discovery of Self-Organized Structures in Block Copolymer Melts by Computer Experiments**
Tomonari Totera
Department of Polymer Chemistry, Graduate School of Engineering, Kyoto University

45. **Theoretical and Computational Studies of Associating Polymers and Thermoreversible Gels**
Tsuyoshi Koga and Fumihiko Tanaka
Department of Polymer Chemistry, Graduate School of Engineering, Kyoto University

46. **Calculation of Resonant Inelastic X-Ray Scattering Spectra: Resonant Inelastic Scattering of Hard X-Ray at Valence Electron of Ge**
Yunori Nisikawa
JAERI SPring-8

47. **Theory of Superconductivity in $PuCoGa_5$**
Kazunori Tanaka
Department of Physics, Graduate School of Science, Kyoto University

48. **Hybrid-DFT Studies on Oxo and Hydroxo Bridged Diiron Compounds**
Mitsuo Shoji, Yusuke Nisiyama, Yusuke Maruno, Kennichi Koizumi, Yasutaka Kitagawa, and Kizashi Yamaguchi
Department of Chemistry, Graduate School of Science, Osaka University

49. **Theoretical Studies on Interaction between Manganese Porphyrin and Oxygen Molecule**
Kennichi Koizumi, Mitsuo Shoji, Yusuke Nisiyama, Yusuke Maruno, Yasutaka Kitagawa, and Kizashi Yamaguchi
Department of Chemistry, Graduate School of Science, Osaka University

50. **Theoretical Study on the Absorption Spectrum of NOCl**
Takefumi Yamashita and Shigeki Kato
Department of Chemistry, Graduate School of Science, Kyoto University

51. **Phonon and Polarization of Crystal Charcogen Compounds**
Masafuyu Matsui, Kazuma Nakamura, and Atsushi Ikawa
Department of Chemistry, Graduate School of Science, Kyoto University

52. **Theoretical Study on Unimolecular Dissociation and Isomerization Reaction of Formaldehyde**
Takehiro Yonehara and Shigeki Kato
Department of Chemistry, Graduate School of Science, Kyoto University

53. **Model Hamiltonian for Ni(II) Electronic Structure in Aqueous Solution**
Satoru Iuchi, Akihiro Morita, and Shigeki Kato
Department of Chemistry, Graduate School of Science, Kyoto University

54. **Theoretical Study of Methyl-, Silyl- and Germyl-Bridged Dinuclear Palladium(I) Complexes: Importance of Agostic and Pd-Pd Bonding Interactions**
Shingo Nakajima, Yoshihide Nakao, Hirofumi Sato, and Shigeyoshi Sakaki
Department of Molecular Engineering, Graduate School of Engineering, Kyoto University

55. **Solvation of cis-Platin and its Aquo Complexes. A Theoretical Study**
Kohei Ono, Hirofumi Sato, and Shigeyoshi Sakaki
Department of Molecular Engineering, Graduate School of Engineering, Kyoto University

56. **Electronic Structures and Absorption Spectra of PbPc and SnPc (Pc=Phthalocyanine). A Theoretical Study**
Michinori Sumimoto[1], Shigeyoshi Sakaki[1], and Hitoshi Fujimoto[2]
[1]*Department of Molecular Engineering, Graduate School of Engineering, Kyoto University*
[2]*Department of Chemistry, Faculty of Science, Kumamoto University*

57. **A Crucial Comparison of Electronic Structure Theories for Solvated Molecule: RISM-SCF versus PCM**
Hirofumi Sato and Shigeyoshi Sakaki
Department of Molecular Engineering, Graduate School of Engineering, Kyoto University

58. **Fine Theoretical Spectroscopy with the SAC-CI Method on Gaussian03**
Masahiro Ehara[1] and Hiroshi Nakatsuji[1,2]
[1]*Department of Synthetic Chemistry and Biological Chemistry, Graduate School of Engineering, Kyoto University*
[2]*Fukui Institute for Fundamental Chemistry, Kyoto University*

59. **Relativistic and Electron Correlation Effects on the Magnetic Shielding Constants of Heavy Elements**
Ryoichi Fukuda[1], Jun Yasui[1], Naoaki Yamada[1], and Hiroshi Nakatsuji[1,2]
[1]*Department of Synthetic Chemistry and Biological Chemistry, Graduate School of Engineering, Kyoto University*
[2]*Fukui Institute for Fundamental Chemistry, Kyoto University*

60. **Photoelectron Spectroscopy of Inner-Shell Ionization and Surface Adsorbates Using SAC-CI General-R Method**
Kei Kuramoto[1], Masahiro Ehara[1], and Hiroshi Nakatsuji[1,2]
[1]*Department of Synthetic Chemistry and Biological Chemistry, Graduate School of Engineering, Kyoto University*
[2]*Fukui Institute for Fundamental Chemistry, Kyoto University*

61. **SAC-CI Spectroscopy for Molecular Biology**
Jun-ya Hasegawa[1], Kazuhiro Fujimoto[1], and Hiroshi Nakatsuji[1,2]
[1]*Department of Synthetic Chemistry and Biological Chemistry, Graduate School of Engineering, Kyoto University*
[2]*Fukui Institute for Fundamental Chemistry, Kyoto University*

62. **Relativistic Effect on Magnetic Circular Dichroism of Halide Molecules**
Y. Honda[1], M. Hada[1], M. Ehara[1], H. Nakatsuji[1,2], and J. Michl[1]
[1]*Department of Synthetic Chemistry and Biological Chemistry, Graduate School of Engineering, Kyoto University*
[2]*Fukui Institute for Fundamental Chemistry, Kyoto University*

63. **Binding of Dioxygen to Fe-Porphyrin, Fe-Porphycene and Fe-Corphycene Complexes**
H. Nakashima[1], J. Hasegawa[1], and H. Nakatsuji[1,2]
[1]*Department of Synthetic Chemistry and Biological Chemistry, Graduate School of Engineering, Kyoto University*
[2]*Fukui Institute for Fundamental Chemistry, Kyoto University*

64. **Analytical Energy Gradient of the SAC-CI Method: Applications to Geometry Optimization of Molecular Excited States**
F. Oyagi[1], J. Yasui[1], M. Ehara[1], and H.Nakatsuji[1,2]
[1]*Department of Synthetic Chemistry and Biological Chemistry, Graduate School of Engineering, Kyoto University*
[2]*Fukui Institute for Fundamental Chemistry, Kyoto University*

65. **Excited States of Green Fluorescent Protein and Mutants: SAC-CI Study**
K. Fujimoto[1], J. Hasegawa[1], and H. Nakatsuji[1,2]
[1]*Department of Synthetic Chemistry and Biological Chemistry, Graduate School of Engineering, Kyoto University*
[2]*Fukui Institute for Fundamental Chemistry, Kyoto University*

66. **Adsorption of NO on Metal Surfaces: Dipped Adcluster Model Study**

N. Matsumune[1], K. Kuramoto[1], and H. Nakatsuji[1,2]
[1]*Department of Synthetic Chemistry and Biological Chemistry, Graduate School of Engineering, Kyoto University*
[2]*Fukui Institute for Fundamental Chemistry, Kyoto University*

67. **Relativistic and Electron Correlation Effects on Magnetic Shielding Constants Based on Dirac-Hartree-Fock Method**

J. Yasui[1], R. Fukuda[1], N. Yamada[1], M. Hada[1], and H. Nakatsuji[1,2]
[1]*Department of Synthetic Chemistry and Biological Chemistry, Graduate School of Engineering, Kyoto University*
[2]*Fukui Institute for Fundamental Chemistry, Kyoto University*