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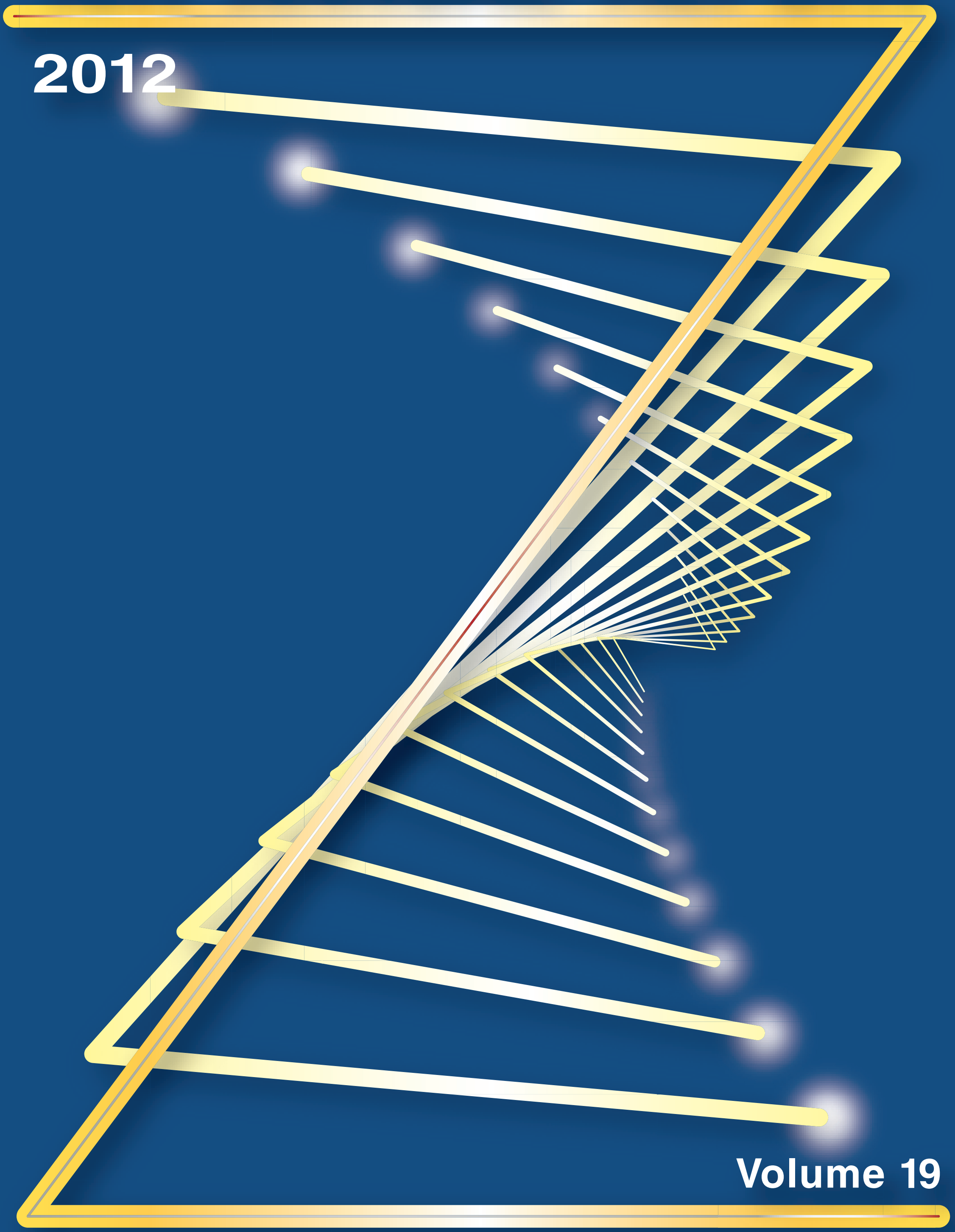
# ICR ANNUAL REPORT

2012



Volume 19

Institute for Chemical Research
Kyoto University

**ICR ANNUAL REPORT 2012 (Volume 19)** - ISSN 1342-0321 -
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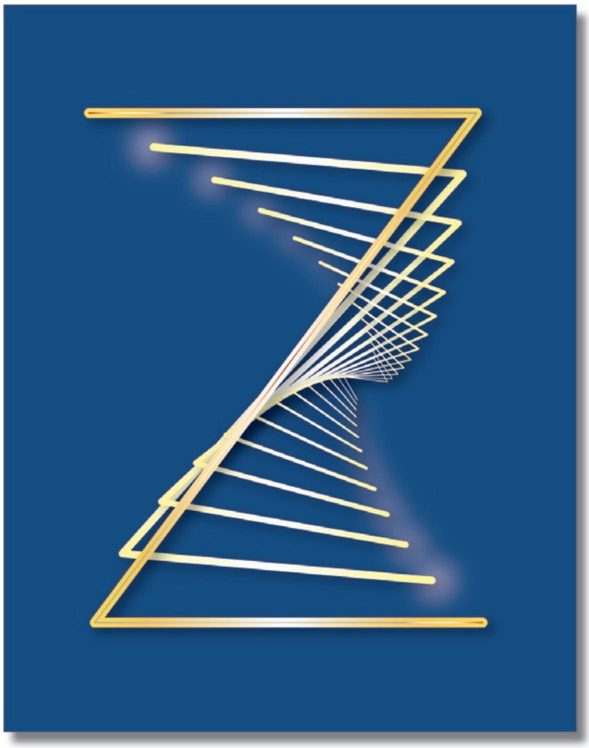
# ICR
# ANNUAL
# REPORT
# 2012



**Institute for Chemical Research**
**Kyoto University**
Volume 19

# Preface

Institute for Chemical Research (ICR), Kyoto University was launched in 1926 as the first research institute at Kyoto University, to mark its 86th anniversary last year; its true roots date back to 1915, that is, the Specialized Center for Chemical Research founded at the College of Science, Kyoto Imperial University. The philosophy at the time of foundation of the ICR above was to "Excel in the Investigation of Basic Principles of Chemistry and Their Applications," and the studies on special medicinal substances "Salvarsans," organometallic chemistry, incendiary reagents, and so on were undertaken at nine research laboratories. Since then, the ICR has continuously produced outstanding research achievements. Now, we have reached the current large-scale organization of five research divisions: Synthetic Chemistry, Materials Chemistry, Biochemistry, Environmental Chemistry, and Multidisciplinary Chemistry and three research centers: Advanced Research Center for Beam Science, International Research Center for Elements Science (IRCELS), and Bioinformatics Center. Currently, about 100 faculty members, 210 graduate students and 50 researchers are engaged in research activities in 32 laboratories in total supervised by full-time professors. Further, we have 5 laboratories supervised by visiting professors and an endowed laboratory.

The research within the ICR encompasses the fields of chemistry, physics, biology, and informatics. The chemical studies core covers fields including physical chemistry, inorganic chemistry, organic chemistry, materials chemistry, and biochemistry. The graduate schools to which our laboratories belong as cooperative ones accepting graduate students cover diverse fields of science, engineering, agriculture, pharmaceutical sciences, medicine, informatics, and human/environmental studies. These laboratories are spearheading leading-edge research, and yielding outstanding results in their own and/or correlated research areas, as examples, a direct electron microscope observation of defects in an organic crystal, a real-time observation of spin-motive force due to a gyrating magnetic vortex, and a discovery of a small molecule promoting cardiac differentiation of human pluripotent stem cells, all achieved in this year. The legacy of our founding philosophy above continues to the present day and describes the essence of our research activities. The ICR has entrusted its members with this vision in mind to choose and pursue research topics at the forefront of advanced chemistry with bottom-up paradigms. Whether or not the human race maintain sustained growth is a key issue of this century. Moreover, we must recover from the Great East Japan Earthquake last year and reform our country from various perspectives in Japan. Hence, the ICR encourages its members to be actively involved in research projects with bottom-up approach in mind, and to value the development of unique interdisciplinary research projects, in order to contribute to the future of our society from materials-related fields.

Besides, the ICR is currently collaborating with domestic/oversea universities and research organizations (with about 55 official international collaboration agreements) and is functioning as a Joint Usage/Research Center proclaiming the Frontier/Interdisciplinary Research Core for Deeping Investigation and Promoting Cooperation in Chemistry-Oriented Fields supported by MEXT (2010-2016). In addition, the ICR, IRCELS in particular, is making a significant contribution to the MEXT Project of Integrated Research on Chemical Synthesis (2010-2016), in collaboration with the Catalysis Research Center at Hokkaido University, the Research Center for Materials Science at Nagoya University and the Institute for Materials Chemistry and Engineering at Kyushu University. Further, we also fully strive to fostering and securing of young researchers through these activities as well as graduate education mentioned above. For instance, this year we restarted an in-house annual grant system named "ICR Grant for Encouraging Promoting Integrated Research," as described later by Professor Futaki, a Vice-Director. The strong collaboration basis so far constructed in-house and also with outside ensures the Institute to serve as the core of global research propellers in chemistry-oriented fields. Finally, we would appreciate your continued encouragement and support.

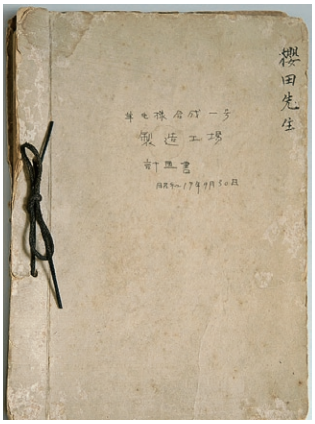
January 2013

Naoki Sato

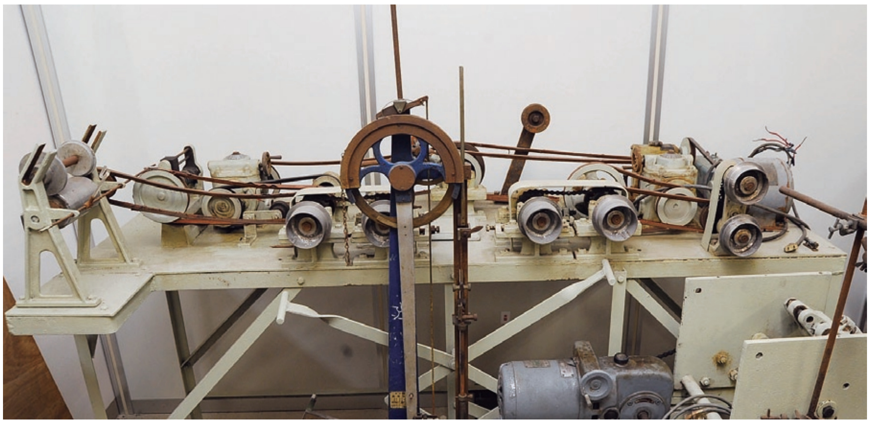
SATO, Naoki
Director

# ICR News 2012

## Materials Related with “Vinylon” in the Institute for Chemical Research Were Approved as Chemical Heritage


半毛様合成一号
製造工場
計画書
昭和17年9月30日
櫻田先生

Plan for first synthetic wool-like manufacturing plant


Laboratory equipment for spinning “Vinylon”

Prof KANAYA, Toshiji

Materials related with “Vinylon” in the Institute for Chemical Research (ICR), Kyoto University, were approved as Chemical Heritage by the Chemical Society of Japan. The plan for industrialization of “Vinylon” and the laboratory equipment for spinning “Vinylon” were certified. On the cover of the plan, “Plan for first synthetic wool-like manufacturing plant” were written in the autograph of Professor Ichiro Sakurada. Synthetic fiber “Vinylon” which was mainly made of polyvinyl alcohol was invented for the first time in domestic technology by Professor Ichiro Sakurada et al., and completed in 1939 at the Institute for Chemical Research (ICR), Kyoto University, which was located in Takatsuki (Takatsuki-cho at that time), Osaka.

Chemical Heritage is one of the most important historical materials related to chemistry and chemical technology in Japan approved by the Chemical Society of Japan. The presentation ceremony of the award was held in the 92nd Spring Annual Meeting of the Chemical Society of Japan at Keio University, Hiyoshi Campus on 26 March 2012. At the same time, 153 fundamental research literatures and the 5 prototype yarns of Unitika Ltd., who was involved in the industrialization of “Vinylon”, and the initial fiber of “Vinylon” (toe) produced by Kuraray Co., Ltd. (at that time, Kurashiki Rayon Co., Ltd.) were also approved as Chemical Heritage.


日本化学会認定化学遺産第016号
日本化学会化学遺産
認定証
A Chemical Heritage
authorized by
The Chemical Society of Japan
京都大学化学研究所 殿
日本のビニロン工業の発祥を示す資料

貴下ご所有の
「日本のビニロン工業の発祥を示す資料」を
日本の化学および化学技術にとって
歴史的に貴重な資料として
日本化学会化学遺産に認定します

平成24年3月26日

公益社団法人 日本化学会
会長 岩澤康裕

Certificate for Chemical Heritage


The certificate presentation ceremony 26 March 2012
(left to right) Norihiro Tokitoh (Director of ICR), Yasuhiro Iwasawa (President of the Chemical Society of Japan), Hitoshi Toyoura (Kuraray Co., Ltd.) and Keiji Yukawa (Unitika Ltd.) at the award ceremony. The positions are at that time.

# 10th International Conference on Heteroatom Chemistry (ICHAC-10)

**Prof TOKITOH, Norihiro**
(Chairman of ICHAC-10)

The International Conference on Heteroatom Chemistry (ICHAC) is an established international forum for the presentation and discussion of research results on the diverse fields of Heteroatom Chemistry. Previous ICHAC meetings have been held in different countries going around Asia, North America, and Europe. This time ICHAC comes back to Japan, the first ICHAC host country (Kobe, 1987), again cerebrating its tenth anniversary. It should be noted that ICHAC-10 was a major scientific event, bringing together organic and inorganic chemists all over the world sharing their interests on the different areas of Heteroatom Chemistry. As usual, this conference served as a professional forum to disseminate scientific knowledge on areas related to all fields of Heteroatom Chemistry.

ICHAC-10 was held during the period of 20-25 May 2012 at Uji Obaku Plaza, Kyoto University, and the conference program consisted of 7 plenary and 17 invited lectures, 3 memorial lectures, as well as 43 short communications and 154 poster presentations. We had 371 participants (92 from abroad) from 28 countries. All the participants may have found a fruitful environment at ICHAC-10 for personal contact and scientific exchange, and experienced useful interactions between chemists of different areas.

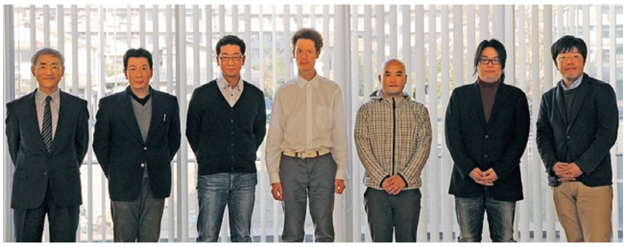
Finally, as a chairman of ICHAC-10, I would like to express my sincere thanks to the kind support by the Institute for Chemical Research, Kyoto University, and the great assistance and contribution from the many members of ICR laboratories related to Heteroatom Chemistry.

Commemorative photo of organizing committee members and guest speakers

# ICR Grant for Promoting Integrated Research

**Prof FUTAKI, Shiroh** (Vice-Director of ICR)

Institute for Chemical Research (ICR), Kyoto University takes pride in the high standard of research cultivated from the academic freedom and the interplays among our staffs and students having various scientific backgrounds. For greater enhancement of pioneering and/or integrated research collaboration research in house, especially among young research staffs, we established an in-house annual grant system named “ICR Grant for Promoting Integrated Research” in the financial year (FY) of 2004; it was suspended in FY 2007-2011 due to a large scale seismic strengthening works of our main building. This year we restarted this system with appreciating its importance. In addition to the original project which promotes the collaboration among young research staffs (under the age of 40) by providing a research grant of 1-3 million JPY in the year for one application, we have laid an additional category to stimulate collaboration involving foreign young researchers in house (1-2 million JPY). Evaluation of research proposals through paper screening and interviews by the selection committee has adopted three research proposals in each category. The awardees are requested to report their results in writing and presentation to our in-house members after the completion.



The representative of each adoption subject in the 2012 with the Director and a public-relations committee member.
The round-table talk was held for the beginning-of-a-book plan of the ICR public relations magazine “Obaku” to exchange of free opinions about this system.

# CONTENTS

**Division of Synthetic Chemistry**

**Division of Materials Chemistry**

**Division of Biochemistry**

**Division of Environmental Chemistry**

**Division of Multidisciplinary Chemistry**

**Advanced Research Center for Beam Science**

**International Research Center for Elements Science**

**Bioinformatics Center**

**Endowed Research Section**

## Abbreviations used in the columns

| | |
|---|---|
| Prof Em | Professor Emeritus |
| Prof | Professor |
| Vis Prof | Visiting Professor |
| Assoc Prof | Associate Professor |
| Vis Assoc Prof | Visiting Associate Professor |
| Assist Prof | Assistant Professor |
| Lect (pt) | Senior Lecturer (part-time) |
| Specially Appointed Prof | Specially Appointed Professor |
| Program-Specific Assoc Prof | Program-Specific Associate Professor |
| Program-Specific Assist Prof | Program-Specific Assistant Professor |
| Program-Specific Res | Program-Specific Researcher |
| Techn Staff | Technical Staff |
| Assist Res Staff | Assistant Research Staff |
| Assist Techn Staff | Assistant Technical Staff |
| Guest Scholar | Guest Scholar |

| | |
|---|---|
| Guest Res Assoc | Guest Research Associate |
| SPD (JSPS) | Special Post-Doctoral Research Fellow (JSPS) |
| PD | Post-Doctoral Research Fellow |
| Res | Researcher |
| Res Support Staff | Research Support Staff |
| Proj Res | Project Researcher |
| RF | Research Fellow |
| D 1～3 | Doctoral Course (Program) 1～3 |
| M1～2 | Master’s Course (Program) 1～2 |
| RS | Research Student |
| UG | Undergraduate Student |
| D Sc | Doctor of Science |
| D Eng | Doctor of Engineering |
| D Agr | Doctor of Agricultural Science |
| D Pharm Sc | Doctor of Pharmaceutical Science |
| D Med Sc | Doctor of Medical Science |
| D Inf | Doctor of Informatics |
| Ph D | Doctor of Philosophy |
| (pt) | part-time |

# ORGANIZATION

# Institute for Chemical Research

## 5 Divisions and 3 Centers

## Laboratories

### Research Divisions

- **Division of Synthetic Chemistry**
  - Organoelement Chemistry
  - Structural Organic Chemistry
  - Synthetic Organic Chemistry
  - Advanced Inorganic Synthesis
- **Division of Materials Chemistry**
  - Chemistry of Polymer Materials
  - Polymer Controlled Synthesis
  - Inorganic Photonics Materials
  - Nanospintronics
- **Division of Biochemistry**
  - Biofunctional Design-Chemistry
  - Chemistry of Molecular Biocatalysts
  - Molecular Biology
  - Chemical Biology
- **Division of Environmental Chemistry**
  - Molecular Materials Chemistry
  - Hydrospheric Environment Analytical Chemistry
  - Solution and Interface Chemistry
  - Molecular Microbial Science
- **Division of Multidisciplinary Chemistry**
  - Polymer Materials Science
  - Molecular Rheology
  - Molecular Aggregation Analysis
  - Supramolecular Biology
  - Interdisciplinary Chemistry for Innovation

### Research Centers

- **Advanced Research Center for Beam Science**
  - Particle Beam Science
  - Laser Matter Interaction Science
  - Electron Microscopy and Crystal Chemistry
  - Structural Molecular Biology
- **International Research Center for Elements Science**
  - Organic Main Group Chemisry
  - Advanced Solid State Chemistry
  - Organotransition Metal Chemistry
  - Photonic Elements Science
- **Bioinformatics Center**
  - Chemical Life Science
  - Mathematical Bioinformatics
  - Bio-knowledge Engineering
  - GenomeNet Project Management Office
- Endowed Research Section
  - Nano-Interface Photonics (SEI Group CSR Foundation)
- Visiting Divisions
- Joint Usage / Research Center
- Supercomputer Laboratory
- Low Temperature Laboratory

# TOPICS AND INTRODUCTORY COLUMNS OF LABORATORIES

# Division of Synthetic Chemistry
## – Organoelement Chemistry –

http://boc.kuicr.kyoto-u.ac.jp/www/index-e.html

Prof
TOKITOH, Norihiro
(D Sc)

Assoc Prof
SASAMORI, Takahiro
(D Sc)

Assist Prof
MIZUHATA, Yoshiyuki
(D Sc)

Assist Prof *
AGOU, Tomohiro
(D Sc)

Techn Staff
HIRANO, Toshiko

PD
MIYAKE, Hideaki
(D Sc)

PD
MAYER, F. J. Ulrich
(Ph D)

PD
SUGAMATA, Koh
(D Sc)

* Also serves as Assist Prof of Pioneering Research Unit for Next Generation

## Students

SAKAGAMI, Michiyasu (D3)
MIYAMOTO, Hisashi (D2)
EGAWA, Yasunobu (D1)
WASANO, Tatsuya (D1)
NAGATA, Koichi (M2)
TSUTSUMI, Yosuke (M2)
AWANE, Hiroyuki (M1)
IKEDA, Shin (M1)
KANESATO, Shuhei (M1)

## Visitors

| | |
|---|---|
| Prof LIPPOLIS, Vito | Department of Inorganic Chemistry, The University of Cagliari, Italy, 21 March |
| Prof APELOIG, Yitzhak | Department of Chemistry, Technion, Israel Institute of Technology, Israel, 16 October |
| Prof SCHESCHKEWITZ, David | Department of Chemistry, Faculty 8: Natural Sciences and Technology III, Saarland-University at Saarbrücken, Germany, 16–17 October |
| Prof RUSSEL, Chris | School of Chemistry, University of Bristol, U.K., 19 November |
| Prof BORDEN, Weston Thatcher | Department of Chemistry, University of North Texas, U.S.A., 26 November |

## Scope of Research

Organic chemistry has been developed as that of second-row elements such as carbon, oxygen, and nitrogen so far, while the synthesis and isolation of the heavier congeners of typical organic molecules as stable compounds have been one of “dreams” for organic chemists. Our main research interest is the elucidation of the similarities and differences in structures and reactivities between organic compounds and the corresponding heavier congeners. These studies are interesting and important from the standpoints of not only fundamental chemistry but also opening the way to more extensive application of main group chemistry.

**KEYWORDS**
Steric Protection
Kinetic Stabilization
Low-coordinated Species
Heteroatom
Transition Metal Complexes

## Selected Publications

Miyake, H.; Sasamori, T.; Tokitoh, N., Synthesis and Properties of 4,5,6-Triphospha[3]radialene, *Angew. Chem. Int. Ed.*, **51,** 3458-3461 (2012).

Agou, T.; Sugiyama, Y.; Sasamori, T.; Sakai, H.; Furukawa, Y.; Takagi, N.; Guo, J. D.; Nagase, S.; Hashizume, D.; Tokitoh, N., Synthesis of Kinetically Stabilized 1,2-Dihydrodisilenes, *J. Am. Chem. Soc.*, **134,** 4120-4123 (2012).

Sugamata, K.; Sasamori, T.; Tokitoh, N., Generation of an Organotellurium(II) Cation, *Eur. J. Inorg. Chem.*, 775-778 (2012).

Sasamori, T.; Sakagami, M.; Niwa, M.; Sakai, H.; Furukawa, Y.; Tokitoh, N., Synthesis of a Stable 1,2-Bis(ferrocenyl)diphosphene, *Chem. Commun.*, **48,** 8562-8564 (2012).

Agou, T.; Nagata, K.; Sakai, H.; Furukawa, Y.; Tokitoh, N., Synthesis, Structure, and Properties of a Stable 1,2-Dibromodialumane(4) Bearing a Bulky Aryl Substituent, *Organometallics*, **31,** 3806-3809 (2012).

## 4,5,6-Triphospha[3]radialene

Radialenes are a unique class of unsaturated hydrocarbons and have attracted much attention from the viewpoint of their cross-conjugated π-electron electronic structures. On the other hand, it was found that P=C bonds have unique characteristics that are different from those of C=C bonds, for example, they have lower LUMO levels relative to compounds with N=N or C=C double bonds. These unique characteristics of radialenes and low-coordinated phosphorus compounds prompted us to research the chemistry of the phosphorus analogues of radialenes, which are an attractive research target as a result of the synergy between the unique nature of radialenes and P=C bonds. We have succeeded in the synthesis of a stable 4,5,6-triphospha[3]radialene. The compound can be easily handled in air under ambient conditions, despite the [3] radialene moiety containing P=C bonds, and exhibits red-shifted absorption as well as high electron-accepting ability. The unique electronic properties are brought about by the synergistic effect of the [3]radialene framework and the phosphorus substitution.

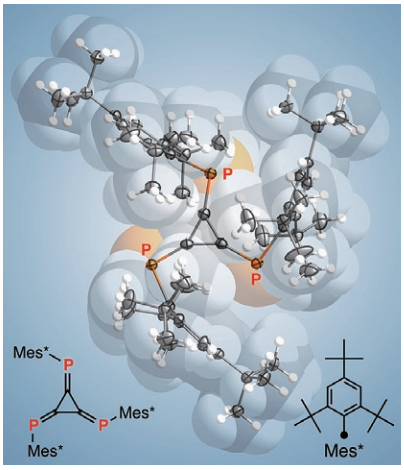


**Figure 1.** Structure of 4,5,6-triphospha[3]radialene.

## 1,2-Dihydorodisilenes

Despite the recent progress in the chemistry of kinetically stabilized multiply bonded silicon compounds, stable disilenes bearing more than one hydrogen substituent still remain elusive. Synthetically, the key challenge for the successful isolation of such multiply hydrogen-substituted disilenes lies in the effective stabilization of the sterically exposed H–Si=Si–H moiety. We have succeeded in the synthesis and isolation of the first stable 1,2-dihydrodisilenes by the introduction of sterically bulky aryl groups (Bbt and Bbp). These 1,2-dihydrodisilenes exhibit distinct Si=Si double-bond character in both solution and the solid state. The Si–H bonds in these 1,2-dihydrodisilenes exhibit higher *s* character than those of typical $\sigma^4,\lambda^4$-hydrosilanes.

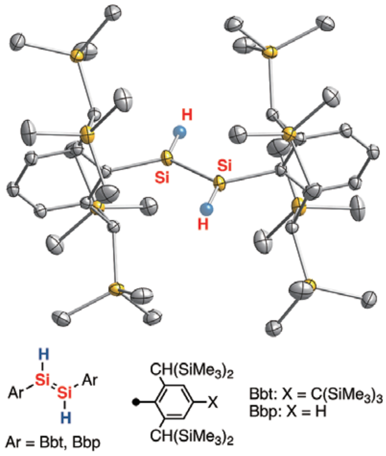


**Figure 2.** Structure of 1,2-dihydrodisilene.

## 1,2-Bis(ferrocenyl)diphosphene

Some d–π electron systems with two ferrocenyl (Fc) groups bridged by a π-bond moiety, *e.g.*, Ph(Fc)C=C(Fc) Ph or Fc–N=N–Fc have been reported and they show the unique properties of multi-step redox systems. A still prevailing limitation for the π-electron systems in these compounds is the restriction to the 2nd row of the p-block elements. We have succeeded in the synthesis and characterization of a stable 1,2-bis(ferrocenyl)diphosphene, wherein a P=P π-bond connects two ferrocenyl units. This represents an unprecedented example for a d–π electron system containing a heavier pnictogen π-spacer group. Stabilization of the highly reactive P=P π-bond was achieved by steric protection using two bulky ferrocenyl moieties. The assessment of its structural parameters and physical properties allowed the conclusion that the P=P π-bond is stable both in the solid state and solution and can act as an efficient π-electron spacer to couple the d-electrons of two ferrocenyl groups.

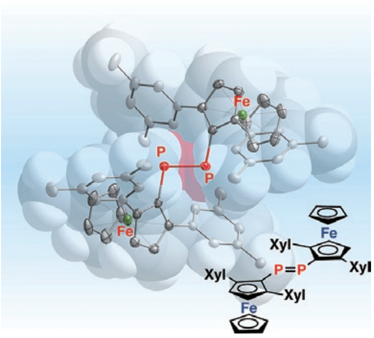


**Figure 3.** Structure of 1,2-bis(ferrocenyl)diphosphene. Xyl=3,5-dimethylphenyl.

# Division of Synthetic Chemistry
## – Structural Organic Chemistry –

http://www.scl.kyoto-u.ac.jp/~kouzou/index.html


Prof
MURATA, Yasujiro
(D Eng)


Assoc Prof
WAKAMIYA, Atsushi
(D Eng)


Assist Prof
MURATA, Michihisa
(D Eng)


PD
TANIGUCHI, Takuhiro
(D Sc)


PD
YOSHIKAWA, Osamu
(D Eng)


PD
ENDO, Masaru
(D Eng)


PD
NAKAIKE, Yumi
(D Eng)

### Students

MORINAKA, Yuta (D3)
MORI, Haruki (M2)
NISHIMURA, Hidetaka (M2)
FUTAGOISHI, Tsukasa (M1)
SHIMOGAWA, Hiroyuki (M1)
ZHANG, Rui (M1)
MA, Jianbo (RS)
SUGANO, Yasunori (UG)
UCHINAGA, Kensuke (UG)

### Visitors

| | |
|---|---|
| Prof LEVITT, Malcolm | School of Chemistry, University of Southampton, 31 October |
| Mr MATEOS GIL, Jaime | Organic Chemistry Department, Complutense University of Madrid, 6 June–8 July |

## Scope of Research

Fundamental studies are being conducted for creation of new functional π-systems with novel structures and properties, and for evaluation of their application as organic semi-conducting materials toward photovoltaic and electroluminescent devices. The major subjects are: organo-chemical transformation of fullerenes $C_{60}$ and $C_{70}$, specifically organic synthesis of endohedral fullerenes by the technique of molecular surgery; generation of ionic fullerene species and their application for the synthesis of functional material; synthesis of new carbon-rich materials by the use of transition metal complex; creation of new functional π-materials with unique photoelectric properties.

### KEYWORDS

π-Conjugated Systems
Open-Cage Fullerenes
Endohedral Fullerenes
Functional Dyes
Organic Solar Cell

### Selected Publications

Kurotobi, K.; Murata, Y., A Single Molecule of Water Encapsulated in Fullerene $C_{60}$, *Science*, **333,** 613-616 (2011).

Murata, M.; Morinaka, Y.; Murata, Y.; Yoshikawa, O.; Sagawa, T.; Yoshikawa, S., Modification of σ-Framework of [60]Fullerene for Bulk-heterojunction Solar Cells, *Chem. Commun.*, **47,** 7335-7337 (2011).

Frunzi, M.; Jockusch, S.; Chen, J. Y.-C.; Calderon, R. K.; Lei, X.; Murata, Y.; Komatsu, K.; Guldi, D. M.; Lawler, R. G.; Turro, N. J., A Photochemical On-Off Switch for Tuning the Equilibrium Mixture of $H_2$ Nuclear Spin Isomers as a Function of Temperature, *J. Am. Chem. Soc.*, **133,** 14232-14235 (2011).

Beduz, C.; Carravetta, M.; Chen, J. Y.-C.; Concistre, M.; Denning, M.; Frunzi, M.; Horsewill, A. J.; Johannessen, O. G.; Lawler, R.; Lei, X.; Levitt, M. H.; Li, Y.; Mamone, S.; Murata, Y.; Nagel, U.; Nishida, T.; Ollivier, J.; Rols, S.; Room, T.; Sarker, R.; Turro, N. J.; Yang, Y., Quantum Rotation of *Ortho* and *Para*-water Encapsulated in a Fullerene Cage, *Proc. Natl. Acad. Sci. USA*, **109,** 12894-12898 (2012).

Zoleo, A.; Lawler, R.; Lei, X.; Li, Y.; Murata, Y.; Komatsu, K.; Valentin, M. D.; Ruzzi, M.; Turro, N. J., ENDOR Evidence of Electron-$H_2$ Interaction in a Fulleride Embedding $H_2$, *J. Am. Chem. Soc.*, **134,** 12881-12884 (2012).

# Topics

## Quantum Rotation of *Ortho* and *Para*-water Encapsulated in a Fullerene Cage

The synthetic procedure known as “molecular surgery” involves opening an orifice in fullerene $C_{60}$ cages by a series of chemical reactions, insertion of small molecules into the cavity, and resealing of the cage by further reactions. This procedure has made available, in macroscopic quantities, a class of pure, stable, substances in which closed fullerene cages encapsulate small molecules. These systems provide “nano-laboratories” in which the small molecules are isolated in a geometrically well-defined, highly symmetrical environment. The recently-synthesized water-endofullerene $H_2O@C_{60}$ is particularly intriguing. Like $H_2$, water exhibits spin isomerism, with *ortho*- and *para*-forms, but unlike $H_2$, water has an electric dipole moment.

We study the energy levels, spin isomerism and quantum dynamics of single water molecules enclosed in fullerene cages, using three complementary physical methods: inelastic neutron scattering (INS), far-infrared spectroscopy (FIR), and nuclear magnetic resonance (NMR). In all cases, the homogeneous and symmetric environment provided by the fullerene cages isolates the *ortho* and *para* spin isomers, and gives rise to relatively narrow and unambiguous spectral features. We observe the existence of metastable *ortho*-water molecules, follow the slow conversion of *ortho*-water into *para*-water, and detect an energy splitting in the *ortho*-water rotational ground state, which is a signature of broken symmetry.

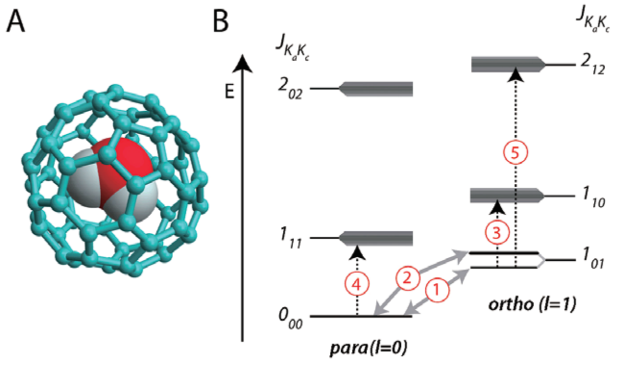


**Figure 1.** (A) Molecular structure of $H_2O@C_{60}$; (B) Energy level diagram, showing the principal transitions detected by INS (grey arrows) and IR spectroscopy (dashed arrows).

## Elucidation of π-Conjugation Modes in Diarene-Fused 1,2-Dihydro-1,2-diborin Dianions

Boron-containing heterocycles have gained widespread attention, not only from a fundamental point of view, but also as potential materials for various applications, such as optoelectronics and sensors. Of particular interest is the fact that the incorporation of an electron-deficient boron atom, which has a vacant p-orbital, into a π-conjugated cyclic skeleton enables the production of an electron-accepting π-system with effective p-π* conjugation.

We have synthesized a series of diarene-fused 1,2-dihydro-1,2-diborins, B-B-bond-containing polycyclic π-electron systems, and investigated their intriguing orbital interactions between the π-framework and the diborane moiety. A dithieno-fused 1,2-dihydro-1,2-diborin derivative with a 3,3’-bithiophene skeleton was synthesized, which showed an absorption band at longer wavelength compared to that of the parent 3,3’-bithiophene. Upon two-electron reduction to the dianion, the 6π aromatic character in the diborin moiety was enhanced. This trend was different from that observed for the 2,2’-bithiophene analogue, the dianion of which had a peripheral π-conjugation that was extended over the tricyclic framework. Moreover, both of these dianions showed significant countercation effects in the absorption spectra, with drastic color changes. These results have provided deep insights into the fundamental nature of boron-containing π-conjugated systems and their potential applicability as a new type of optoelectronic materials.

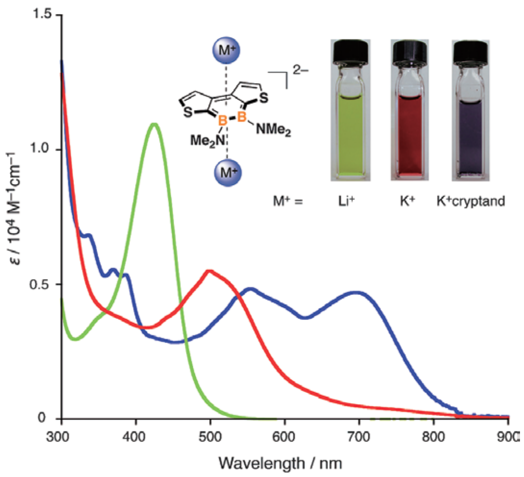


**Figure 2.** Absorption spectra of salts of 1,2-diborin dianion ($Li^+$, $K^+$, and $K^+$-([2.2.2]cryptand) in THF, together with photographs of their solutions in THF.

# Division of Synthetic Chemistry
## – Synthetic Organic Chemistry –

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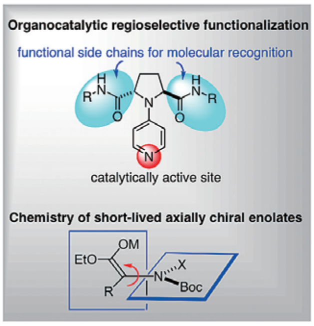
## Scope of Research

The research interests of the laboratory include the development of advanced molecular transformation, total synthesis of biologically active products, and molecular recognition. Programs are active in the areas of asymmetric alkylation of carbonyl compounds based on "memory of chirality", organocatalysis for fine organic syntheses, synthesis of unusual amino acids and nitrogen heterocycles, regioselective functionalization of carbohydrates, and the structural and functional investigation of heterochiral oligomers.

**KEYWORDS**
Organocatalysis
Regioselective Functionalization
Dynamic Chirality
Unusual Amino Acid
Molecular Recognition



### Selected Publications

Kawabata, T.; Matsuda, S.; Kawakami, S.; Monguchi, D.; Moriyama, K., Stereochemical Diversity in Asymmetric Cyclization via Memory of Chirality, *J. Am. Chem. Soc.*, **128,** 15394-15395 (2006).

Kawabata, T.; Muramatsu, W.; Nishio, T.; Shibata,T.; Schedel, H., A Catalytic One-Step Process for the Chemo- and Regiocelective Acylation of Monosaccharides, *J. Am. Chem. Soc.*, **129,** 12890-12895 (2007).

Kawabata, T.; Moriyama, K.; Kawakami, S. Tsubaki, K., Powdered KOH in DMSO: An Efficient Base for Asymmetric Cyclization via Memory of Chirality at Ambient Temperature, *J. Am. Chem. Soc.*, **130,** 4153-4157 (2008).

Kawabata, T.; Jiang, C.; Hayashi, K.; Tsubaki, K.; Yoshimura, T.; Majumdar, S.; Sasamori, T.; Tokitoh, N., Axially Chiral Binaphthyl Surrogates with an Inner N-H-N Hydrogen Bond, *J. Am. Chem Soc.*, **131,** 54-55 (2009).

Yoshida, K.; Furuta, T.; Kawabata, T., Organocatalytic Chemoselective Monoacylation of 1,n-Linear Diol, *Angew. Chem. Int. Ed.*, **50,** 4888-4892 (2011).

Yoshida, K.; Mishiro, K.; Ueda, Y.; Shigeta, T.; Furuta, T.; Kawabata, T., Nonenzymatic Geometry-Selective Acylation of Tri- and Tetrasubstituted α,α'-Alkenediols, *Adv. Syn. Catal.*, **354,** 3291-3298 (2012).

Yoshimura, T.; Takuwa, M.; Tomohara, K.; Uyama, M.; Hayashi, K.; Yang, P.; Hyakutake, R.; Sasamori, T.; Tokitoh, N.; Kawabata, T., Protonation-Assisted Conjugate Addition of Axially Chiral Enolates: Asymmetric Synthesis of Multisubstituted β-Lactams from α-Amino Acids, *Chem. Eur. J.*, **18,** 15330-15336 (2012).

## The First Example of Nonenzymatic Geometry-Selective Acylation of Tetrasubstituted α,α’-Alkenediols

Selective functionalization of hydroxy groups in polyol substrates is important in organic transformation. Differentiation of hydroxy groups of unsymmetrically substituted 2-alkylidene-1,3-propanediols has been expected to be difficult due to the similar intrinsic reactivity of the two primary hydroxy groups. In accordance with the expectation, nonenzymatic methods for geometry-selective acylation of unsymmetrically *trisubstituted* 2-alkylidene-1,3-propanediols has never been reported, while highly selective enzymatic acylation of the diols and deacylation of the corresponding diesters have been reported. However, no methods including enzymatic protocols for the *differentiation of primary hydroxy groups of tetrasubstituted 2-alkylidene-1,3-propanediols* have been reported. Here we report the first example of the highly geometry-selective acylation of tetrasubstituted 2-alkylidene-1,3-propanediols promoted by artificial catalysts. Highly *E*-selective acylation of various tetrasubstituted 2-alkylidene-1,3-propanediols was achieved in 96~>99 % selectivity by treatment of the diol substrates with acetic anhydride in the presence of 10 mol% of organocatalyst **1**.

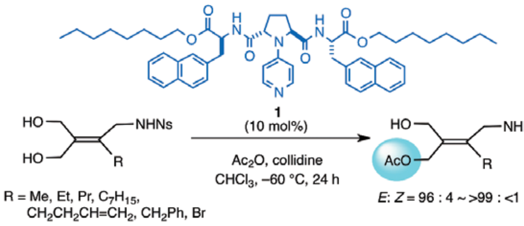


**Figure 1.** Geometry-selective acylation of tetrasubstituted α,α’-alkenediols promoted by organocatalyst **1**.

## A Catalytic One-Step Method for Regioselective Manipulation of Biologically Active Complex Natural Products

Chemo- and regioselective manipulation of one of the multiple hydroxy groups of polyol natural products has been a fundamental challenge in organic synthesis. We describe here a regiochemical profile of acylaion of a complex polyol natural product possessing eight free hydroxy groups, lanatoside C (**2**), a clinically used cardiac glycoside, which is composed of a tetrasaccharide containing a terminal glucopyranoside and an aglycon named digoxigenin. The acylation of **2** was examined with catalyst **3** and DMAP. In the presence of 10 mol% of **3**, acylation took place predominantly at C(4’’’’)-OH in 90% regioselectivity and 87% yield for monoacylation on treatment of **2** with isobutyric anhydride in $CHCl_3$-THF (9:1) at –60 °C. On the other hand, DMAP catalyzed acylation of **2** gave the C(3’’’’)-*O*-acylate in up to 97% regioselectivity. Thus, diverse regioselective introduction of acyl groups among eight free hydroxy groups of lanatoside C was achieved. Various functionalyzed acyl groups were also regioselectively introduced at C(4’’’’)-OH by employing an mixed anhyride method in the presence of catalyst **3** and the related organocatalyst.

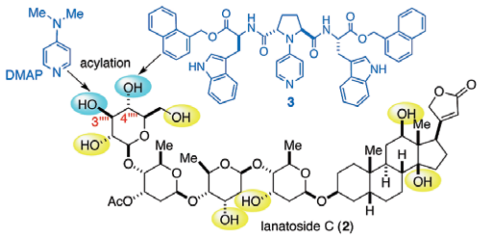
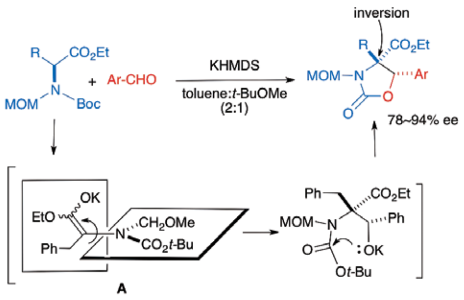


**Figure 2.** One-step regioselective introduction of acyl groups into lanatoside C (**2**) by organocatalysis.

## Asymmetric Aldol Reaction via Memory of Chirality

Asymmetric aldol reaction of α-amino acid derivatives via memory of chirality has been developed. Although asymmetric aldol reactions have extensively developed, the present method has unique characteristics in which asymmetric induction is controlled solely by the enolate chirality in the absence of chiral catalysts or chiral auxiliaries. The reaction was assumed to proceed via axially chiral enolate intermediate **A** to give the chiral aldolate in inversion of the configutaion at the newly formed tetrasubstituted carbon center. Chiral oxazolidones were obtained by intramolecular acylation of the aldolate. Thus, chiral oxazolidone derivatives with contiguous tetra- and tri-substituted chiral centers were readily obtained from abundant α-amino acids in a highly diastereoselective and enantioselective manner. Chiral oxazolidones have been known to be useful chiral auxiliaries in organic synthesis, and recently disclosed to be a novel class of antibiotics. Oxazolidones obtained by the present method are the structural equivalent to β-hydroxy-α-amino acids with a tetrasubstituted carbon center, which are the frequently observed structural subunits in biologically active natural products.



# Division of Synthetic Chemistry
## –Advanced Inorganic Synthesis–

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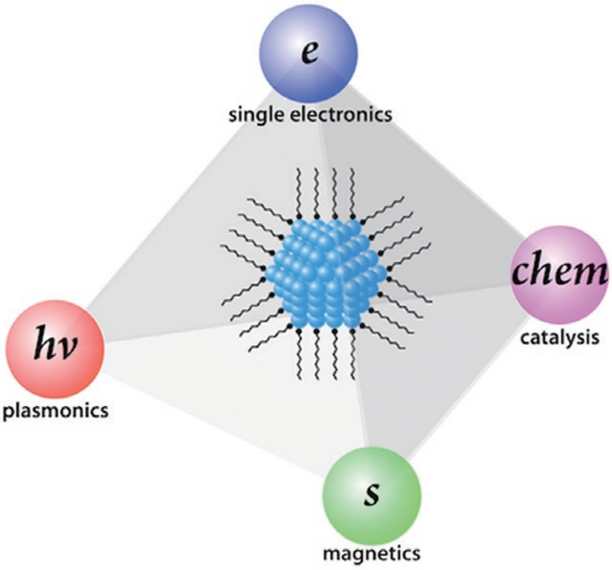
## Scope of Research

We are focusing on the precise synthesis of inorganic nanoparticles by controlling the primary (size, shape, composition, etc.) and secondary (spatial arrangement) structures to tune their properties, such as electron confinement, carrier oscillation, spin, and catalysis. These high quality inorganic nanoparticles are applied to both high-performance nanodevices (single electron transistor, plasmon waveguide, nanocomposite magnet) and photo-energy conversion materials (overall water splitting, solar cell).



**KEYWORDS**
Inorganic Nanoparticles
Single Electronics
Plasmonics
Nanocomposite Magnet
Photocatalysts

### Selected Publications

Sakamoto, M.; Tanaka, D.; Tsunoyama, H.; Tsukuda, T.; Minagawa, Y.; Majima, Y.; Teranishi, T., Platonic Hexahedron Composed of Six Organic Faces with an Inscribed Au Cluster, *J. Am. Chem. Soc.*, **134**, 816-819 (2012).

Furube, A.; Yoshinaga, T.; Kanehara, M.; Teranishi, T., Electric Field Enhancement in NIR Two-Photon Absorption by Indium Tin Oxide Nanoparticle Film, *Angew. Chem. Int. Ed.*, **51,** 2640-2642 (2012).

Maeda, K.; Okabayashi, N.; Kano, S.; Takeshita, S.; Tanaka, D.; Sakamoto, M.; Teranishi, T.; Majima. Y., Logic Operations of Chemically Assembled Single-Electron Transistor, *ACS Nano*, **6,** 2798-2803 (2012).

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Kanehara, M.; Arakawa, H.; Honda, T.; Saruyama, M.; Teranishi, T., Large-Scale Synthesis of High-Quality Metal Sulfide Semiconductor Quantum Dots with Tunable Surface-Plasmon Resonance Frequencies, *Chem. Eur. J.*, **18,** 9230-9238(2012).

Ikeda, T.; Xiong, A.; Yoshinaga, T.; Maeda, K.; Domen, K.; Teranishi, T., Polyol Synthesis of Size-controlled Rh Nanoparticles and Their Application to Photocatalytic Overall Water Splitting under Visible Light, *J. Phys. Chem. C* (in press).

## Platonic Hexahedron Composed of Six Organic Faces with an Inscribed Au Cluster

The structures of nanomaterials determine their individual properties and the suprastructures they can form. Introducing anisotropic shapes and/or interaction sites to isotropic nanoparticles has been proposed to extend the functionality and possible suprastructure motifs. Because of symmetric anisotropy, Platonic solids with regular polygon faces are one of the most promising nanoscale structures. Introduction of Platonic solid anisotropy to isotropic nanomaterials would expand the functionality and range of possible suprastructure motifs. We demonstrate a novel strategy to obtain nano-Platonic solids through the face coordination of square porphyrins on an inscribed Au sphere with adequate size. The face coordination of the multidentate macrocyclic porphyrin thioester derivatives: tetrakis-5α,10α,15α,20α-(2-acetylthiomethylphenyl) porphyrin ($SC_1P$), and tetrakis-5α,10α,15α,20α-(2-acetylthioethylphenyl) porphyrin ($SC_2P$) (Figure 1a), with four acetylthio groups facing the same direction, on the Au cluster encased the Au cluster in a Platonic hexahedron with six porphyrin faces (Figure 1). These hexahedra are regarded as novel “artificial atoms” with anisotropically interactive faces. We believe that this approach using spherical nanoparticles is a novel self-assembly technique, because the formation of Platonic solid is automatically determined by the relationship between the diameter of the inscribed sphere and shapes/sizes of the polygonal faces.

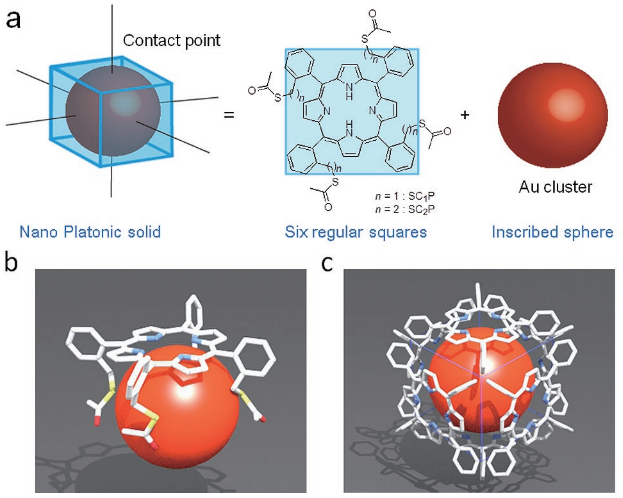

**Figure 1.** (a) Strategy for assembling the platonic solid from porphyrins and a Au cluster. Chemical structures of $SC_nP$ are also shown. (b) Schematic illustration of the coordination fashion of $SC_1P$ on the Au cluster. Hydrogen atoms are omitted for clarity. (c) Schematic illustration of the Platonic hexahedron constructed with six porphyrin faces and an inscribed Au sphere. Only the tetraphenylporphyrin moieties are shown for clarity.

## Electric-Field Enhancement in an Indium–Tin Oxide (ITO) Nanoparticle Film

Nanoparticles (NPs) of noble metals such as gold and silver are well-known to have strong plasmon bands in the visible region and show unique optical characteristics because of an enhanced near-field electric field at the NP surface. We have recently reported that indium–tin oxide (ITO) NPs have a unique plasmon property in the near-infrared (NIR) range and the peak wavelength can be easily tuned by controlling the amount of Sn doping. Here, we have applied transient absorption spectroscopy to a dye-coated ITO NP film, where dye absorption is present at half the wavelength of the plasmon resonance so that two-photon-induced transient absorption can be expected. Since a two-photon process occurs only in a strong electric field, we can selectively observe the near field generated by ITO NPs.

The enhancement of the electric properties of a dye molecule (IR26) by indium–tin oxide nanoparticles (ITO NPs, Figure 2) has been shown by measuring the near-infrared two-photon-excited transient absorption spectra. It was found that the dye molecules were excited much more efficiently in the presence of an ITO NP layer by a factor of 30 compared to the control sample without ITO NPs. The results show that NPs of transparent conductive metal oxides can possibly be applied in plasmonic sensors and solar cells, because in general NIR light interacts weakly with chemical substances in the wavelength window ranging from the UV/Vis electronic transition region and the IR vibrational region.

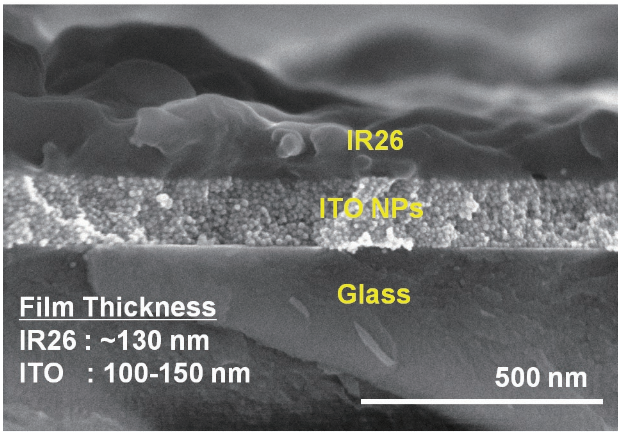

**Figure 2.** SEM image of IR26-coated ITO NP layer on a glass substrate.

# Division of Materials Chemistry
## – Chemistry of Polymer Materials –

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### Visitor

Mr FERRIER, Robert University of Pennsylvania, U.S.A., 19 June–21 August

## Scope of Research

Kinetic and mechanistic analyses are made for better understandings of the chemical and physicochemical reactions occurring in polymerization systems and for better routes to the synthesis of well-defined polymers. By various polymerization techniques, in particular, living polymerizations, new well-defined polymers or polymer assemblies are prepared, and their structure/properties relationships are precisely analyzed. Projects in progress include: (1) Kinetics and mechanisms of living radical polymerization (LRP). (2) Synthesis of new polymeric materials by living polymerizations and their structure/properties studies. (3) Synthesis, properties, and applications of concentrated polymer brushes (CPB).

### KEYWORDS

Precision Polymerization
Living Radical Polymerization
Polymer Brush
Hybrid Materials
Biointerface

### Selected Publications

Tsujii, Y.; Nomura, Y.; Okayasu, K.; Gao, W.; Ohno, K.; Fukuda, T., AFM Studies on Microtribology of Concentrated Polymer Brushes in Solvents, *J. Phys.: Conf. Ser.*, **184,** no. 012031 (2009).

Arita, T.; Kayama, Y.; Ohno, K.; Tsujii, Y.; Fukuda, T., High-Pressure Atom Transfer Radical Polymerization of Methyl Methacrylate for Well-Defined Ultrahigh Molecular-Weight Polymers, *Polymer*, **49,** 2426-2429 (2008).

Tsujii, Y.; Ohno, K.; Yamamoto, S.; Goto, A.; Fukuda, T., Structure and Properties of High-Density Polymer Brushes Prepared by Surface-Initiated Living Radical Polymerization, *Adv. Polym. Sci.*, **197,** 1-45 (2006).

Ohno, K.; Morinaga, T.; Takeno, S.; Tsujii, Y.; Fukuda, T., Suspension of Silica Particles Grafted with Concentrated Polymer Brush: Effects of Graft Chain Length on Brush Layer Thickness and Colloidal Crystallization, *Macromolecules*, **40,** 9143-9150 (2007).

Ohno, K.; Morinaga, T.; Koh, K.; Tsujii, Y.; Fukuda, T., Synthesis of Monodisperse Silica Particles Coated with Well-Defined, High-Density Polymer Brushes by Surface-Initiated Atom Transfer Radical Polymerization, *Macromolecules*, **38,** 2137-2147 (2005).

## Novel Tribomaterials of Cellulosic-Nanofiber Sheets with Well-Defined Bottle-Brushes

Previously, we developed a novel graft-type of gels, i.e., a gel of cross-linked bottle brushes, having an excellent-lubricating property. The key to success was to keep the side-chain length short enough to achieve the CPB effects (including super lubrication) originating from the highly stretched-chain conformation and high-density segmental density in a solvent, where CPB represents the concentrated polymer brush (successfully and systematically synthesized by controlled radical polymerization techniques). In order to further improve the mechanical property, we have attempted to reinforce it by nano-fibers; in brief, the bacteria-producing hydrogel containing cellulosic nanofibers (CNF) was hot-pressed into a non-woven sheet with an excellent mechanical strength, which was filled up with bottle brushes of short side chains of poly(styrene) (PS). Figure 1 shows the scanning electron micrographs on the surface of the CNF sheet before and after incorporating the bottle brush, suggesting the well-defined, higher-order structure. The frictional property was measured in toluene, a good solvent for PS, on the surfaces of the composite as well as original CNF sheets. Figure 1 plots the frictional coefficient $\mu$ as a function of shear velocity $v$, clearly suggesting that the filling with the bottle brush much improves the lubricating property. Similar structure can be found in the articular cartilage of a human joint, but the difference is the mechanism for lubrication, that is the electrostatic interaction of charged groups but not the CPB effect. We believe that this study will open up a new route to novel tribomaterials on the based on the CPB concept.

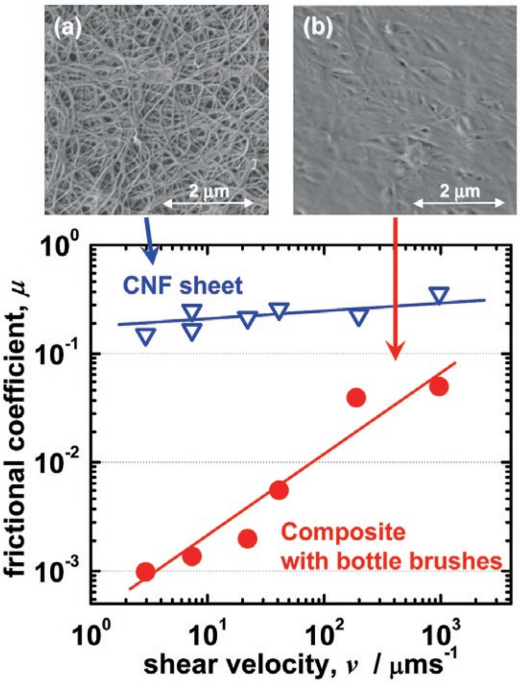

**Figure 1.** SEM images (a, b) and frictional property (plot of $\mu$ vs $v$ in toluene) on the surfaces of the CNF sheets with and without bottle brushes insides.

## Blood Clearance and Biodistribution of Polymer Brush-Afforded Silica Particles Prepared by Surface-Initiated Living Radical Polymerization

The physiological properties of polymer brush-afforded silica particles prepared by surface-initiated living radical polymerization were investigated in terms of the circulation lifetime in the blood and distribution in tissues. A series of hybrid particles were synthesized by varying the diameter of the silica core and the chain length of the polymer brush in order to examine the relationship between their physicochemical and physiological properties. The hybrid particles were injected intravenously into mice to systematically investigate their blood clearance and body distribution. It was revealed that the structural features of the hybrid particles significantly affected their *in vivo* pharmacokinetics. Some hybrid particles exhibited an excellently prolonged circulation lifetime in the blood with a half-life of about 20 h. When such hybrid particles were injected intravenously into a tumor-bearing mouse, they preferentially accumulated in tumor tissue. The tumor-targeted delivery was optically visualized using hybrid particles grafted with fluorescence-labeled polymer brushes.

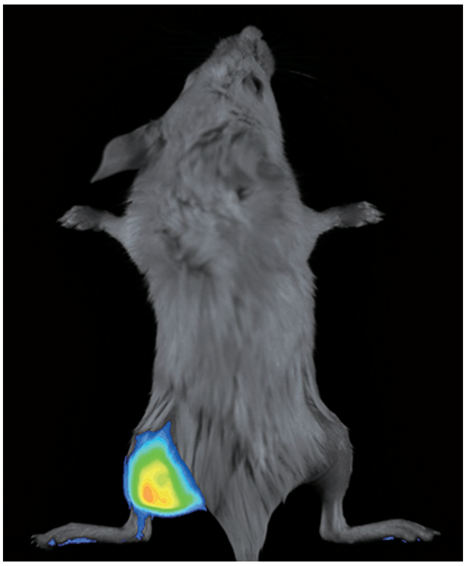

**Figure 2.** Optical fluorescence image of tumor-bearing mouse taken at 24 h post-injection of hybrid particles grafted with fluorescence-labeled polymer brush.

# Division of Materials Chemistry
## – Polymer Controlled Synthesis –

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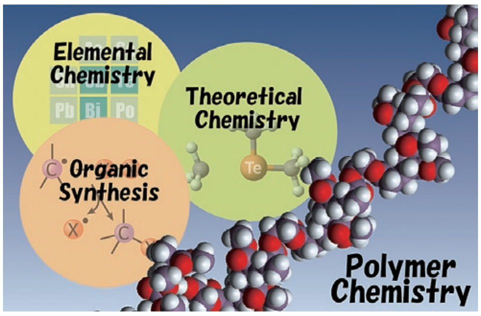
TAKU, Setsu (M1)
FUJII, Akira (M1)
CHEN, Tao (RS)
KURACHI, Daisuke (UG)
NOGUCHI, Naoki (UG)
MAEDA ,Yuuki (UG)

## Visitors

| | |
|---|---|
| Dr LUTZ, Jean-François | Institut Charles Sadron, Strasbourg, France, 18 January |
| Prof CRUDDEN, Cathleen M | Department of Chemistry, Queen's University, Kingston, Canada, 1 March |
| Prof WAGENER, Kenneth B | University of Florida, Florida, U.S.A., 17 May |
| Prof MUÑIZ, Kilian | Institute of Chemical Research of Catalonia (ICIQ), Tarragona, Spain, 20 November |
| Assoc Prof ZETTERLUND, Per B | Centre for Advanced Macromolecular Design (CAMD), The University of New South Wales, Australia, 20 December |

## Scope of Research

Our research focuses on creation of new organic molecules which would become key reagents and materials for future science and technologies. Furthermore, we have been developing new organic and polymeric materials based on our tailor-made molecules. One such topic is the development of new living radical polymerization method utilizing heavier heteroatom compounds as controlling agents. The other topic is the synthesis of cycloparaphenylenes, hoop-shaped $\pi$-conjugated molecules, based on new synthetic strategy. We also study various polymer condensed states by both static and dynamic methods to understand the relation of physical properties and structures.



**KEYWORDS**
Organic Synthesis
Polymer Synthesis
Living Radical Polymerization
Polymer Properties
Conjugated $\pi$-molecules

## Selected Publications

Nakamura, Y.; Arima, T.; Tomita, S.; Yamago, S., Photoinduced Swiching from Living Radical Polymerization to a Radical Coupling Reaction Mediated by Organotellurium Compounds, *J. Am. Chem. Soc.*, **134**, 5536-5539 (2012).

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Kayahara, E.; Yamada, H.; Yamago, S., Generation of Carbanions via Stibin-Metal and Bismuthine-Metal Exchange Reaction and Its Applications to Precision Synthesis of $\omega$-End Functionaized Polymers, *Chem. Eur. J.*, **17,** 5272-5280 (2011).

Nakamura, Y.; Kitada, Y.; Kobayashi, Y.; Ray, B.; Yamago, S., Quantitative Analysis of the Effect of Azo Initiators on the Structure of $\alpha$-Polymer Chain Ends in Degenerative Chain Transfer-Mediated Living Radical Polymerization Reactions, *Macromolecules*, **44,** 8388-8397 (2011).

## Photoinduced Switching from Living Radical Polymerization to a Radical Coupling Reaction Mediated by Organotellurium Compounds

Modulation of the reaction pathway using external stimuli has been a significant challenge in organic and polymer syntheses, because such methods would considerably expand the structural diversity of products from a limited number of precursors. Although a variety of chemical stimuli have been used for this purpose, physical stimuli, such as thermal and photochemical stimuli, like those used in the pericyclic reactions, are attractive due to their “green” character.

We have already reported that organotellurium-mediated living radical polymerization (TERP) possesses several synthetic advantages such as high monomer versatility, high compatibility toward functional groups and solvents, and ease of the living-end transformation for the synthesis of block copolymers and end-functionalized polymers. While expanding the synthetic applicability of TERP to dienes, we found that the reaction pathway can be selectively switched from LRP to a radical-coupling reaction (RC) by using photostimuli (Figure 1). Structurally well-defined telechelic polyisoprenes and ABA-triblock copolymers were prepared by successive organotellurium-mediated living radical polymerization (TERP) under thermal conditions, followed by a polymer-end radical coupling reaction under photoirradiation.

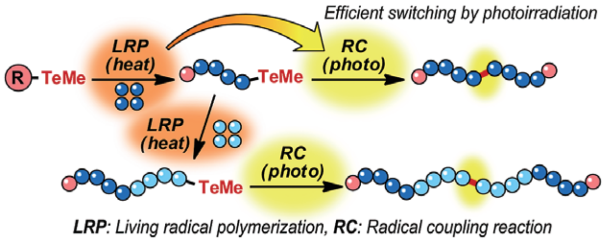

**Figure 1.** Switching of reaction pathway.

## Formation of the Shortest Fullerene-Peapod

Cycloparaphenylenes (CPPs) are hoop-shaped π-conjugated molecules in which paraphenylene units are linked in a cyclic manner (Figure 2). They represent the simplest structural unit of armchair carbon nanotubes. Based on the analogy to layered carbon networks with curved surfaces, the concave cavity of the CPPs should act as a host for π-conjugated molecules with a convex surface, such as fullerenes. Such a host–guest complex would be a suitable model for elucidating convex–concave π–π interactions. We found that [10]CPP selectively encapsulated $C_{60}$ forming the shortest fullerene-peapod, [10] CPP $\supset$ $C_{60}$, among several CPPs prepared by the method we have developed (Figure 3). This finding opens the possibility of utilizing CPPs as size- and shape-selective host molecules for various guest molecules, such as higher fullerenes, metallofullerenes, and carbon nanotubes. Such complementary host–guest chemistry will be useful for the size- and shape-selective separation of higher fullerenes and carbon nanotubes.

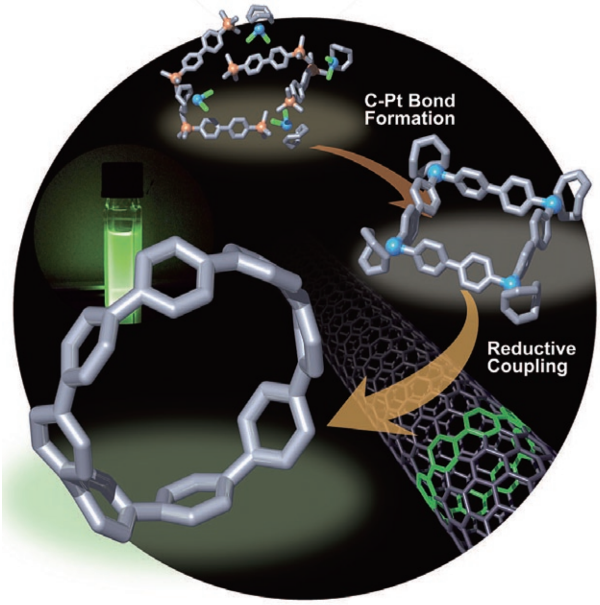

**Figure 2.** Synthesis of CPP.

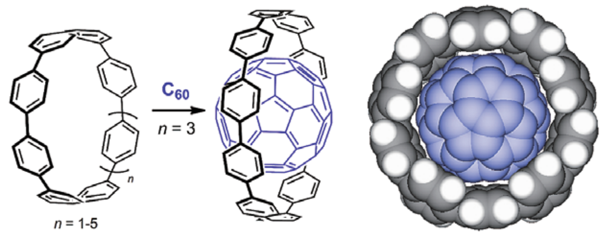

**Figure 3.** Formation of the shortest fullerene-peapod.

# Division of Materials Chemistry
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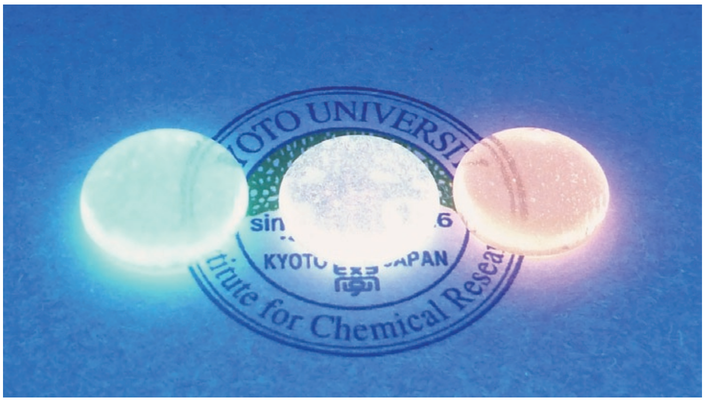
## Scope of Research

In the laboratory, the main subject is to create novel functional amorphous materials such as organic-inorganic hybrids, polycrystalline and amorphous inorganic oxides. For obtaining such materials, the amorphous structure and the property are investigated by XRD, MAS NMR, thermal and optical analysis and quantum chemical calculations. Currently, we are trying to prepare novel amorphous-based optical functional materials such as proton conducting membrane, optical biosensor, and amorphous phosphor.

**KEYWORDS**
Amorphous Oxide Phosphor
Low Melting Glass
Organic-Inorganic Hybrid Materials
Optical Microbiosensor
Proton Conducting Membrane



## Selected Publications

Tokuda, Y.; Oka, T.; Takahashi, M.; Yoko, T., Inhomogeneous Distribution of $Na^+$ in Alkali Silicate Glasses, *J. Ceram. Soc. Japan*, **199,** 909-915 (2011).

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Masai, H.; Takahashi, Y.; Fujiwara, T.; Matsumoto, S.; Yoko, T., High Photoluminescent Property of Low-Melting Sn-Doped Phosphate Glass, *Applied Physics Express*, **3,** [082102-1]-[082102-3] (2010).

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## Preparation of Proton Conductive Membranes with Graded Monomer Conversion

Future advances in fuel cell technology are contingent on the development of new materials. One such material is the Nafion membrane (DuPont); it is a proton-conducting membrane and has been employed in polymer electrolyte fuel cells (PEFCs). However, the PEFC faces problems including poor carbon monoxide tolerance and heat rejection in temperatures between 60 and 80°C. In order to overcome these drawbacks, a proton-conducting membrane is required to operate at intermediate temperatures around 100–150°C and should possess good durability and thermal stability.

In this study, we describe a novel technique to prepare a membrane with a graded monomer conversion using ultraviolet light (UV) irradiation during radical photo-polymerization. A schematic procedure is shown in Figure 1. High conversion at the surface of the membrane enhanced durability while low conversion at the inner part of the membrane facilitated proton conductivity. This incremental change in the proton conductivity is possible because p$K_{a1}$ of vinylphosphonic acid (VPA) is 2.74 and p$K_{a2}$ is 7.34, while p$K_a$ of PVPA is around 5–6. Copolymerization of VPA with an additive monomer of hydrophobic nature having a low chain transfer constant leads to an increase in the conversion of the additive polymer.

The proton conductivity of the present membrane was $6.3\times10^{-4}$ Scm$^{-1}$ at 150°C even under dry conditions. The durability of the membrane VET-ht was much higher than that of polyvinylphosphonic acid, PVPA. The membrane was also thermally stable up to 200°C. These properties contribute to overcome the conventional problems associated with decreases in proton conductivity of polymer electrolytes at intermediate temperatures between 100 and 150°C.

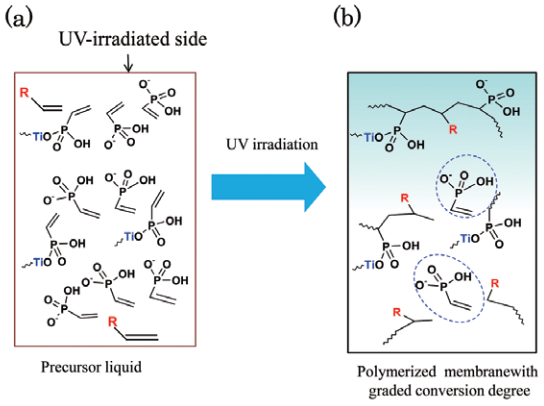

**Figure 1.** Schematic representation of membrane with graded degrees of polymerization:
(a) titanophosphite precursor.
(b) copolymerized membrane with graded degrees of polymerization.

## Fabrication of Rare Earth-free Amorphous Oxide Phosphor

Nowadays, rare earth (RE)-containing materials have been used as white-emitting devices. However, these white-emitting devices consisting of sharp emission bands of RE possess lower color rendering than the conventional broad band emission device. Moreover, since there is uncertainty about the stable supply of RE over the future, it is worthwhile to examine RE-free emitting material. We have focused on the RE-free phosphors that have been used for white fluorescent lamp. It is expected that white light emission can be attained by RE-free phosphor, for example $Sb^{3+}$, $Mn^{2+}$-doped calcium halophosphate. On the other hand, if glass material without the RE cation shows white light emission comparable to the crystalline phosphor, it will be considered a novel emitting material capable of much broader emission and good formability that is quite important in the industrial manufacturing process.

Recently, we have reported the highest quantum efficiency (QE) for amorphous SnO-ZnO-$P_2O_5$ low-melting glass. It is notable that the transparent oxide glass containing no RE cation shows high UV-excited emission that is comparable to crystal phosphor such as $MgWO_4$; further, this was the largest efficiency of glass material without RE cation ever reported. The broad emission is brought about by $Sn^{2+}$, which is the most conventional and harmless ns$^2$ type center. Our group has also demonstrated white light emission of RE-free Mn-doped SnO-ZnO-$P_2O_5$ glass. The transparent glass showed blue ~ white ~ red emission, which depended on the amount of MnO (Figure 2). In particular, some glasses showed white light emission with a high value of quantum efficiency comparable to $MgWO_4$ crystalline phosphor, which suggests that RE-free glass phosphor is very fascinating material from the viewpoint of unique emission mechanisms in a random matrix.

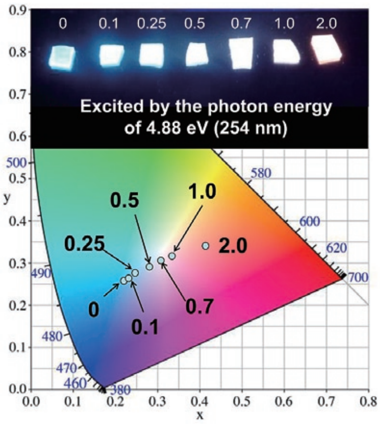

**Figure 2.** Chromaticity coordinates of the $x$MnO-2.5SnO-57.5ZnO-40$P_2O_5$ glasses. Inset shows a photograph of these glasses under exposure to the photon energy of 4.88 eV (254 nm).

# Division of Materials Chemistry
## – Nanospintronics –

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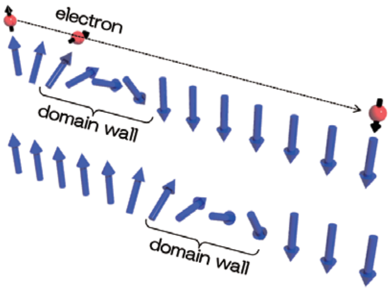
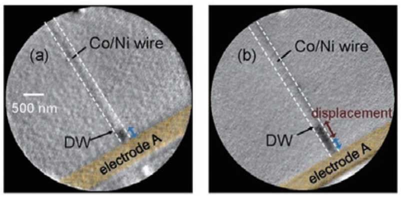
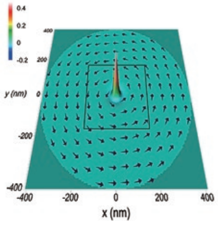
## Scope of Research

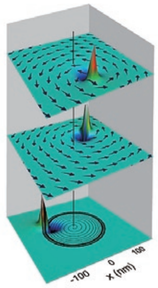
The conventional electronics utilizes only the "charge" of electrons, while the traditional magnetic devices use only "spin" degree of freedom of electrons. Aiming at the complete control of both charge and spin in single solid-state devices, an emerging field called *spintronics* is rapidly developing and impacting on information technologies. By combining the atomic-layer deposition with nanofabrication, we focus on the development of spin properties of various materials and the control of quantum effects in mesoscopic systems for novel spintronics devices.

**KEYWORDS**
Spintronics
Quantum Transport
Nano-fabrication
Artificial Materials









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## Enhancement in Switching Speed of Magnetic Domain Wall by Voltage Application

Controlling the displacement of a magnetic domain wall is potentially useful for information processing in magnetic non-volatile memories and logic devices. A magnetic domain wall can be moved by applying an external magnetic field and/or electric current, and its velocity depends on their magnitudes. We showed that the applying an electric field could change the velocity of a magnetic domain wall significantly. A field-effect device, consisting of a top-gate electrode, a dielectric insulator layer, and a wire-shaped ferromagnetic Co thin layer with perpendicular magnetization, was used to observe it in a finite magnetic field (Figure 1). We found that the application of the electric fields can change the magnetic domain wall velocity by more than an order of magnitude (Figure 2). This significant change is due to electrical modulation of the energy barrier for the magnetic domain wall motion. We think that the concept presented here will be useful in reducing the energy consumption of magnetic recording media and logic devices.

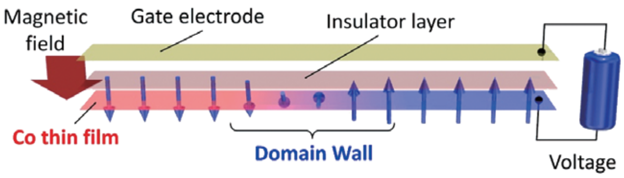

**Figure 1.** Schematic illustration of the device structure. The device consists of a Co microwire, an insulator layer, and a gate electrode on top. The magnetic domain wall was prepared in the wire to investigate the speed of it under applying voltage.

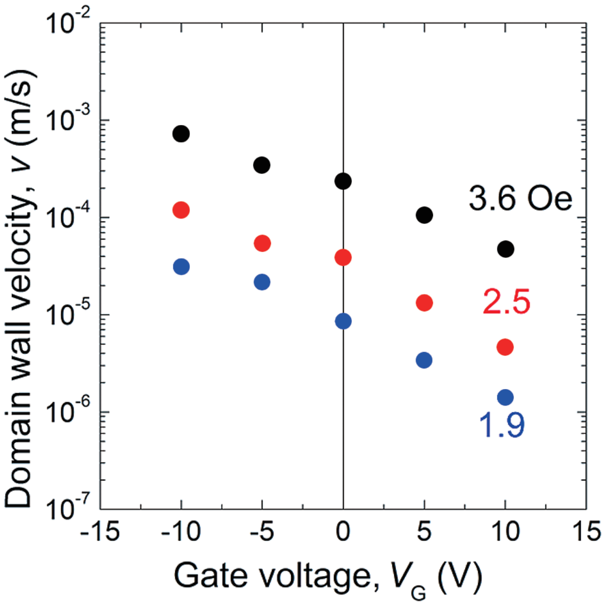

**Figure 2.** Applied voltage dependence of the domain wall speed.

## Spin-motive Force Due to a Gyrating Magnetic Vortex

A change of magnetic flux through a circuit induces an electromotive force. By analogy, a recently predicted force that results from the motion of non-uniform spin structures has been termed the spin-motive force (Figure 3). Although recent experiments seem to confirm its presence, a direct signature of the spin-motive force has remained elusive. We report the observation of a real-time spin-motive force produced by the gyration of a magnetic vortex core (Figure 4). We find a good agreement between the experimental results, theory and micromagnetic simulations, which taken as a whole provide strong evidence in favour of a spin-motive force.

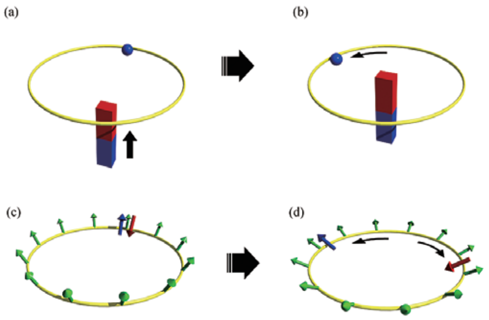

**Figure 3.** (a-b) A change of magnetic flux through a closed circuit induces an electromotive force which drives an electron flow (c-d) A motion of non-uniform spin structures induces the spin-motive force which drives a spin current flow.

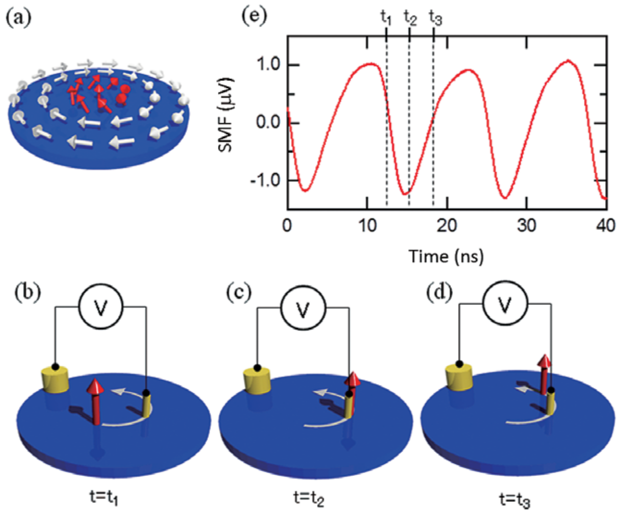

**Figure 4.** (a) A vortex state in a micron-size magnetic disk. (b)-(d) Illustrations of the time domain measurements in a gyrating vortex core at a time t. The vortex core is indicated by the red arrow. (e) Experimentally observed spin motive force (SMF) as a function of time.

# Division of Biochemistry
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### Visitors

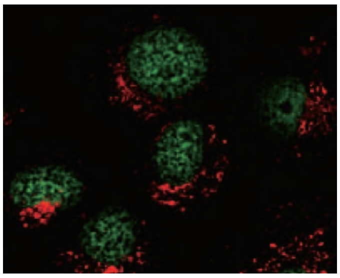
| | |
|---|---|
| Prof GRÄSLUND, Astrid | Stockholm University, Sweden, 23 January |
| Prof NEUNDORF, Ines | University of Cologne, Germany, 15 September |
| Prof XIA, Jiang | The Chinese University of Hong Kong, China, P.R., 15 September |

## Scope of Research

The ultimate goal of our research is the regulation of cellular functions by designed peptides and proteins. Current research subjects include (1) development of novel intracellular delivery systems aiming at elucidation and control of cellular functions using designed membrane permeable peptide vectors, (2) elucidation of the DNA binding and recognition modes of C2H2-type zinc finger proteins and design of artificial transcription factors with various DNA binding specificities, and (3) design of stimulation-responsible artificial peptides and proteins.

**KEYWORDS**

Membrane-Permeable Peptides
Intracellular Delivery
Peptide Design
Zinc Finger Protein



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Nakase, I.; Okumura, S.; Katayama, S.; Hirose, H.; Pujals, S.; Yamaguchi, H.; Arakawa, S.; Shimizu, S.; Futaki, S., Transformation of an Antimicrobial Peptide into a Plasma Membrane-Permeable, Mitochondria-Targeted Peptide via the Substitution of Lysine with Arginine, *Chem. Commun.*, **48,** 11097-11099 (2012).

Nakase, I.; Okumura, S.; Tanaka, G.; Osaki, K.; Imanishi, M.; Futaki, S., Signal Transduction Using an Artificial Receptor System that Undergoes Dimerization upon Addition of a Bivalent Leucine-Zipper Ligand, *Angew. Chem. Int. Ed.*, **51,** 7464-7477 (2012).

Hirose, H.; Takeuchi, T.; Osakada, H.; Pujals, S.; Katayama, S.; Nakase, I.; Kobayashi, S.; Haraguchi, T.; Futaki, S., Transient Focal Membrane Deformation Induced by Arginine-rich Peptides Leads to Their Direct Penetration into Cells, *Mol. Ther.*, **20,** 984-993 (2012).

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Imanishi, M.; Yamamoto, K.; Yamada, H.; Hirose, Y.; Okamura, H.; Futaki, S., Construction of a Rhythm Transfer System That Mimics the Cellular Clock, *ACS Chem. Biol.*, **7,** 1817-1821 (2012).

## Creation of Artificial Epidermal Growth Factor Receptor Activated by Coiled-Coil Peptides

Epidermal growth factor receptor (EGFR) regulates various signaling pathways to induce cellular functions (e.g. proliferation, survival). If activation of this receptor could be controlled on demand, the techniques contribute to a lot of valuable aspects of cellular regulations. However, because overexpression and overactivation of the EGFR lead to cancer-like modality, the control is difficult using intact receptor and ligands. From this point of view, our research objectives are to create artificial EGFR on cell membranes, which can be specifically activated with artificial ligands.

Coiled-coil has been used in numerous applications such as affinity purification, miniaturized antibodies, and receptor imaging. Using advantage of the coiled-coil peculiarities, we designed artificial EGFR, of which the receptor dimerization can be controlled by coiled-coil interactions. Growth factor binding to the extracellular region of EGFR promotes dimerization of the receptor and increases the tyrosine kinase activity of its intracellular domain. To create artificial EGFR and ligands, coiled-coil peptides (E3 and K4) were used. We designed surface-exposed tag sequence E3 fused EGFR (E3-EGFR) lacking domains I~III and a portion of domain IV, which participate in dimerization of the EGFR after binding of natural ligand (e.g. EGF) to the receptor. To dimerize the E3-EGFR, we synthesized conjugates of two K4 peptides (K4-conjugates), and the linker lengths (~10 angstrom) mimic distance during dimerization of the EGFR (Figure 1).

To test receptor activation, E3-EGFR expressed CHO cells were treated with the K4-conjugates, and this was followed by western blot assay for detection of receptor phosphorylation. Treatment of the cells with the K4-conjugates increased level of the phosphorylation in ~5 min, and enhanced lamellipodia formations and cell migrations were observed. This model-receptor system should be applicable to design of various receptors and other membrane-associated proteins to attain control of cellular functions.

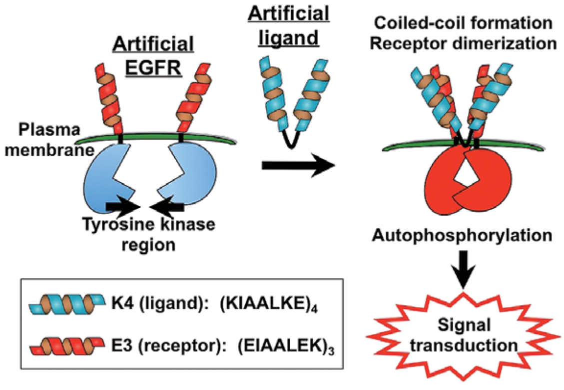

**Figure 1**. Concept of artificial EGFR activated by a helix peptide ligand via a coiled-coil formation.

## CXCR4 is a Receptor Stimulating the Cellular Uptake of Arginine-rich Cell-penetrating Peptides: the Relevance to Macropinocytosis and HIV Infection

The CXCR4 chemokine receptor is a co-receptor of HIV-1 infection in host cells. It has been reported that ligand binding to CXCR4 leads to its internalization via clathrin-dependent endocytosis. Here, through the photo-cross-linking study to identify receptors involved in internalization of oligoarginine cell-penetrating peptides (CPPs), we found that CXCR4 serves as a receptor that stimulates internalization of the arginine 12-mer peptide (R12), in which actin-driven fluid-phase endocytosis (macropinocytosis) plays an important role in cellular uptake. Interestingly, CXCR4 was responsible for the uptake of R12 (Figure 2), but there was no significant effect for the uptake of the arginine 8-mer (R8) or the HIV-1 TAT derived CPP. We also found that stimulating CXCR4 with its intrinsic ligands, stromal cell-derived factor 1α (SDF-1α) and HIV-1 envelope glycoprotein 120 (gp120), induced macropinocytosis. R12 had activity to prevent viral infection for HIV-1$_{\mathrm{IIIB}}$, a subtype of HIV-1 that uses CXCR4 as a co-receptor for entry into susceptible cells. On the other hand, the addition of macropinocytosis inhibitor, dimethylamiloride (DMA), resulted in enhancement of viral infection. Thus, the present study showed that CXCR4 triggers macropinocytosis, which may have implications for the cellular uptake of oligoarginine CPPs and internalization of HIV.

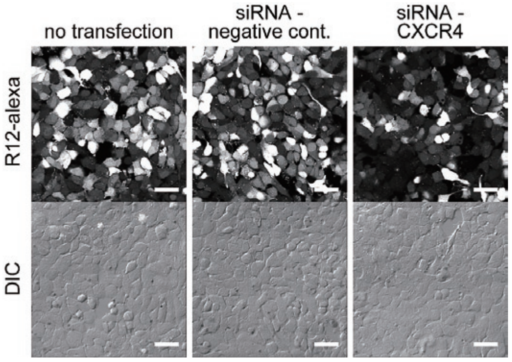

**Figure 2.** Down-regulation of CXCR4 led to diminished cellular uptake of R12-alexa. HeLa cells were transfected with 10 nM CXCR4-targeted siRNA for 24 h followed by treatment with 10 μM R12-alexa for 30 min at 37°C. Cellular internalization of R12-alexa was analyzed by confocal microscopy.

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## Scope of Research

Our research focuses on the molecular design and synthesis of specific inhibitors of physiologically important enzymes (biocatalysts). The enzyme inhibitors are used for probing the reaction mechanisms, three-dimensional structures and identifying the physiological roles of the enzymes. The finely designed inhibitors are further elaborated to develop useful bioactive substances that could knockout the specific enzyme *in vivo* and to develop lead compounds for novel pharmaceuticals, agrochemicals and cosmetic ingredients. Our current research includes the design, synthesis and applications of transition-state analog and/or mechanism-based inhibitors of such enzymes as γ-glutamyl transpeptidase, a key enzyme in glutathione metabolism, asparagine synthetase, an important enzyme for cancer chemotherapy, and 4-coumaroyl CoA ligase that plays a pivotal role in the biosynthesis of a vast array of phenylpropanoid in plants. The identification of the genes of hitherto unknown enzymes for biosynthesis of phenylpropanoid volatiles in plants are also pursued to shed light on the detailed reaction mechanisms and the physiological function of the biosynthetic enzymes in plant secondary metabolites.

### KEYWORDS

Enzyme Reaction Mechanisms
Transition-State Analogue Inhibitors
Glutathione Homeostasis
Bioactive Substance
Plant Secondary Metabolite Biosynthesis

### Selected Publications

Ikeuchi, H.; Ahn, Y. M.; Otokawa, T.; Watanabe, B.; Hegazy, L.; Hiratake, J.; Richards, N. G., A Sulfoximine-based Inhibitor of Human Asparagine Synthetase Kills L-asparaginase-resistant Leukemia Cells, *Bioorg. Med. Chem.*, **20,** 5915-5927 (2012).

Sato, S.; Kawamoto, J.; Sato, S. B.; Watanabe, B.; Hiratake, J.; Esaki, N.; Kurihara, T., Occurrence of a Bacterial Membrane Microdomain at the Cell Division Site Enriched in Phospholipids with Polyunsaturated Hydrocarbon Chains, *J. Biol. Chem.*, **287,** 24113-24121 (2012).

Joyce-Brady, M.; Hiratake, J., Inhibiting Glutathione Metabolism in Lung Lining Fluid as a Strategy to Augment Antioxidant Defense, *Current Enzyme Inhibition*, **7,** 71-77 (2011).

Koeduka, T.; Watanabe, B.; Suzuki, S.; Hiratake, J.; Mano, J.; Yazaki, K., Characterization of Raspberry Ketone/Zingerone Synthase, Catalyzing the Alpha, Beta-Hydrogenation of Phenylbutenones in Raspberry Fruits, *Biochem. Biophys. Res. Commun.*, **412,** 104-108 (2011).

Ikeuchi, H.; Meyer, M. E.; Ding, Y.; Hiratake, J.; Richards, N. G. J., A Critical Electrostatic Interaction Mediates Inhibitor Recognition by Human Asparagine Synthetase, *Bioorg. Med. Chem.*, **17,** 6641-6650 (2009).

## Inhibitors Targeting Human Asparagine Synthetase for Cancer Chemotherapy

A standard current clinical protocol for acute lymphoblastic leukemia (ALL) is the use of the enzyme L-asparagine amidohydrolase (ASNase) that catalyzes the hydrolysis of L-Asn to deplete circulating L-Asn in blood. This chemotherapy is unique in that the proliferation of leukemia cells is suppressed by cutting off the supply of nutrient for rapid growth. The efficacy of ASNase chemotherapy, however, is hampered by the emergence of ASNase-resistant leukemic blasts; 10–12% of patients who initially go into remission undergo subsequent relapse. One widely-accepted hypothesis for ASNase resistance is the up-regulation of glutamine- and ATP-dependent asparagine synthetase (ASNS) that enables the leukemia cells to synthesize L-Asn necessary for their growth. Hence the inhibition of human ASNS is highly important in cancer chemotherapy, and we have synthesized a specific inhibitor of human ASNS. According to the proposed reaction mechanism of ASNS in which the β-carboxy group of L-Asp is activated by adenylation followed by nucleophilic substitution by ammonia to yield L-Asn, AMP and PPi, an *N*-adenylated sulfoximine **1** was synthesized as a transition-state analogue inhibitor of ASNS (Figure 1).

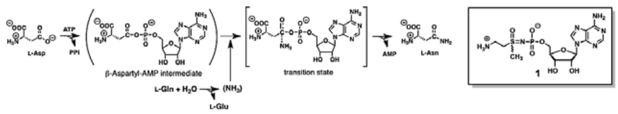

**Figure 1.** Reaction mechanism of asparagine synthetase and its transition-state analogue 1.

Compound **1** was found to be an extremely potent inhibitor of human ASNS; it inhibited the enzyme in a time-dependent manner with an overall $K_i$* of 8 nM (Figure 2). Furthermore, the inhibitor **1** suppressed cell proliferation of ASNase-resistant MOLT-4R leukemia cells (Figure 3). The suppression of cell proliferation was dose-dependent with an IC$_{50}$ of ca. 0.1 mM. Surprisingly, compound **1** induced cell death as well as suppression of cell proliferation at higher concentrations. ASNase-sensitive leukemia cells with low ASNS activity were much less sensitive toward compound **1**, suggesting that ASNS in itself was an essential enzyme for leukemia cells and was an important drug target for cancer chemotherapy.

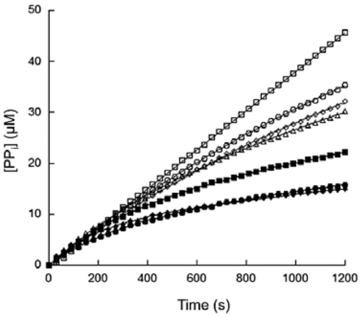

**Figure 2.** Time-dependent inhibition of human ASNS by compound **1** (0–5 μM).

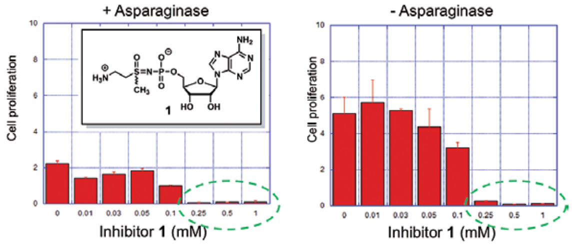

**Figure 3.** The effect of ASNS inhibitor **1** on the proliferation of ASNase-resistant MOLT-4 leukemia cells in the presence and absence of 1U asparaginase. (Left) MOLT-4 cells with ASNase; (right) MOLT-4R cells without ASNase. Cell proliferation is defined as the number of viable cells after 48 h incubation.

## Biosynthetic Pathway of Phenylpropanoid Volatiles in Plants

Phenylpropanoid volatiles including raspberry ketone and zingerone, are produced in plants, and are characteristic constituents in many fruits and spices, and floral bouquet. Double bond reductases, which recognize secondary metabolites such as (2*E*)-nonenal, (+)-pulegone, and furaneol derivatives, have been identified, but little is known about the presumably similar enzymes responsible for the biosynthesis of phenylpropanoid volatiles. By using a homology-based PCR, we isolated a cDNA encoding raspberry ketone/zingerone synthase (RZS) from raspberry fruits. The protein encoded by this cDNA can catalyze the NADPH-dependent reduction of 4-hydroxybenzalacetone and 3-methoxy-4-hydroxybenzalacetone to raspberry ketone and zingerone, respectively. The substrate specificity experiments suggested that RZS strictly discriminates the methyl group in the side chain of substrates. We are currently investigating other double-bond reductases that may be responsible for the branching of the biosynthetic pathway of phenylpropanoid volatiles in petunia flowers.

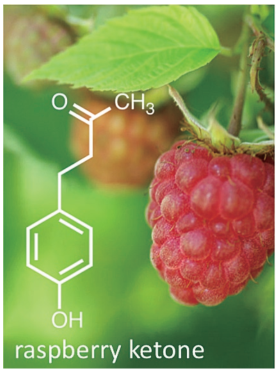

**Figure 4.** Characteristic aroma of raspberry fruits.

# Division of Biochemistry
## – Molecular Biology –

http://www.scl.kyoto-u.ac.jp/~molbio/index_e.html

Prof
AOYAMA, Takashi
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Assoc Prof
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TSUGE, Tomohiko
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Techn Staff
YASUDA, Keiko

Res
FUJIWARA-KATO, Mariko
(D Agr)

## Students

NAKAI, Hideto (D3)  WADA, Yukika (D3)  GOTO, Kakeru (M1)

## Visitors

| | |
|---|---|
| Prof QU, Li-Jia | College of Life Science, Peking University, China, P.R., 28 February–3 March |
| Assist Prof KANG, Juqing | College of Life Science, Peking University, China, P.R., 27–29 October |
| Ms LI, Jieru | College of Life Science, Peking University, China, P.R., 14 December 2011–13 January 2013 |
| Ms ZHANG, Jun | College of Life Science, Peking University, China, P.R., 27 September 2012–26 September 2013 |
| Ms LIN, Qing | College of Life Science, Peking University, China, P.R., 7 December 2012–6 June 2013 |

## Scope of Research

This laboratory aims at clarifying molecular bases of regulatory mechanisms for plant development, especially plant morphogenesis, with techniques of forward and reverse genetics, molecular biology, and biochemistry. Current major subjects are phospholipid signalings in cell morphogenesis, the transcriptional network for cytokinin responses, COP9 signalosome modulating signal transduction in the nuclei, and the endoreduplication cell cycle in cell differentiation.

### KEYWORDS

Morphogenesis
Signal Transduction
Phospholipid
COP9 Signalosome
Cytokinin

## Selected Publications

Lin, Q.; Aoyama, T., Pathways for Epidermal Cell Differentiation via the Homeobox Gene GLABRA2: Update on the Roles of the Classic Regulator, *J. Integr. Plant Biol.*, **54,** 729-737 (2012).

Aki, S.; Nakai, H.; Aoyama, T.; Oka, A.; Tsuge, T., *AtSAP130/AtSF3b-3* Function is Required for Reproduction in *Arabidopsis thaliana*, *Plant Cell Physiol.*, **52,** 1330-1339 (2011).

Taniguchi, Y. Y.; Taniguchi, M.; Tsuge, T.; Oka, A.; Aoyama, T., Involvement of *Arabidopsis thaliana* Phospholipase Dζ2 in Root Hydrotropism through the Suppression of Root Gravitropism, *Planta*, **231,** 491-497 (2010).

Kusano, H.; Testerink, C.; Vermeer, J. E. M.; Tsuge, T.; Shimada, H.; Oka, A.; Munnik, T.; Aoyama, T., The *Arabidopsis* Phosphatidylinositol Phosphate 5-kinase PIP5K3 Is a Key Regulator of Root Hair Tip Growth, *Plant Cell*, **20,** 367-380 (2008).

Menon, S.; Tsuge, T.; Dohmae, N.; Takio, K.; Wei, N., Association of SAP130/SF3b-3 with Cullin-RING Ubiquitin Ligase Complexes and Its Regulation by the COP9 Signalosome, *BMC Biochem.*, **9,** 1 (2008).

Taniguchi, M.; Sasaki, N.; Tsuge, T.; Aoyama, T.; Oka, A., ARR1 Directly Activates Cytokinin Response Genes That Encode Proteins with Diverse Regulatory Functions, *Plant Cell Physiol.*, **48,** 263-277 (2007).

## Regulatory Network for Epidermal Cell Differentiation in Plants

The epidermal cells of *Arabidopsis thaliana*, including trichomes and root hairs, are excellent subjects for studies on pattern formation and morphological differentiation in plant cells. It has been revealed that the regulation of cell differentiation pattern involves cell lineage, positional cues from subepidermal tissues, and lateral inhibition between neighboring cells, and that elaborate transcriptional networks play an integrative role in the regulation. Interestingly, of such transcriptional networks, those for various epidermal tissues share a common structure consisting of transcription factor genes encoding MYB proteins, bHLH proteins, the WD40 protein TRANSPARENT TESTA GLABRA1 (TTG1), and the homeodomain leucine-zipper protein GLABRA2 (GL2) (Figure 1). In the conserved network structure, the *GL2* gene is placed furthest downstream, targeted by a transactivating complex consisting of R2R3-type MYB, bHLH, and TTG1 proteins, and negatively regulated by R3-type MYB proteins. Although *GL2* is assumed to be a bottleneck in the regulatory pathway for cell differentiation in various epidermal tissues, both its physiological outputs in cell differentiation and downstream target genes of GL2 almost remain unclear. Therefore, the total picture of the regulatory pathway for differentiation into each cell type is still obscure.

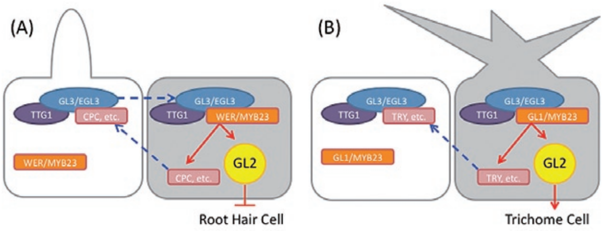

**Figure 1.** Regulatory Pathways for Epidermal Cell Differentiation. Pathways upstream of GL2 are schematically illustrated for hair and non-hair cells in the root epidermis (A), pavement and trichome cells in the leaf epidermis (B). Red arrows and T-bars indicate positive and negative transcriptional regulation, respectively. Blue arrows indicate protein movement between cells. Arrows with dashed lines indicate assumed regulation and movement. Cells that strongly express the *GL2* gene are shown in glay color.

To clarify the regulatory pathway for epidermal cell differentiation in plants, we are studying on the transcriptional network downstream of GL2, and have identified several its direct target genes, including a phospholipase D (PLD) gene, *PLDζ1*. PLDs are known to play roles in intracellular signal transduction via their product, phosphatidic acid (PA). Artificial down-regulation of the *PLDζ1* gene caused abnormalities in root hair cell morphogenesis. Recent studies on plant signal transduction revealed that PA signaling links to protein kinase cascades containing the 3'-phosphoinositide-dependent kinase PDK1 and AGCVIII-type kinases in plant cells. The finding suggests that AGCVIII-type kinases mediate the PA signal produced by PLDζ1 to promote root hair cell development in *Arabidopsis*. Candidate AGCVIII-type kinases include AGC2-1/OXI1 and PID, which have been reported to be involved in signals of reactive oxygen species (ROS) and the phytohormone auxin, respectively. PLDζ1-RFP fusion protein expressed using the *PLDζ1* promoter was localized to inner membrane structures in root hair cells, suggesting that PA activates PDK1 on the inner membrane (Figure 2). Downstream of *GL2*, PLDζ1 may accelerate signal transduction, including those mediated by ROS and auxin, which are involved in root hair development.

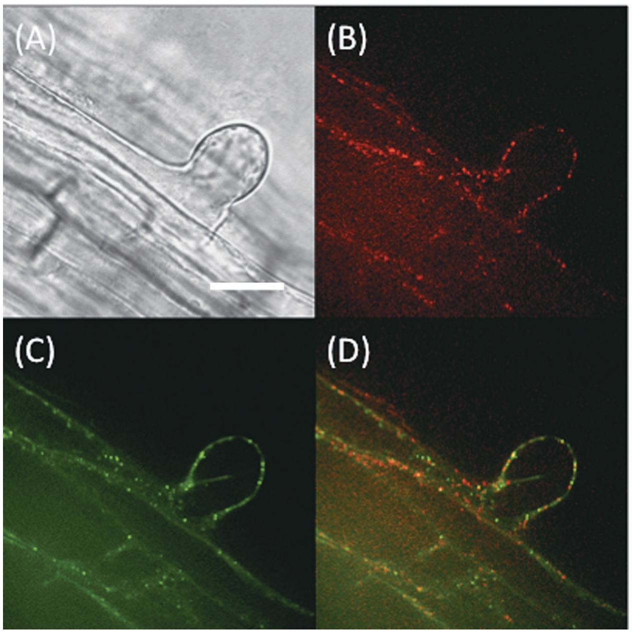

**Figure 2.** Intracellular Localization Pattern of PLDζ1-RFP. Fluorescence signals of PLDζ1-RFP and GFP-ARA7, an endosome marker, in a root hair cell were observed with confocal laser scanning microscopy. A bright field image (A), and fluorescence images of PLDζ1-RFP (B), GFP-ARA7 (C), and their overlay are shown. PLDζ1-RFP was partially co-localized with GFP-ARA7. Bar = 20 μm.

# Division of Biochemistry
## – Chemical Biology –

http://www.scl.kyoto-u.ac.jp/~uesugi/e/index.php

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Proj Res**
HIRATA, Nao
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Proj Res***
WATANABE, Mizuki
(D Pharm Sc)

Proj Res**
JIN, Guihua
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Proj Res**
KUO, Ting-Fang
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Proj Res**
KATSUDA, Yousuke
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Proj Res***
TAKENOYA, Mihoko
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Proj Res (PD, iCeMS)**
PERRON, Amelie
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### Assist Res Staff

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MAO, Di (D1)
TAKAYA, Junichiro (D1)
RYODEN, Yuta (M2)

* Program-Specific Research Center Assist Prof of iCeMS
** PD (NEXT Program) of iCeMS
*** Res (WPI) of iCeMS
**** iCeMS

### Visitors

| | |
|---|---|
| Assoc Prof HOW, Siew Eng | Universiti Malaysia Sabah, Malaysia, 4 April |
| Prof LEI, Xiaoguang | National Institute of Biological Sciences, China, P.R., 31 October–1 November |
| Prof SCHÄRER, Orlando D. | Stony Brook University, U.S.A., 29 November |

## Scope of Research

Chemical biology is an interdisciplinary field of study that is often defined as "chemistry-initiated biology." As biological processes all stem from chemical events, it should be possible to understand or manipulate biological events by using chemistry. Our laboratory has been discovering or designing unique organic molecules that modulate fundamental processes in human cells. Such synthetic organic molecules often serve as tools for basic cell biology. Discovery or design of small molecules with unique biological activity permits small-molecule initiated exploration of complex cellular events. Our mission is to create a new world of bioactive synthetic molecules: their new way to use, their new shapes, and their new sizes. We hope to open new avenues for small-molecule applications in a range of fields, including future concepts in drug discovery and use of small molecules for cell therapy.

KEYWORDS
Cell Therapy
Chemical Biology
Small Molecules
Chemical Library
Chemical Genetics

### Selected Publications

Minami, I.; Yamada, K.; Otsuji, T. G.; Yamamoto, T.; Shen, Y.; Otsuka, S.; Kadota, S.; Morone, N.; Barve, M.; Asai, Y.; Tenkova-Heuser, T.; Heuser, J. E.; Uesugi, M.; Aiba, K.; Nakatsuji, N., A Small Molecule That Promotes Cardiac Differentiation of Human Pluripotent Stem Cells under Defined Cytokine- and Xeno-free Conditions, *Cell Reports*, (in press) (2012).
Jung, D.; Abu-Elheiga, L.; Ayuzawa, R.; Gu, Z.; Shirakawa, T.; Fujiki, Y.; Nakatsuji, N.; Wakil, S. J.; Uesugi, M., Mis-localization and Inhibition of ACC1 by a Synthetic Small Molecule, *Biochem J.*, **448 (3),** 409-416 (2012).
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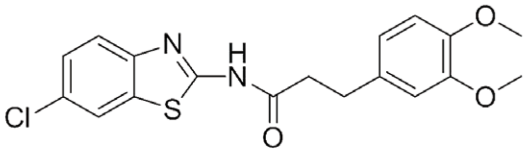
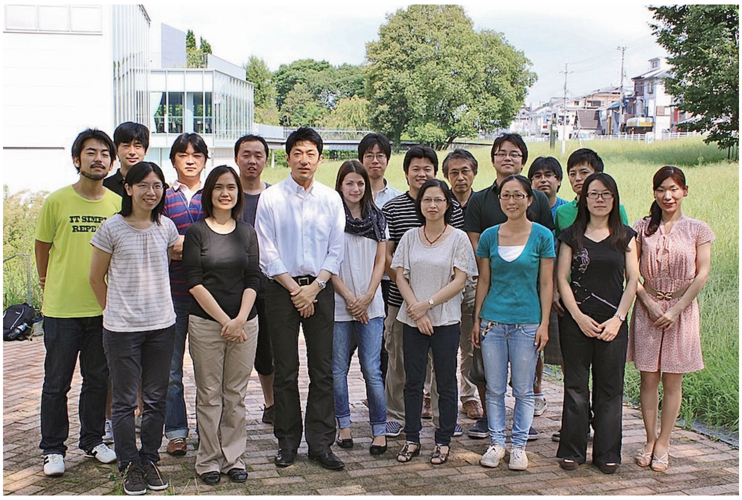
Shirakawa, T.; Kawazoe, Y.; Tsujikawa, T.; Jung, D.; Sato, S.; Uesugi, M., Deactivation of STAT6 through Serine 707 Phosphorylation by JNK, *J. Biol. Chem.*, **286,** 4003-4010 (2011).

## A Small Molecule That Promotes Cardiac Differentiation of Human Pluripotent Stem Cells under Defined Cytokine- and Xeno-free Conditions

Human pluripotent stem cells (hPSCs), including embryonic stem cells and induced pluripotent stem cells, are potentially useful in regenerative therapies for heart disease. For medical applications, clinical-grade cardiac cells must be produced from hPSCs in a defined, cost-effective manner. Cell-based screening led to the discovery of KY02111, a small molecule that promotes differentiation of hPSCs to cardiomyocytes. Although the direct target of KY02111 remains unknown, results of the present study suggest that KY02111 promotes differentiation by inhibiting WNT signaling in hPSCs but in a manner that is distinct from that of previously studied WNT inhibitors. Combined use of KY02111 and WNT signaling modulators produced robust cardiac differentiation of hPSCs in a xeno-free, defined medium, devoid of serum and any kind of recombinant cytokines and hormones, such as BMP4, Activin A, or insulin. The methodology has potential as a means for the practical production of human cardiomyocytes for regeneration therapies.

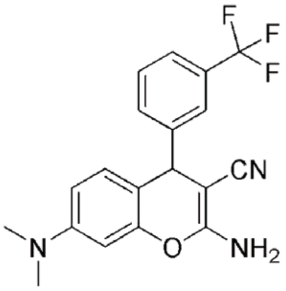


KY02111



## Mis-localization and Inhibition of ACC1 by a Synthetic Small Molecule

Chromeceptin is a synthetic small molecule that inhibits insulin-induced adipogenesis of 3T3-L1 cells and impairs the function of insulin-like growth factor 2 (IGF2). The molecular target of this benzochromene derivative is multifunctional protein 2 (MFP-2). The interaction between chromeceptin and MFP-2 activates the signal transducer and activator of transcription 6 (STAT6), which subsequently induces IGF inhibitory genes. It was not previously known how the binding of chromeceptin with MFP-2 blocks adipogenesis and activates STAT6. Results of the present study showed that the chromeceptin/MFP-2 complex binds to and inhibits acetyl-CoA carboxylase 1 (ACC1), an enzyme important for the de novo synthesis of malonyl-CoA and fatty acids. The formation of this ternary complex removes ACC1 from the cytosol and sequesters it in peroxisomes through guidance of Pex5p. As a result, chromeceptin impairs fatty acid synthesis from acetate where ACC1 is a rate limiting enzyme. Overexpression of malonyl-CoA decarboxylase or siRNA knockdown of ACC1 resulted in STAT6 activation, suggesting a role of malonyl-CoA in STAT6 signaling. The molecular mechanism of chromeceptin may provide a new pharmacological approach to selective inhibition of ACC1 for biological studies and pharmaceutical development.



Chromeceptin

# Division of Environmental Chemistry
## – Molecular Materials Chemistry –

http://www.molmat.kuicr.kyoto-u.ac.jp/index-e.html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Techn Staff
OHMINE, Kyoko


Techn Staff
MAENO, Ayaka


PD
OHTSUKI, Akimichi
(D Sc)

### Lect (pt)

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TANISHIMA, Miho

### Students

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FUJIMURA, Subaru (M2)
FURUKAWA, Shinya (M2)
SUZUKI, Hajime (M1)
DETANI, Masahiro (M1)
OKUDA, Takashi(UG)
TANAKA, Fumiya (UG)

## Scope of Research

Our research target is to develop high-performance organic electroluminescence devices, organic solar cells, and polymer materials. For the purpose, we have carried out syntheses, device fabrications, precise structure characterizations, and quantum chemical calculations for high functional organic materials. Along with exploring novel synthetic routes and novel devices, detailed analyses of structures and dynamics are performed mainly by sophisticated solid-state NMR spectroscopy in order to obtain structure-dynamics-property relationships.

### KEYWORDS

Solid-State NMR
Amorphous Materials
Organic Light-Emitting Diodes
Organic Solar Cells
Living Radical Polymerization
Quantum Chemical Calculation

### Selected Publications

Fukushima, T.; Kaji, H., Green- and Blue-Emitting Tris(8-hydroxyquinoline) Aluminum(III) ($Alq_3$) Crystalline Polymorphs: Preparation and Application to Organic Light Emitting Diodes, *Organic Electronics*, **13,** 2985-2990 (2012).

Nishiyama, Y.; Fukushima, T.; Fukuchi, M.; Fujimura, S.; Kaji, H., Sensitivity Boosting in Solid-State NMR of Thin Organic Semiconductors by a Paramagnetic Dopant of Copper Phthalocyanine, *Chem. Phys. Lett.*, (in press).

Sato, T.; Shizu, K.; Tanaka, K.; Kaji, H., Theoretical Design for Carrier-Transporting Molecules in View of Vibronic Couplings, *Journal of Photonics for Energy*, **2,** [021201-1]-[021201-10] **(**2012).

Goto, A.; Tsujii, Y.; Kaji, H., Reversible Complexation Mediated Polymerization (RCMP) of Methyl Methacrylate, *ACS Symp. Ser.*, **1100,** 305-315 (2012).

Yazawa, K.; Suzuki, F.; Nishiyama, Y.; Ohata, T.; Aoki, A.; Nishimura, K.; Kaji, H.; Asakura, T., Probing Intermolecular Structures of β Sheet of Alanine Oligomer and Silk Fibroin by High Resolution $^1$H NMR Spectroscopy with Ultra Fast MAS under Ultra High Field $^1$H Resonant Frequency, *Chem. Comm.*, **48,** 11199-11201 (2012).

## Green- and Blue-Emitting Organic LED Materials: Preparation of Polymorphs and Application to Organic LEDs

Tris(8-hydroxyquinoline) aluminum(III) ($Alq_3$) is known to have two isomeric states, namely meridional and facial isomers. Typical $Alq_3$ crystals composed of meridional and facial isomers are $\alpha$- and $\delta$-form crystals, respectively. First, we investigate the temperature change in the crystalline forms of $\alpha$-$Alq_3$ and $\delta$-$Alq_3$ in X-ray diffraction experiments in a vacuum. $\alpha$-$Alq_3$ remains in $\alpha$-form up to 300ºC, immediately before sublimation. In contrast, $\delta$-$Alq_3$ is found to transform into $\gamma$-form at ~180ºC, and remain in $\gamma$-form immediately before sublimation. Both $\gamma$-$Alq_3$ and $\delta$-$Alq_3$ are composed of facial isomers and emit blue luminescence, which is different from the typical green emissions of $\alpha$-$Alq_3$. Second, we fabricate organic light-emitting diodes (OLEDs) from different crystals as source powders; i.e., from 1) $\alpha$-$Alq_3$, 2) $\delta$-$Alq_3$, and 3) a mixture of $\alpha$-, $\gamma$-, and $\delta$-$Alq_3$. All the OLEDs exhibit green electroluminescence with almost the same maximum wavelength, suggesting that some facial isomers become meridional while $Alq_3$ is in the gas phase. In contrast, electroluminescence efficiency depends on the $Alq_3$ crystalline polymorph; the OLED fabricated from the mixture of $\alpha$-, $\gamma$-, and $\delta$-$Alq_3$ has up to 1.4 times the efficiency of the OLED fabricated from $\alpha$-$Alq_3$ for the same device structure.

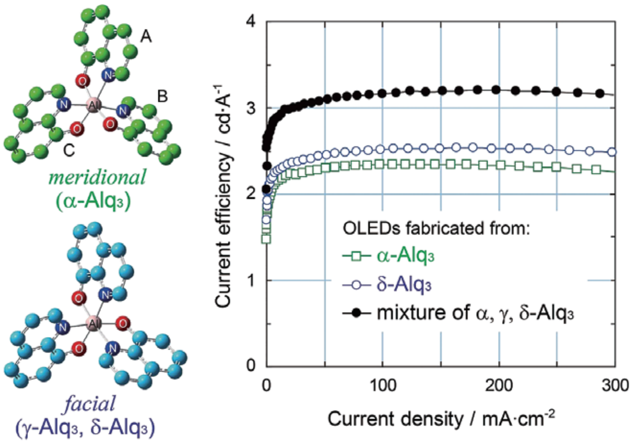

**Figure 1.** Current efficiency-current density characteristics of OLEDs fabricated from $\alpha$-$Alq_3$, $\delta$-$Alq_3$, and the mixture of $\alpha$-, $\gamma$-, and $\delta$-$Alq_3$.

## Visible-Light-Induced Living Radical Polymerization with Organic Catalysts

A photo-induced living radical polymerization (photo-LRP) using organic catalysts was developed. It is among the most simple and robust photo-LRPs, as it uses iodine as a capping agent and the catalysts are such common compounds as tributylamine. Under visible-light-irradiation at 350-600 nm, the polymer molecular weight and its distribution ($M_w/M_n$ = 1.1–1.4) were well controlled for methyl methacrylate and some functional methacrylates up to fairly high conversions in many cases. Perfectly no polymerization took place without photo-irradiation, meaning that the system is an ideal polymerization switched "on" and "off" by external photo-stimulus. The polymerization rate was also finely tunable by the external irradiation power. The uses of inexpensive compounds and visible light, good polydispersity control, good tolerance to functional groups, and fine response to external photo-irradiation may be useful features of this system.

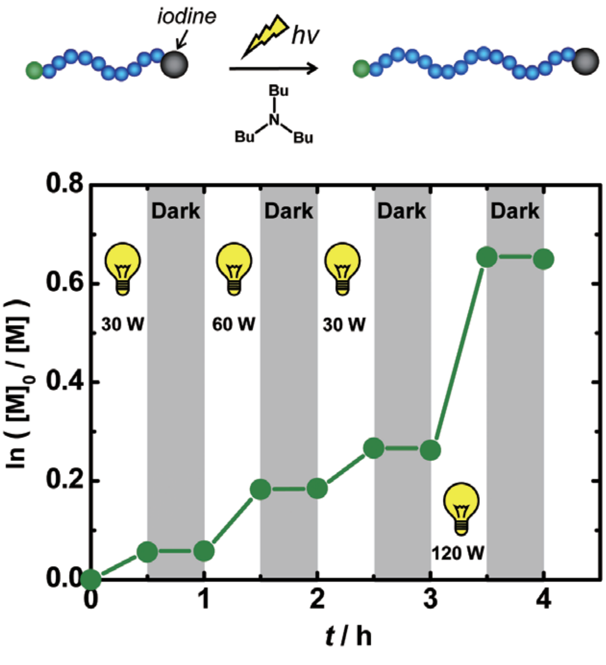

**Figure 2.** Schematic illustration of photo-LRP using iodine as a capping agent and tributylamine as a catalyst, and first-order-plot of monomer concentration (monomer conversion index) for temporal control by external visible-light-irradiation.

# Division of Environmental Chemistry
## – Hydrospheric Environment Analytical Chemistry –

http://inter3.kuicr.kyoto-u.ac.jp/scope_E.html

Prof
SOHRIN, Yoshiki
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Assoc Prof
UMETANI, Shigeo
(D Sc)

Assist Prof
NORISUYE, Kazuhiro
(D Sc)

Techn Staff
MINAMI, Tomoharu
(D Eng)

## Students

| | | |
|---|---|---|
| TAKANO, Shotaro (D1) | FUJISAKA, Hiroaki (M2) | KAWAHARA, Shimpei (M1) |
| YAMAMOTO, Jun (D1) | ICHIWAKI, Shouhei (M2) | KONAGAYA, Wataru (M1) |

## Visitor

| | |
|---|---|
| Dr HO, Tung-Yuan | Research Center for Environmental Changes, Academia Sinica, Taiwan, 13 July |

## Scope of Research

(i) Biogeochemistry of trace elements in the hydrosphere: Novel analytical methods are developed for trace metals and its isotopes. Distribution of trace elements in the hydrosphere and its effects on ecosystem are investigated. The study also covers hydrothermal activity, deep biosphere and paleocean.

(ii) Ion recognition: Novel ligands and ion recognition system are designed, synthesized and characterized.

### KEYWORDS

| | |
|---|---|
| Analytical Chemistry | Stable Isotopes |
| Marine Chemistry | Metal Ion Recognition |
| Trace Elements | |

## Selected Publications

Norisuye, K.; Sohrin, Y., Determination of Bismuth in Open Ocean Waters by Inductively Coupled Plasma Sector-Field Mass Spectrometry after Chelating Resin Column Preconcentration, *Analytica Chimica Acta*, **727,** 71-77 (2012).

Nakagawa, Y.; Takano, S.; Firdaus, M. L.; Norisuye, K.; Hirata, T.; Vance, D.; Sohrin, Y., The Molybdenum Isotopic Composition of the Modern Ocean, *Geochemical Journal*, **46,** 131-141 (2012).

Cid, A. P.; Nakatsuka, S.; Sohrin, Y., Stoichiometry among Bioactive Trace Metals in the Chukchi and Beaufort Seas, *Journal of Oceanography*, **68,** 985-1001 (2012).

Okamura, H.; Ikeda-Ohno, A.; Saito, T.; Aoyagi, N.; Naganawa, H.; Hirayama, N.; Umetani, S.; Imura, H.; Shimojo, K., Specific Cooperative Effect of a Macrocyclic Receptor for Metal Ion Transfer into an Ionic Liquid, *Analytical Chemistry*, **84,** 9332-9339 (2012).

Tsurubou, S.; Umetani, S.; Komatsu, Y., Separation of Alkaline Earth Metal Ions with a Strongly Acidic Cation Exchange Resin Using the Diazapolyoxabicyclic Ligand as an Ion Size Selective Masking Reagent, *Solvent Extraction Research and Development, Japan*, **19,** 177-181 (2012).

## Stoichiometry among Bioactive Trace Metals in the Arctic Ocean

The distribution of Al, Mn, Fe, Co, Ni, Cu, Zn, Cd, and Pb in seawater was investigated in the Chukchi and Beaufort Seas in September 2000. The unfiltered and filtered seawater samples were used for determination of total dissolvable metal (TDM) and dissolved metal (DM), respectively. The concentrations of TDAl, TDMn, TDFe, TDCo, and TDPb varied substantially in the study area. The high concentrations occurred at stations near the Bering Strait, in the Mackenzie delta, and above reductive sediments on the shelf and slope. These elements were mostly dominated by labile particulate species, such as Fe-Mn oxides and species adsorbed on terrestrial clay. DCo was correlated with DMn over the study area. TDNi, TDCu, TDZn, and TDCd showed relatively small variations and were generally dominated by dissolved species. There was a moderate correlation between DCd and phosphate for all samples, whereas there were no significant correlation between the other DMs and nutrients. TDNi and TDCu showed a remarkable linearity for most stations except those near the Bering Strait. These results suggest that biogeochemical cycling including uptake by phytoplankton and remineralization from settling particles has only minor control over the distribution of trace metals in this area. Using the present data, the annual input of bioactive trace metals from the Bering Strait and the Mackenzie River was estimated. Also the trace metal compositions of major water masses were evaluated. The DM/P ratios were significantly different from those for Pacific deep water and Bering Sea water, suggesting substantial modification of the trace metal compositions of seawater in the study area.

**Figure 1.** Observation in the Arctic Ocean during the R/V Mirai MR00-K06 cruise in September 2000.

## High-Throughput Method for the Determination of Bismuth in Open Ocean Waters

Bismuth is a unique and useful tracer for the input of volcanogenic and/or anthropogenic materials to the surface oceans and also for vertical processes in the ocean. However, the number of oceanic data is scarce and little is known about the marine biogeochemical cycle of this element. It is necessary to develop a method that satisfies high throughput as well as high precision, good accuracy, and low blank and detection limit. We have developed a novel low-blank method for the analysis of bismuth in open ocean waters based on preconcentration using an ethylenediaminetriacetic acid (EDTriA) chelating resin column followed by determination with inductively coupled plasma sector-field mass spectrometry (ICPSFMS). A sample is siphoned into and drains through the column with the flow rate being kept constant by using a water bath device. Bi in 250 mL of acidified seawater is extracted onto the column in this process and eluted with 2 mL of 3 M $HNO_3$ followed by 3 mL of ultra-high purity water. The concentration of Bi in the eluate is measured by ICPSFMS. The benefits of the present method relative to others are its simplicity, a smaller amount of seawater, and lower blanks and detection limits at fmol $kg^{-1}$ levels. Another advantage is that it allows a simultaneous run of large numbers of samples depending on the number of column lines.

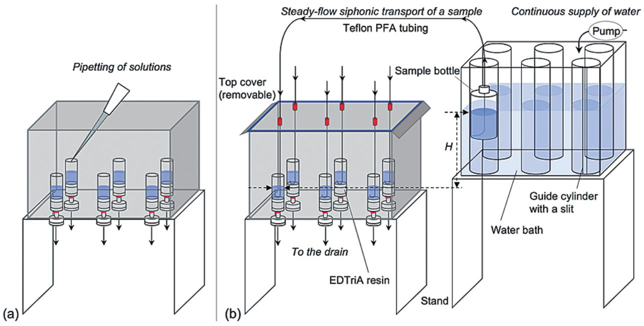

**Figure 2.** The preconcentration system. (a) Pipetting of solutions for conditioning, removal of sea salt and elution. (b) Steady-flow siphonic transport of seawater samples using the flotation device. H is the water level difference of a sample solution between the bottle and column.

# Division of Environmental Chemistry
## – Solution and Interface Chemistry –

http://www.scl.kyoto-u.ac.jp/~yoeki/


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TU, Kai-min (D2)
NORIMOTO, Shingo (M1)
MORIMINE, Seiya (M1)

## Scope of Research

We investigate chemical phenomena in condensed phases. (1) To understand the chemical structure, property and reactions in a two-dimensional molecular aggregate, the keywords of molecular interactions and orientation are focused on, and the fluctuated molecular aggregates are investigated by using originally developed spectroscopic and theoretical techniques. (2) The structure, dynamics, and reaction of solutions with nano-scale inhomogeneity and/or with fine tunability are investigated by computer simulation, and statistical-mechanical theory of solutions, and NMR spectroscopy.

### KEYWORDS

Infrared and Raman Spectroscopy
Surface and Interface Chemistry
Nano Particle and Fibril Analysis
Free Energy
Solvation
Solution Theory

### Selected Publications

Shimoaka, T.; Itoh, Y.; Hasegawa, T., Dynamic Rearrangement of Stearic Acid Molecules Adsorbed on a Gold Surface Induced by Ambient Water Molecules Studied by Infrared Spectroscopy, *J. Phys. Chem. C*, **116,** 17142-17148 (2012).

Itoh, Y.; Hasegawa, T., Polarization Dependence of Raman Scattering from a Thin Film Involving Optical Anisotropy Theorized for Molecular Orientation Analysis, *J. Phys. Chem. A*, **116,** 5560-5570 (2012).

Muro, M.; Harada, M.; Okada, T.; Hasegawa, T., Molecular Rearrangement in a Zinc Stearate Langmuir Film Dependent on a Film Preparation Method Studied Using Polarization-Modulation Infrared Reflection Absorption Spectroscopy and X-ray Absorption Fine Structure, *J. Phys. Chem. B*, **116,** 3148-3154 (2012).

Matubayasi, N.; Takahashi, H., Free-energy Analysis of the Electron-density Fluctuation in the Quantum-mechanical/Molecular-mechanical Simulation Combined with the Theory of Energy Rrepresentation, *J. Chem. Phys.*, **136,** [044505-1]-[044505-10] (2012).

Shintani, M.; Matsuo, Y.; Sakuraba, S.; Matubayasi, N., Interaction of Naphthalene Derivatives with Lipid in Membrane Studied by $^1$H-Nuclear Overhauser Effect and Molecular Dynamics Simulation, *Phys. Chem. Chem. Phys.*, **114,** 14049-14060 (2012).

Kimura, H.; Yasaka, Y.; Nakahara, M.; Matubayasi, N., Nuclear Magnetic Resonance Study on Rotational Dynamics of Water and Benzene in a Series of IonicLliquids: Anion and Cation Effects, *J. Chem. Phys.*, **137,** [194503-1]-[194503-10] (2012).

## Spectroscopic Observation of Dynamic Rearrangement of Adsorbed Molecules on Imperfectly Hydrophilic Gold Surface

Molecular adsorbates of stearic acid on a imperfectly hydrophilic gold surface prepared as an imperfect Langmuir-Blodgett (LB) film is found to exhibit dynamic molecular rearrangement when the humid atmosphere about the sample is changed. The gold surface was prepared by solvent cleaning in a sonication bath. The molecular adsorbates stored in a thoroughly dried sample room of FT-IR is found to have a unique adsorption structure; the hydrocarbon chains have a nearly parallel orientation to the substrate surface while the molecules are highly packed to have the orthorhombic subcell packing, which is confirmed by infrared reflection-absorption (RA) spectrometry. When the sample is pulled into an ambient air, the adsorption structure exhibits a drastic change in about only fifteen minutes, which is pursued by polarization-modulation infrared reflection-absorption spectrometry (PM-IRRAS). The spectra clearly indicate that the molecular stance has largely been changed to have a standing-up orientation, whereas the molecular conformation is largely degraded. When the sample is got back to the dried sample room, the molecular conformation largely improves while the standing orientation is kept. These irreversible changes are induced by ambient water molecules adsorbed on the lying stearic acid molecules, which was monitored by analyzing absorption bands of the hydronium ion.

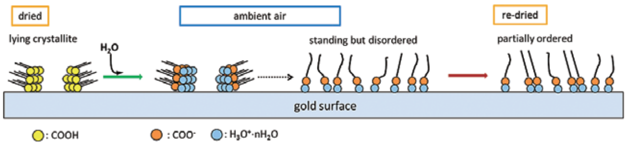

**Figure 1.** Schematic illustrations of the adsorbed stearic acid molecules on gold as a function of the environmental condition.

## Interaction of Small Molecule with Lipid Membrane through Combined $^1$H-Nuclear Overhauser Effect Measurement and Molecular Dynamics Simulation

The location, orientation, and dynamics of hydrophobic small molecule in lipid membrane are studied through combined use of the solution-state $^1$H-NMR and MD simulation. 1-Naphthol and 1-methylnaphthalene were adopted as the small molecule with or without hydrophilic group. The nuclear Overhauser effect (NOE) measurement was performed for large unilamellar vesicle (100 nm in diameter) composed of dimyristoylphosphatidylcholine (DMPC) and the naphthalene derivative. The transient NOE-SE (spin echo) scheme was employed to quantitatively determine the NOE cross relaxation rate constant between DMPC and the naphthalene derivative. The observed NOE shows that both the naphthalene derivatives distribute over wide domain across the normal of the essentially planar membrane ranging from the hydrophobic core to the hydrophilic headgroup. The experimental NOE information was further refined in combination with the analysis of time correlation functions in MD simulation. It was found that 1-naphthol exhibits slight preference of its OH group pointing toward the hydrophilic domain of membrane and that no definite preference can be concluded for the orientation of 1-methylnaphthalene. When 1-naphthol and 1-methylnaphthalene are compared, the NOE is the stronger for 1-naphthol due to the restricted motion by the OH group. The slowdown of the 1-naphthol motion is also evidenced by the $^1$H spectral line width.

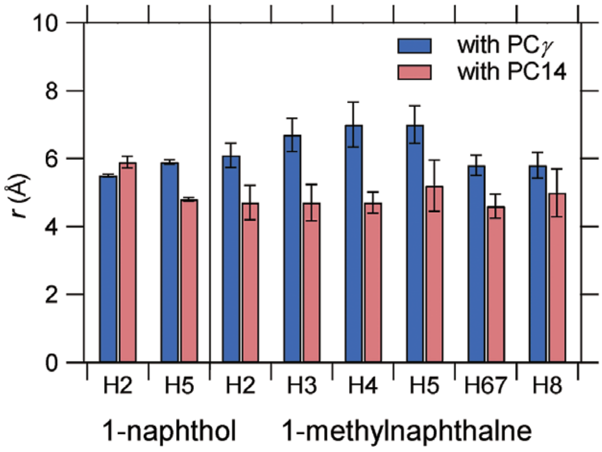

**Figure 2.** The distances $r$ from DMPC terminal positions (PC$\gamma$ and PC14) estimated by combining the experimental NOE cross relaxation rate constant and the simulated correlation time.

# Division of Environmental Chemistry
## – Molecular Microbial Science –

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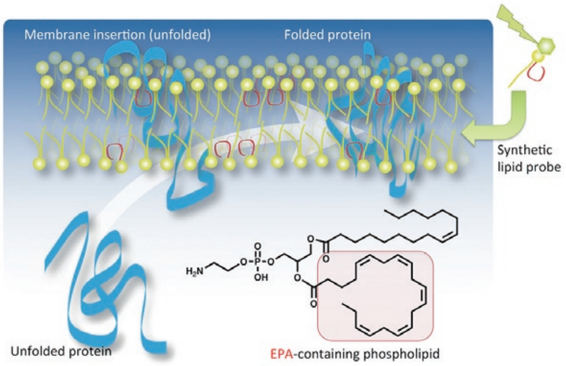
## Scope of Research

Microorganisms are found almost anywhere on Earth. They have a great diversity of capacities to adapt to various environments including chemically and physically unusual environments. Our main subject is to clarify the molecular basis of environmental adaptation of microorganisms and their application. Specific functions of proteins and lipids that play essential roles in environmental adaptation of extremophilic microorganisms are of our particular interest. Mechanistic analysis of microbial enzymes, in particular those involved in unique metabolic pathways, and their application are also undertaken.



### KEYWORDS

Molecular Microbial Science
Biochemistry
Psychrotroph
Polyunsaturated Fatty Acid
Bioengineering

### Selected Publications

Sato, S.; Kawamoto, J.; Sato, S. B.; Watanabe, B.; Hiratake, J.; Esaki, N.; Kurihara, T., Occurrence of Bacterial Membrane Microdomain at the Cell Division Site Enriched in Phospholipids with Polyunsaturated Hydrocarbon Chain, *Journal of Biological Chemistry*, **287,** 24113-24121 (2012).

Park, J.; Kawamoto, J.; Esaki, N.; Kurihara, T., Identification of Cold-inducible Inner Membrane Proteins of the Psychrotrophic Bacterium, *Shewanella livingstonensis* Ac10, by Proteomic Analysis, *Extremophiles*, **16,** 227-236 (2012).

Dai, X.-Z.; Kawamoto, J.; Sato, S. B., Esaki, N.; Kurihara, T., Eicosapentaenoic Acid Facilitates the Folding of an Outer Membrane Protein of the Psychrotrophic Bacterium, *Shewanella livingstonensis* Ac10, *Biochemical and Biophysical Research Communications*, **425,** 363-367 (2012).

Nakayama, T.; Kamachi, T.; Jitsumori, K.; Omi, R.; Hirotsu, K.; Esaki, N.; Kurihara, T.; Yoshizawa, K., Substrate Specificity of Fluoroacetate Dehalogenase: An Insight from Crystallographic Analysis, Fluorescence Spectroscopy, and Theoretical Computations, *Chemistry*, **27,** 8392-8402 (2012).

Sato, S. B.; Park, J.; Kawamoto, J.; Sato, S.; Kurihara, T., Inhibition of Constitutive Akt (PKB) Phosphorylation by Docosahexaenoic Acid in the Human Breast Cancer Cell Line MDA-MB-453, *Biochimica et Biophysica Acta*, **1831,** 306-313 (2013).

## Characterization of 1-Acyl-*sn*-glycerol-3-phosphate Acyltransferase from a Polyunsaturated Fatty Acid-producing Bacterium, *Shewanella Livingstonensis* Ac10

*Shewanella livingstonensis* Ac10, a psychrotrophic bacterium, produces the omega-3 polyunsaturated fatty acid eicosapentaenoic acid (EPA), as a fatty acyl chain of phospholipids at low temperatures. EPA is incorporated into the *sn*-2 position of phospholipids. 1-Acyl-sn-glycerol-3-phosphate acyltransferase (PlsC) catalyzes the acylation at the *sn*-2 position of 1-acyl-sn-glycerol-3-phosphate to form phosphatidic acid (PA). We found that 5 genes code for proteins homologous to *Escherichia coli* PlsC (named PlsC1 through PlsC5), suggesting that these PlsCs are involved in the synthesis of EPA-containing phospholipids. To examine the role of these putative PlsCs, we constructed the knockout mutants of each plsC gene (ΔplsC1 to ΔplsC5). In the mutant ΔplsC1, the amount of phospholipids containing EPA was less. Functional expression studies in a temperature-sensitive mutant of PlsC, *E. coli* JC201, showed that PlsC1 has a PlsC activity with a broad acyl-coenzyme A (acyl-CoA) specificity including EPA-CoA. These results indicate that PlsC1 is a key enzyme in the synthesis of EPA-containing PA in *S. livingstonensis* Ac10.

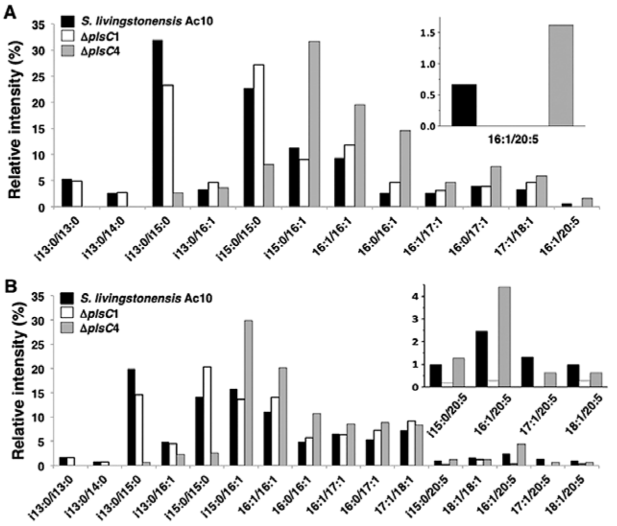


**Figure 1.** Composition of phosphatidylethanolamine (A) and phosfatidylglicerol (B) of *S. livingstonensis* Ac10 cultivated at 4°C.

## Eicosapentaenoic Acid Regulates the Membrane Localization of Cell Division Proteins of a Psychrotrophic Bacterium, *Shewanella Livingstonensis* Ac10

A cold-adapted microorganism, *Shewanella livingstonensis* Ac10 isolated from Antarctic seawater, produces eicosapentaenoic acid (EPA) as an acyl chain of its membrane phospholipids at 4˚C. When EPA-biosynthesis genes were disrupted, the EPA-lacking mutant showed the growth retardation and filamentous cells at 4˚C, but not at 18˚C, suggesting that EPA-containing phospholipids have an important role in the cell division of this bacterium at low temperatures. We also found that, in the absence of EPA, the membrane localization of a cell division-related protein, FtsE, was changed, and supplementation of EPA-containing phospholipids suppressed the defect of membrane localized FtsE. To confirm the involvement of EPA with FtsE and its partner protein, FtsX, *in vivo* localization of these proteins was analyzed. In the wild type, FtsE was localized at cell division site. On the other hand, spiral formed FtsE was observed only from the EPA-less mutant (Figure 2). These results indicate that EPA-containing phospholipids regulate the membrane localization of FtsE and the assembly of FtsEX complex during its cell division at low temperatures.

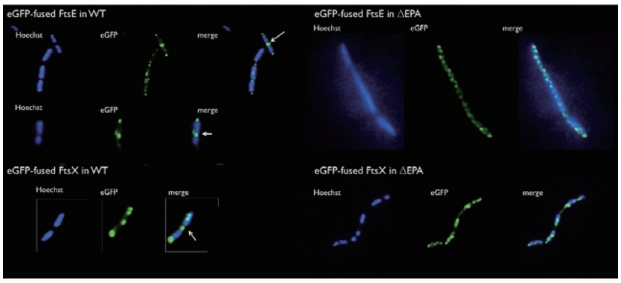


**Figure 2.** Localization of eGFP-fused FtsE and FtsX in *Shewanella livingstonensis* Ac10 and the EPA-less mutant.

# Division of Multidisciplinary Chemistry
## – Polymer Materials Science –

http://www.scl.kyoto-u.ac.jp/~kanaya2/e_index.html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HIRANO, Tatsumasa (M1)
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SHIRAISHI, Yasuhiro (UG)
TAKEDA, Kazuki (UG)
MAEDE, Tadahiko (UG)

## Scope of Research

The structure and molecular motion of polymer substances are studied using mainly scattering methods such as neutron, X-ray and light with intension of solving fundamentally important problems in polymer science. The main projects are the mechanism of structural development in crystalline polymers from glassy or molten state to spherulites, the dynamics in disordered polymer materials including low-energy excitation, glass transition and local segmental motions; formation processes and structure of polymer gels; the structure and molecular motion of polyelectrolyte solutions.

**KEYWORDS**

Polymer Physics
Polymer Properties
Scattering
Neutron Scattering

### Selected Publications

Asakawa, H.; Nishida, K.; Yamamoto, J.; Inoue, R.; Kanaya, T., Heating Rate Effects on the Crystallization Behavior of Isotactic Polypropylene from Mesophase–A De-polarized Light Transmission Study, *Polymer*, **53,** 2777-2782 (2012).

Polec, I.; Fujiwara, T.; Kanaya, T.; Deng, C., Simultaneous SAXS/WAXS Experiments on Shear Induced iPP Crystallization near Nominal Melting Temperature, *Polymer*, **53,** 3540-3547 (2012).

Deng, C.; Fujiwara, T.; Polec, I.; Matsuba, G.; Jin, L.; Inoue, R.; Nishida, K.; Kanaya, T., Precursor of Shish-Kebab in Atactic Polystyrene/Isotactic Polystyrene Blend above Nominal Melting Temperature, *Macromolecules*, **45,** 4360-4367 (2012).

Inoue, R.; Kanaya, T.; Masuda, T.; Nishida, K.; Yamamuro, O., Relationship between the Local Dynamics and Gas Permeability of Para-Substituted Poly(1-chloro-2-phenylacetylenes), *Macromolecules*, **45,** 6008-6014 (2012).

Kanaya, T.; Takahashi, N.; Takeshita, H.; Ohkura, M.; Nishida, K.; Kaji, K., Structure and Dynamics of Poly(vinylalchol) Gels in Mixture of Dimethyl Sulfoxide and Water, *Polymer J.*, **44,** 83-94 (2012).

## Effects of Non-crystalline Atactic Polystyrene on the Shear-induced Crystallization of Isotacitic Polystyrene

We studied effects of non-crystalline high molecular weight atactic polystyrene (aPS) on the shear-induced crystallization of isotacitic polystyrene (iPS) above the nominal melting temperature $T_m$ (=223°C) using polarized optical microscope (POM). It was found that the non-crystalline aPS accelerated the crystallization of iPS in some concentration range. An influence of aPS on the shear-induced crystallization of iPS was also examined as functions of shear rate, shear strain and concentration of aPS. It was also found that aPS enhanced the crystallization at around 4 wt % of aPS most effectively in any shear conditions (see Figure 1). These experimental findings suggest that the orientation and relaxation of non-crystalline high molecular weight aPS might have significant impact on the enhancement of crystallization under shear flow. The corresponding mechanism presents new insights into the shear-induced crystallization of polymers.

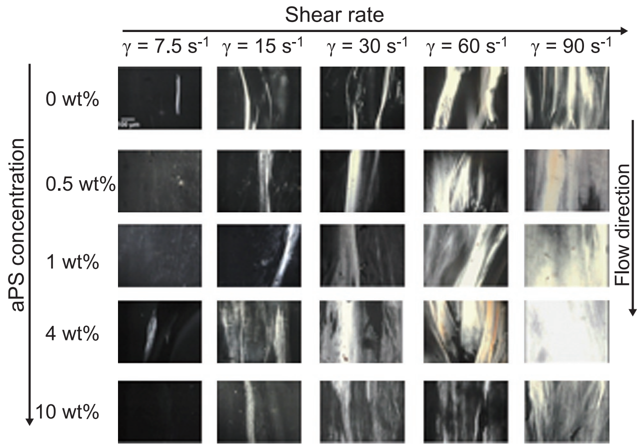

**Figure 1.** POM pictures of shear-induced precursors formed at different shear rates during shear flow at 250°C in iPS and aPS/iPS blends.

## Relationship between the Local Dynamics and Gas Permeability of Substituted Polyacetylenes

It is well known that some polyacetylenes with bulky substittuents exhibit high gas permeability among the synthetic polymers. It is considered that the physical origin of highly gas-permeable substituted polyacetylens is attributed to low apparent density due to the existence of microvoids. Recently the poly-(1-chloro-2-phenylacetylene) (PCPA) derivatives were synthesized and their gas permeability were investigated taking the advantage of excellent solubility to common organic solvents. Interestingly some PCPA derivatives exhibit high gas permeability despite of low fractional free volume (FFV), implying the existence of other controlling parameter for gas permeability other than microvoids. In order to disclose the unknown controlling parameter of gas permeability, we studied the local dynamics of PCPA derivatives by quasielastic neutron scattering (QENS). Broadening of the dynamic scattering law was clearly observed for PCPA derivatives and the observed dynamic scattering law was well fitted with the combination of slow and fast motions. Only the relaxation rate from narrow component exhibited with a positive correlation between local dynamics probed by QENS and gas permeability, as shown in Figure 2. It implies that the local dynamics with the time scale of several tens of ps play a main role for gas permeability of substituted polyacetylenes in glassy state.

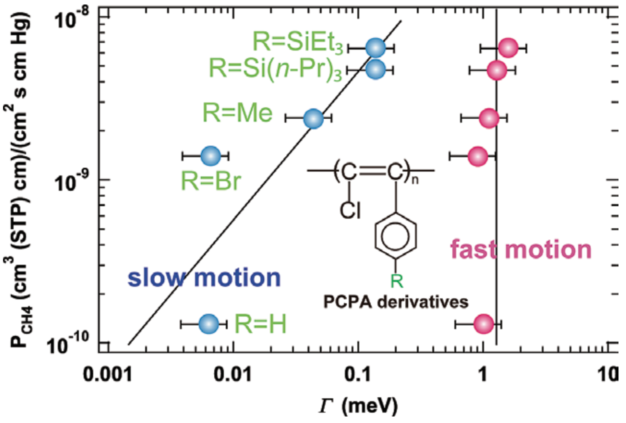

**Figure 2.** Correlation between $P_{CH4}$ and the relaxation rates ($\Gamma$) for the narrow and broad components.

# Division of Multidisciplinary Chemistry
## – Molecular Rheology –

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NAGAO, Masahiro (M1)
TSUBOTA, Takuya (M1)
KATSUO, Soichiro (UG)
KUMAZAWA, Kazuki (UG)

### Visitors

| | |
|---|---|
| Prof HASSAGER, Ole | Technical University of Denmark, Denmark, 12 March |
| Prof LIKHTMAN, Alexey | University of Reading, U.K., 1 April–30 June |
| Dr SHAUKAT, Asima | University of Leeds, U.K., 22 June–20 July, 17–30 December |
| Prof MCKENNA, Greg | Texas Tech University, U.S.A.,12 November |
| Prof MCLEISH, Tom | Durham University, U.K., 27–29 November |
| Prof KUNIN, Seth | Durham University, U.K., 27–29 November |
| Prof ASUTAY, Mehmet | Durham University, U.K., 27–29 November |
| Prof PETLEY, David | Durham University, U.K., 27–29 November |
| Prof SAUL, Nicholas | Durham University, U.K., 27–29 November |
| Prof HENDRY, Robin | Durham University, U.K., 27–29 November |
| Prof QUINLAN, Roy | Durham University, U.K., 27–29 November |
| Prof BENHAM, Adam | Durham University, U.K., 27–29 November |
| Prof STRANG, Veronica | Durham University, U.K., 27–29 November |
| Prof GARNETT, Philip | Durham University, U.K., 27–29 November |
| Prof ROBERTS, David | Durham University, U.K., 27–29 November |
| Prof PETEKIDIS, George | University of Crete, Greece, 30 November |
| Prof LODGE, Tim | University of Minnesota, U.S.A., 10 December |

## Scope of Research

**KEYWORDS**

Rheology Dielectric Spectroscopy Softmatter
Primitive Chain Network Simulation

The molecular origin of various rheological properties of material is studied. Depending on time and temperature, homogeneous polymeric materials exhibit typical features of glass, rubber, and viscous fluid while heterogeneous polymeric systems exhibit plasticity in addition to these features. For a basic understanding of the features, the molecular motion and structures of various scales are studied for polymeric systems in deformed state. Measurements are performed of rheological properties with various rheometers, of isochronal molecular orientation with flow birefringence, and of auto-correlation of the orientation with dynamic dielectric spectroscopy. Direct observation of molecular motion is also carried out with fluorescent microscopy and molecular simulations.

### Selected Publications

Yaoita, T.; Isaki, T.; Masubuchi, Y.; Watanabe, H.; Ianniruberto, G.; Marrucci, G., Primitive Chain Network Simulation of Elongational Flows of Entangled Linear Chains: Stretch/Orientation-induced Reduction of Monomeric Friction, *Macromolecules*, **45,** 2773-2782 (2012).

Masubuchi, Y.; Matsumiya, Y.; Watanabe, H.; Shiromoto, S.; Tsutsubuchi, M.; Togawa, Y., Primitive Chain Network Simulations for Comb-branched Polymer under Step Shear Deformations, *Rheo. Acta*, **51,** 193-200 (2012).

Suzuki, S.; Uneyama, T.; Inoue, T.; Watanabe, H., Nonlinear Rheology of Telechelic Associative Polymer Networks: Shear Thickening and Thinning Behavior of Hydrophobically Modified Ethoxylated Urethane (HEUR) in Aqueous Solution, *Macromolecules*, **45,** 888-898 (2012).

Matsumiya, Y.; Chen, Q.; Uno, A.; Watanabe, H.; Takano, A.; Matsuoka, K.; Matsushita, Y., Dielectric Behavior of Styrene–Isoprene (SI) Diblock and SIIS Triblock Copolymers: Global Dynamics of I Blocks in Spherical and Cylindrical Domains Embedded in Glassy S Matrix, *Macromolecules*, **45,** 7050-7060 (2012).

Uneyama, T.; Masubuchi, Y., Multi-chain Slip-spring Model for Entangled Polymer Dynamics, *J. Chem. Phys.*, **137,** 154902 (2012).

## Primitive Chain Network Simulation of Elongational Flows of Entangled Linear Chains: Stretch/Orientation-induced Reduction of Monomeric Friction

Well-entangled monodisperse linear polystyrene melts exhibit monotonic thinning of the steady state elongational viscosity with increasing the strain rate $\dot{\varepsilon}$ even beyond the Rouse relaxation frequency, $\tau_R^{-1}$. This behavior is quite different from the thinning followed by hardening at $\dot{\varepsilon}>\tau_R^{-1}$ observed for entangled semidilute solutions. We attempt to elucidate the molecular origin of this difference by focusing on the concept of stretch/orientation-dependent monomeric friction $\zeta$ recently proposed by Ianniruberto and co-workers. Specifically, literature data of the stress relaxation after cessation of transient elongational flow, reported for both PS melts and solutions, are analyzed to evaluate the stretch/orientation-dependent decrease of $\zeta$. In our working hypothesis, $\zeta$ is expressed as a function of the factor $F_{so} = \tilde{\lambda}^2\bar{S}$, where $\tilde{\lambda}$ is the normalized stretch ratio of entangled subchains defined with respect to the fully stretched state, and $\bar{S}$ is an average orientational anisotropy of the components (polymer plus solvent if any) in the system. The factor $F_{so}$ was estimated from the stress decay data after flow cessation. The resulting functional form of $\zeta(F_{so})$ was then used in the primitive chain network (PCN) simulation including finite extensible nonlinear elasticity (FENE) to examine the elongational behavior of melts and solutions. For melts the simulation indicates that $\zeta$ decreases significantly under fast elongation because the entangled subchains are short and approach the fully stretched (and fully oriented) limit rather easily. Hence, the steady elongational viscosity $\eta_E$ follows this decrease of $\zeta$ to exhibit the monotonic thinning even at $\dot{\varepsilon}>\tau_R^{-1}$. In contrast, for solutions, the simulated $\eta_E$ exhibits thickening at $\dot{\varepsilon}>\tau_R^{-1}$ because the average anisotropy $\bar{S}$ is governed by the solvent and remains small, thus overwhelming the increase of the subchain stretch $\tilde{\lambda}$. The simulated results proved to be in satisfactory agreement with the experiments.

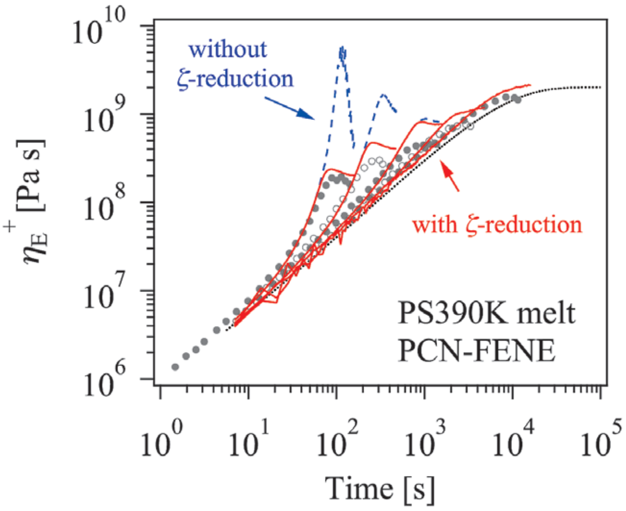
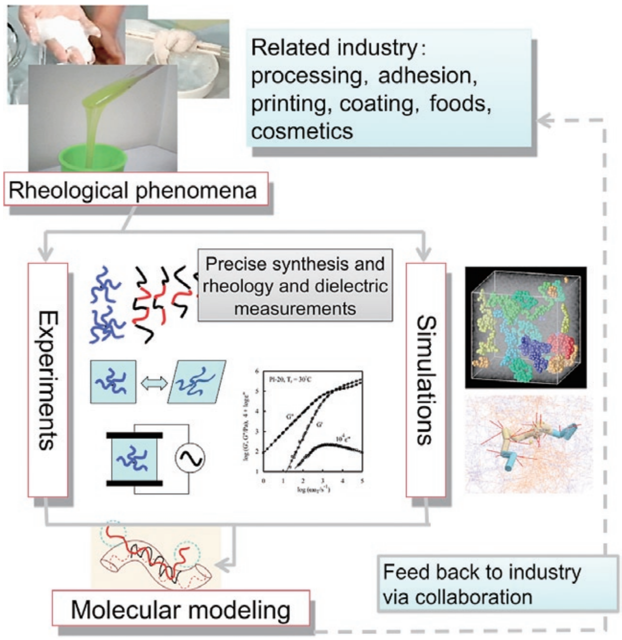


**Figure 1.** Uniaxial viscosity growth data for linear polymer melt (PS, $M$ = 390K) at various strain rates (open circles). Simulation results with (red solid curves) and without (black dash curves) stretch/orientation-dependent monomeric friction reduction are shown. The former agrees well with the experimental data.



# Division of Multidisciplinary Chemistry
## – Molecular Aggregation Analysis –

http://www.kuicr.kyoto-u.ac.jp/labos/is2/scope.html


Prof
SATO, Naoki
(D Sc)


Assoc Prof
ASAMI, Koji
(D Sc)


Assist Prof
YOSHIDA, Hiroyuki
(D Sc)


Assist Prof
MURDEY, Richard James
(Ph D)

### Students

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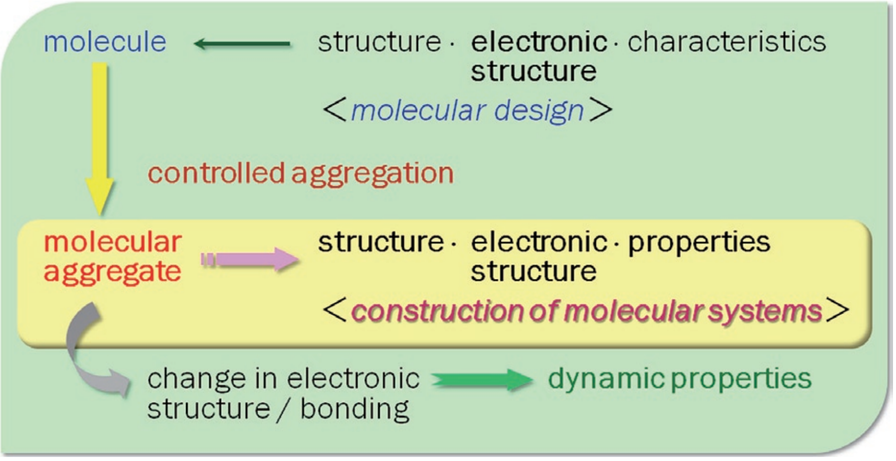
HIDAKA, Yuta (M1)
SHIRAISHI, Ryo (M1)

## Scope of Research

The research at this subdivision is devoted to correlation studies on structures and properties of both natural and artificial molecular aggregates from two main standpoints: photoelectric and dielectric properties. The electronic structure of organic thin films is studied using photoemission and inverse photoemission spectrosocpies in connection with the former, and its results are applied to create novel molecular systems with characteristic electronic functions. The latter is concerned with heterogeneous sturcutres in mocrocapsules, boipolymers, biological membranes and biological cells, and the nonlinearity in their dielectric properties is also studied in relation to molecular motions.

**KEYWORDS**
α-Dispersion
Cell Suspension
Core Level Energy
Film Surface
Organic Semiconductor



### Selected Publications

Yoshida, H.; Sato, N., A Precise Analysis of the Core-Level Energy Difference between the Surface and Bulk Region of Organic Semiconductor Thin Films, *J. Phys. Chem. C*, **116,** 10033-10038 (2012).

Yoshida, H.; Ito, E.; Hara, M.; Sato, N., Core Level Energy Differences between the Surface and Bulk of Organic Semiconductor Films: The Effect of Electrostatic Polarization Energy, *Synth. Met.*, **161,** 2549-2553 (2012).

Yoshida, H.; Ito, E.; Hara, M.; Sato, N., Electronic Structure of the Buried Interface between an Organic Semiconductor, *N,N'*-Bis(3-methylphenyl)-*N,N'*-diphenylbenzidine (TPD), and Metal Surfaces, *J. Nanosci. Nanotechnol.*, **12,** 494-498 (2012).

Yoshida, H., Near-Ultraviolet Inverse Photoemission Spectroscopy Using Ultra-Low Energy Electrons, *Chem. Phys. Lett.*, **539-540,** 180-185 (2012).

Daoud, J.; Asami, K.; Rosenberg, L.; Tabrizian, M., Dielectric Spectroscopy for Non-Invasive Monitoring of Epithelial Cell Differentiation within Three Dimensional Scaffolds, *Phys. Med. Biol.*, **57,** 5097-5112 (2012).

Murdey, R.; Sato, N., Voltage Stress Induced Reversible Diode Behavior in Pentacene Thin Films, *J. Chem. Phys.*, **137,** [234703-1]-[234703-5] (2012).

## A Precise Analysis of the Core-Level Energy Difference between the Surface and Bulk Regions of Organic Semiconductor Thin Films

We have presented a precise analysis of the angle-resolved X-ray photoemission spectra to evaluate the energy difference for a particular electronic level between the surface and bulk layers of organic thin films. In contrast to the method employed in the earlier studies, the present analysis allows us to determine the energy difference precisely as well as the thickness of the surface region as a result of the following features:

(1) Photoemission spectra were measured at more than 10 different detection angles $\theta$.

(2) Subtle spectral differences were efficiently detected using principal component analysis (PCA).

(3) The determined spectral differences were expressed as the Taylor series expansion of the coefficients of which are calculated by the target transformation of the PCA results without losing information.

(4) By comparing the spectral differences expressed in the form of the Taylor series expansion with the two-layer model, the energy difference of the C1s level between the surface and bulk layers, $E_2$–$E_1$, and the thickness of surface layer $z$ are obtained, where $E_1$ and $E_2$ are assumed to be the energies of the C1s level in the surface and the other regions in the organic layer, respectively.

The method was applied to the organic films of tris(8-hydroxyquinoline)aluminum ($Alq_3$), bathocuprine (BCP), and copper phthalocyanine (CuPc) vacuum-deposited on polycrystalline gold surfaces. We determined the energy difference between the surface and the bulk to be ranging from 0.2 to 0.4 eV and the thickness of the surface region to be comparable to that of one monolayer. These values agree with the theoretically estimated values, suggesting that the observed energy difference arises from the difference in the electrostatic polarization energy. The larger energy differences observed for the polar molecules suggest, however, that their permanent dipole moments may also play a role.

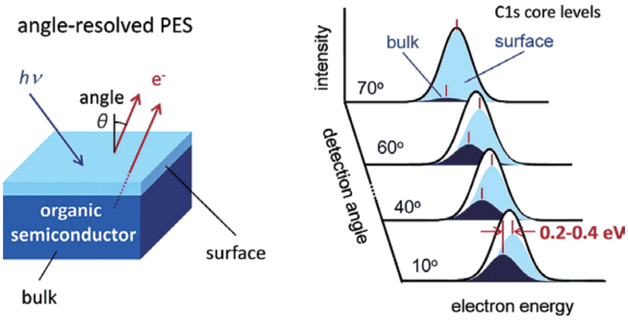


**Figure 1.** Schematic of angle-resolved photoemission spectroscopy to show core level spectra for an organic semiconductor thin film.

## Low-Frequency Dielectric Dispersion of Biological Cell Suspensions

It is known that some cell suspensions show low-frequency dispersion below 10 kHz, which is called $\alpha$-dispersion. The origin of the $\alpha$-dispersion has not been well understood and it seems unlikely that all the $\alpha$-dispersions are interpreted by a unique polarization mechanism. The $\alpha$-dispersion of bacteria may be due to displacement of counterions around charged cell surfaces, i.e., counterion polarization. The $\alpha$-dispersion of erythrocyte ghosts (that are erythrocytes lysed in hypotonic media) has been lately interpreted in terms of interfacial polarization by taking into account the presence of a nano-size hole on each ghost. Another candidate for the origin of the $\alpha$-dispersion is movement of charges and/or reorientation of dipoles in the membranes. To test the possibility erythrocytes were doped with dipicrylamine (DPA) ions that readily translocate in the membrane because of their lipophilic nature. The DPA-doped cell suspensions showed the low-frequency dispersion around a few kHz as expected (Figure 2). The dispersion was accounted for by displacement of the mobile charges in the membrane.

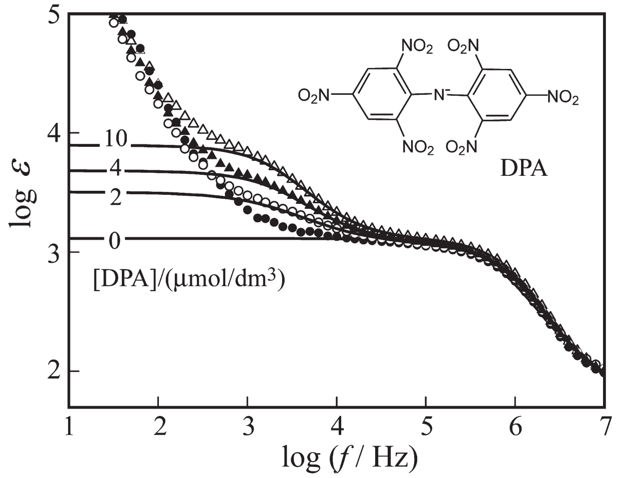


**Figure 2.** Dielectric spectra of DPA-doped erythrocyte suspensions.

# Division of Multidisciplinary Chemistry
## – Interdisciplinary Chemistry for Innovation –

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### Students

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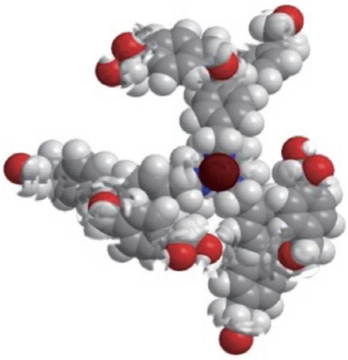
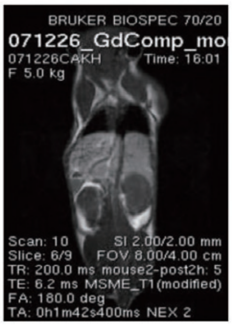
SUGII, Hiroaki (M1)
IURA, Yoshihito (UG)
KAMEDA, Tetsurou (UG)

## Scope of Research

Organic chemistry can contribute to the innovation through the design and synthesis of molecules those are valuable to human society. Our methodology possesses advantage in heteroatom chemistry, transition metal-catalyzed reactions, and asymmetric synthesis. As for the synthetic procedure, we take note to develop atom-economic as well as environment-benign reactions. We recognize the importance of the collaboration with various fields of technology of industry and academia. Recent examples of our projects include design, synthesis, and evaluation of aromatic compounds used in light-emitting field-effect transistors, sugar-fullerene linked compounds used in photodynamic therapy of cancers, and gadolinium complex of chiral dendrimers used in magnetic resonance imaging of cancers (shown in the figure).





**KEYWORDS**
Innovation
Organic Synthesis
Heteroatom Chemistry
Transition Metal Catalyst
Asymmetric Synthesis

## Selected Publications

Miyake, Y.; Kimura, Y.; Ishikawa, S.; Tsujita, H.; Miura, H.; Narazaki, M.; Matsuda, T.; Tabata, Y.; Yano, T.; Toshimitsu, A.; Kondo, T., Synthesis and Functional Evaluation of Chiral Dendrimer-Triamine-Coordinated Gd Complexes as Highly Sensitive MRI Contrast Agents, *Tetrahedron Lett.*, **53,** 4580-4583(2012).

Kondo, T.; Kimura, Y.; Kanda, T.; Takagi, D.; Wada, K.; Toshimitsu, A., Simple and Practical Aerobic Oxidation of Alcohols Catalyzed by a (μ-Oxo)tetraruthenium Cluster, *Green Sus. Chem.*, **1,** 149-154 (2011).

Kondo, T.; Niimi, M.; Yoshida, Y.; Wada, K.; Mitsudo, T.; Kimira, Y.; Toshimitsu, A., Rhodium-catalyzed Linear Codimerization and Cycloaddition of Ketenes with Alkynes, *Molecules*, **15,** 4189-4200 (2010).

Sakanoue, T.; Yahiro, M.; Adachi, C.; Takimiya, K.; Toshimitsu, A., Electrical Characteristics of Single-component Ambipolar Organic Field-effect Transistors and Effects of Air Exposure of Them, *J. Appl. Phys.*, **103,** [094509-1]-[094509-6] (2008).

Sakanoue, T.; Yahiro, M.; Adachi, C.; Uchiuzou, H.; Takahashi, T.; Toshimitsu, A., Ambipolar Light-emitting Organic Field-effect Transistors Using a Wide-band-gap Blue-emitting Small Molecule, *Appl. Phys. Lett.*, **90,** [171118-1]-[171118-3] (2007).

## Synthesis and Functional Evaluation of Chiral Dendrimer-Triamine-Coordinated Gd Complexes as Highly Sensitive MRI Contrast Agents

MRI constitutes a prominent non-invasive imaging technique for disease diagnosis. Low-molecular-weight contrast agents based on Gd-DTPA (DTPA = diethylenetriaminepentaacetic acid) has been approved by the U.S. Food and Drug Administration (FDA) and the European Medicines Agency (EMEA), and is widely used in the clinical diagnosis of tumors. However, the non-specificity, low contrast efficiency and rapid renal excretion of this low-molecular-weight contrast agent necessitate a high dosage (*ca*. 0.5 M), which imposes a great physical strain on the patient. The main reason for the low contrast efficiency is that, among the 9 coordination sites of Gd, up to 8 are solidly occupied with ionic chelating ligands, and thus only 1 remains for coordination with free water molecules, which is observed by MRI. In addition, the rotational motion of Gd metal in the center of existing small ligands cannot be suppressed, and as a result the image contrast is considerably reduced.

In order to overcome these difficulties, we prepared *chiral* dendrimer-triamine-coordinated Gd complexes **1-(*R*)** and **1-(*S*)** shown in Figure 1. Complexes **1-(*R*)** and **1-(*S*)** have a triamine ligand and three chloride ligands, which stably occupy 6 coordination sites of Gd. Accordingly, 3 coordination sites remain vacant for coordination with water molecules, which will be observed by MRI. In addition, large dendrimer in the periphery of Gd will suppress the molecular tumbling and rotation of Gd to result in the increase of the image contrast.

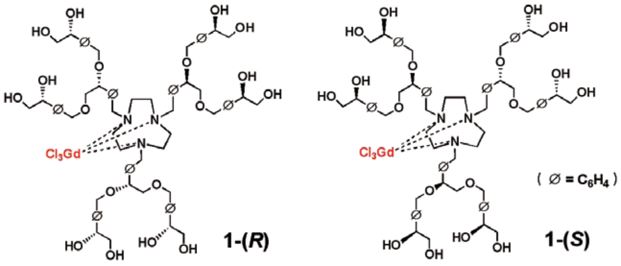


**Figure 1.** Structure of chiral dendrimer-triamine-coordinated Gd compleses, **1-(*R*)** and **1-(*S*)**.

The ability as the imaging agents *in vitro* was evaluated by the longitudinal relaxivities (r1) of Gd complexes (**1-(*R*)** and **1-(*S*)**), $GdCl_3 \cdot 6H_2O$, and Gd-DTPA (Figure 2). As expected, the r1 values of **1-(*R*)** and **1-(*S*)** were 11.4 and 11.1 $mM^{-1}$ $s^{-1}$, respectively, which are approximately 3 times higher than that of Gd-DTPA (r1 = 4.6 $mM^{-1}$ $s^{-1}$).

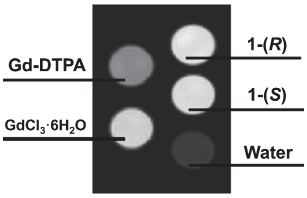


**Figure 2.** T1-weighted MR images of Gd-DTPA, $GdCl_36H_2O$, **1-(*R*)**, **1-(*S*)** (0.50 mM) and water.

Contrast enhancement by **1-(*R*)** and **1-(*S*)** was also evaluated *in vivo*. Figure 3 shows T1-weighted MR images of mice before and after intravenous injection of **1-(*R*)**, **1-(*S*)**, and Gd-DTPA (0.10 mmol Gd/kg). Since most of the injected Gd-DTPA was excreted through the kidney, and accumulated in the bladder within 30 min, little contrast enhancement was observed except for the kidney. In contrast, no accumulation of **1-(*R*)** or **1-(*S*)** in specific organs, such as the liver and kidney, was observed with high and prolonged contrast enhancement throughout the entire bodies of mice. They also showed improved vascular retention and a moderate renal excretion rate (completely excreted after 24 h).

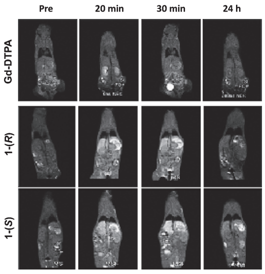


**Figure 3.** T1-weighted MR images before and after intravenous injection of Gd-DTPA (top), **1-(*R*)** (middle), and **1-(*S*)** (bottom).

In order to discuss the differences between optical isomers, the time-course of the signal intensities (SI) at the blood vessels in MR images was measured to indicate that the rate of clearance of **1-(*R*)** was faster than that of **1-(*S*)** (Figure 4). In addition, the concentrations of $Gd^{3+}$ in the blood and urine, 60 minutes after the injection of **1-(*R*)** and **1-(*S*)**, were quantified by an atomic absorption spectroscopy, which showed that 30.2% of **1-(*R*)** and 20.6% of **1-(*S*)** were transferred to urine, while 22.9% of **1-(*R*)** and 27.8% of **1-(*S*)** were retained in the blood, respectively. All results obtained strongly support that **1-(*S*)** is retained in vasculature for longer than **1-(*R*)** after administration in a mouse body.

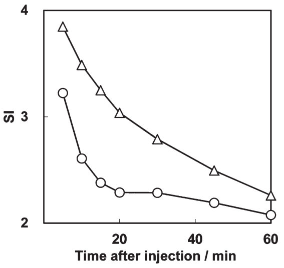


**Figure 4.** Time-course of the signal intensities (SI) at the blood vessels in MR images after injection of **1-(*R*)** (circular symbol) and **1-(*S*)** (triangular symbol).

# Advanced Research Center for Beam Science
## – Particle Beam Science –

http://wwwal.kuicr.kyoto-u.ac.jp/www/index-e.htmlx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IWASHITA, Yoshihisa
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Assist Prof
SOUDA, Hikaru


Techn Staff
TONGU, Hiromu

### Lect (pt)

| | |
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KAZAMA, Ichiro

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NASU, Yuji (M2)
FUWA, Yasuhiro (M2)
KITAHARA, Ryunosuke (M1)
IKEDA, Hideki (M1)

### Visitors

| | |
|---|---|
| Prof MADSEN, Niels | Swansea University, Department of Physics, U.K., 1–8 October |
| Mr PLOSTINAR, Ciprian | Rutherford Appleton Laboratory, Romania, 15–17 October |

## Scope of Research

The Following Subjects are being studied: Beam dynamics related to space charge force in accelerators: Beam handling during the injection and extraction processes of the accelerator ring: Ultra-low Emittance state of a proton beam created by the electron cooling: Laser cooling of $Mg^+$ ion beam: Irradiation of short bunch proton beam by electron cooling and phase rotation: Research and development of permanent quadrupole magnets for final focusing of International Linear Collider(ILC): Development of electron-cyclotron resonance(ECR) ion source for small neutron source.

**KEYWORDS**
Beam Physics
Accelerator Physics
Beam Cooling
Phase Rotation
Neutron Optics

### Selected Publications

Noda, A., Ion Beam Cooling at S-LSR Project, *Nucl. Instrum. Meth.*, **A532,** 150-156 (2004).
Shirai, T.; Ikegami, M.; Fujimoto, S.; Souda, H.; Tanabe, M.; Tongu, H.; Noda, A.; Fujimoto, T.; Iwata, S.; Shibuya, S.; Smirnov, A.; Meshkov, I.; Fadil, H.; Grieser, M., One Dimensional Beam Ordering of Protons in a Storage Ring, *Phys. Rev. Lett.*, **98,** [204801-1]-[204801-4] (2007).
Nakamura, S.; Ikegami, M.; Iwashita, Y.; Shirai, T.; Tongu, H.; Souda, H.; Daido, H.; Mori, M.; Kado, M.; Sagisaka, A.; Ogura, K.; Nishiuchi, M.; Orimo, S.; Hayashi, Y.; Yogo, A.; Pirozhkov, A. S.; Buranov, S. V.; Esirkepov, T.; Nagashima, A.; Kimura, T.; Tajima, T.; Takeuchi, T.; Fukumi, A.; Li, Z.; Noda, A., High-Quality Laser-Produced Proton Beam Realized by the Application of a Synchronous RF Electric Field, *Jpn. J. Appl. Phys.*, **46,** L717-L720 (2007).
Wakasugi, M.; Emoto, T.; Furukawa, Y.; Ishii, K.; Ito, S.; Koseki, T.; Kurita, K.; Kuwajima, A.; Masuda, T.; Morikawa, A.; Nakamura, M.; Noda, A.; Ohnishi, T.; Shirai, T.; Suda, T.; Takeda, H.; Tamae, T.; Tongu, H.; Wang, A.; Yano, Y., Novel Internal Target for Electron Scattering off Unstable Nuclei, *Phys. Rev. Lett.*, **100,** [164801-1]-[164801-4] (2008).
Iwashita, Y.; Tajima, Y.; Hayano, H., Development of High Resolution Camera for Observations of Superconducting Cavities, *Phys. Rev. S.T.-Accel. Beams*, **11,** [093501-1]-[093501-6] (2008).
Arimoto, Y.; Geltenbort, P.; Imajo, S.; Iwashita, Y.; Kitaguchi, M.; Seki, Y.; Shimizu, H. M.; Yoshioka, T., Demonstration of Focusing by a Neutron Accelerator, *Phys. Rev. A*, **86,** 023843 (2012).

## Efficiency Enhancement of Indirect Transverse Laser Cooling by Synchro-Betatron Resonance Coupling with Suppression of Circulating Ion Beam Intensity

The capability to cool down the transverse temperature of the circulating $^{24}Mg^+$ ion beam with the kinetic energy of 40 keV by application of “Synchro-Betatron Resonance Coupling” (SBRC) [1] has already been experimentally demonstrated [2]. The transverse cooling rate, however, was so slow to reach crystalline string state [3] that an approach to enhance the efficiency of the indirect transverse laser cooling by SBRC with suppression of the circulating ion beam current using scraping has been proposed and tested [4] After suppression of the circulating beam intensity, the transverse beam profiles were measured using another scrapers with the measurement of survival rate for various scraper positions, which enabled us to observe the beam size for the circulating beam intensity down to $10^4$. In Figure 1(a) the cooled beam sizes for various beam intensities are shown. Together with recent optimization of overlapping between the laser and the ion beam using adjusters by piezo-driven mirrors, the cooling time of the transverse beam size has been reduced by suppression of the circulating ion numbers as shown in Figure 1 [5].

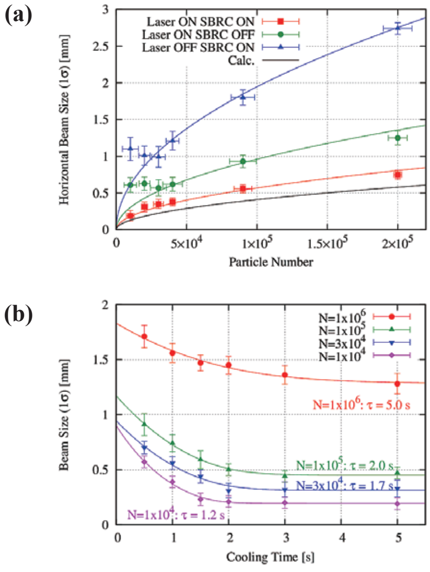

**Figure 1.** Circulating beam intensity dependence of the indirectly transverse cooled $^{24}Mg^+$ ion beam size.

**References**

[1] H. Okamoto, A.M. Sessler, D. Mohl, *Phys. Rev. Lett.*, **72** (1994) 3977-3980.

[2] M. Nakao et al., *Phys. Rer. ST Accel. Beam*, **15,** 110102.

[3] J. Wei, H. Okamoto, A.M. Sessler, *Phys. Rev. Lett.*, **80** (1998) 2606-2609.

[4] A. Noda et al. *Proc. of the 23rd Russian Particle Accelerator Conference*, St. Petersburg, Russia, 24-28 September 2012, 48-52.

[5] H. Souda et al., *Jpn. J. Appl. Phys*., 52 (2013) 030202.

## Controlled Acceleration of Neutrons

Today, neutron beam is utilized widely, for example investigations of material structure and cancer therapy. The utilizing efficiency, however, is limited because controlling neutrons, which have no electric charge, is difficult with the conventional accelerator technique. On the other hand, a neutron has the magnetic dipole moment, which feels a force in a gradient magnetic field. Already developed neutron lens exerts the force for transverse direction by sextupole magnetic field, which focuses neutron beams and improves the efficiency on the small angle neutron scattering (SANS) experiments. Although such a force in the longitudinal direction has been well known, net velocity change is not available when the magnetic field strengths of initial and final positions are the same (it acts as the magnetic potential) if the spin preserves. Combination of a static gradient magnetic field and an RF field, whose frequency is well modulated, makes the spin flip in the static magnetic field to change the sign of the force. The demonstration experiment was performed at ILL, France and a space-time focusing of neutrons (can increase space density at an experimental area) are successfully observed by controlling the velocities of the neutrons. This will be a powerful technique for variety of measurements that require high density of neutrons, for example, the search of the permanent electric dipole moment of neutrons, which relates to the violation of time-reversal invariance in particle physics.

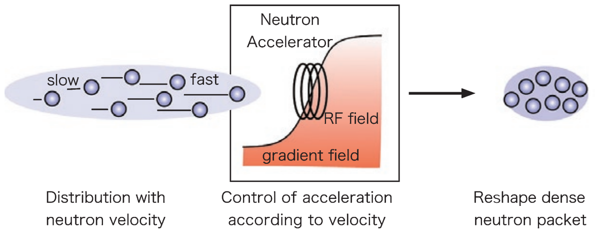

**Figure 2.** Our neutron accelerator system can reshape the neutron bunch at the experimental position by using gradient magnetic field and RF field.

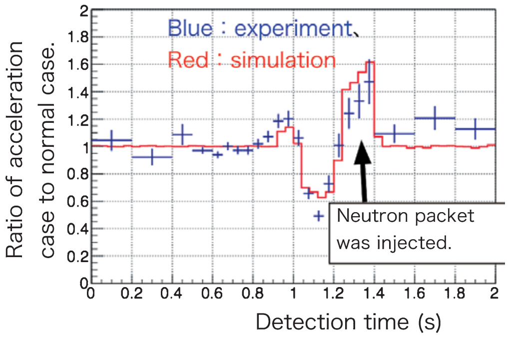

**Figure 3.** The neutron packet was injected and made the peak in the graph.

# Advanced Research Center for Beam Science
## – Laser Matter Interaction Science –

http://laser.kuicr.kyoto-u.ac.jp/e-index.html

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## Students

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MIYASAKA, Yasuhiro (D2)
NAKAJIMA, Hiroaki (M2)
IKEDA, Daiki (M1)
KAWAMOTO, Mao (M1)
MAEDA, Kazuya (M1)
MORI, Kazuaki (M1)

## Visitor

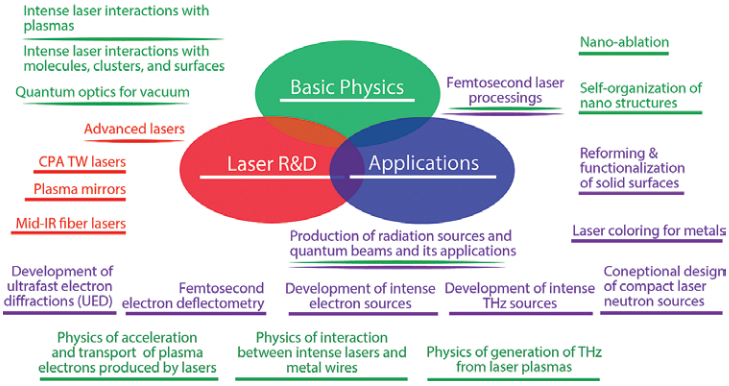
Ms GEMINI, Laura    Czech Technical University, Czech R., 15 September–30 November

## Scope of Research

The interaction of femtosecond laser pulses with matters involves interesting physics, which does not appear in that of nanosecond laser pulses. Investigating the interaction physics, potential of intense femtosecond lasers for new applications is being developed (such as laser produced radiations and laser processing). Ultra-intense lasers can produce intense radiations (electrons, ions, THz, and so on), which can be expected as the next-generation radiation sources. Ultra-short lasers are available to process any matters without thermal dissociation. The femtosecond laser processing is also the next-generation laser processing. In our laboratory ultra intense femtosecond laser named $T^6$-laser is equipped, and the physics of intense laser matter interactions and its applications are researched.

### KEYWORDS

Intense Laser Science
Laser Plasma Radiations
(Electrons, Ions, and THz)
Ultrafast Electron Diffraction (UED)
Laser Nano-ablation Physics
Femtosecond Laser Processing
Mid-infrared Fiber Lasers



## Selected Publications

Inoue, S.; Tokita, S.; Otani, K.; Hashida, M.; Hata, M.; Sakagami, H.; Taguchi, T.; Sakabe, S., Autocorrelation Measurement of Fast Electron Pulses Emitted through the Interaction of Femtosecond Laser Pulses with a Solid Target, *Phys. Rev. Lett.*, **109,** 185001 (2012).

Miyasaka, Y.; Hashida, M.; Ikuta, Y.; Otani, K.; Tokita, S.; Sakabe, S., Nonthermal Emission of Energetic Ions from a Metal Surface Irradiated by Extremely Low-Fluence Femtosecond Laser Pulses, *Physical Review B*, **86,** 75431 (2012).

Jahangiri, F.; Hashida, M.; Tokita, S.; Nagashima, T.; Ohtani, K.; Hangyo, M.; Sakabe, S., Directional Terahertz Emission from Air Plasma Generated by Linearly Polarized Intense Femtosecond Laser Pulses, *Appl. Phys. Express*, **5,** 26201 (2012).

Inoue, S.; Tokita, S.; Otani, K.; Hashida, M.; Sakabe, S., Femtosecond Electron Deflectometry for Measuring Transient Fields Generated by Laser-accelerated Fast Electrons, *Appl. Phys. Lett.*, **99,** 31501 (2011).

Tokita, S.; Otani, K.; Nishoji, T.; Inoue, S.; Hashida, M.; Sakabe, S., Collimated Fast Electron Emission from Long Wires Irradiated by Intense Femtosecond Laser Pulses, *Phys. Rev. Lett.*, **106,** 255001 (2011).

## Upgraded Laser System for Higher Quality Pulse Generation

The $T^6$-laser has been operated for the study of laser-matter interaction physics and its applications since 1987 (since 2004 at ICR), and lots of fruits were obtained by not only our laboratory members but also the collaboration with another universities and industrial enterprises. For more advanced research, a major upgrade of the laser system was made from April to August 2012. The upgraded points are (1) install of a plasma-mirror pulse cleaner, (2) shortening of pulse duration, (3) accompanying increase of peak power, and (4) install of a programmable femtosecond pulse shaper. Especially for the first point, it is the first development of a high-repetition-rate plasma mirror setup in Japan. The new laser system (Figure 1) delivers 30 fs, 0.5 J pulses (15 TW) with 5 Hz repetition rate. Its frontend incorporates a 10-fs mode-locked laser oscillator, an Offner-triplet-type pulse stretcher, the programmable spectral pulse shaper allowing to optimize the group delay dispersion of the whole system, a 8-pass preamplifier, and a picosecond Pockels cell system for a high contrast ratio of the ASE (amplified spontaneous emission) prepulse to the femtosecond main pulse. The backend of the laser system incorporates the plasma mirror to further improve the contrast ratio, resulting in an estimated contrast ratio of $10^{-12}$ at 1 ns before the main pulse.

**Figure 1.** A photograph of the new laser system.

## Nonthermal Emission of Energetic Ions from a Metal Surface Irradiated by Extremely Low-fluence Femtosecond Laser Pulses

We have found a new phenomenon of energetic ion emission in extremely low-fluence range. In this research, ions emitted from a copper surface are studied by energy spectroscopy. The energy spectra of ions are investigated considering surface state changes with respect to the number of laser pulses. Singly charged ions with energies of 180 eV are produced at low fluences of 80 mJ/cm$^2$, and the ion energy spectrum does not follow a shifted Maxwell-Boltzmann (SMB) distribution (Figure 2). A new mechanism of ion acceleration, namely, Coulomb explosion of nanoparticles (CENs), is proposed to explain the energy spectra of ions. This mechanism is supported by the relationships of surface-state (self-organized nanostructures) with ion energy and ion emission amounts.

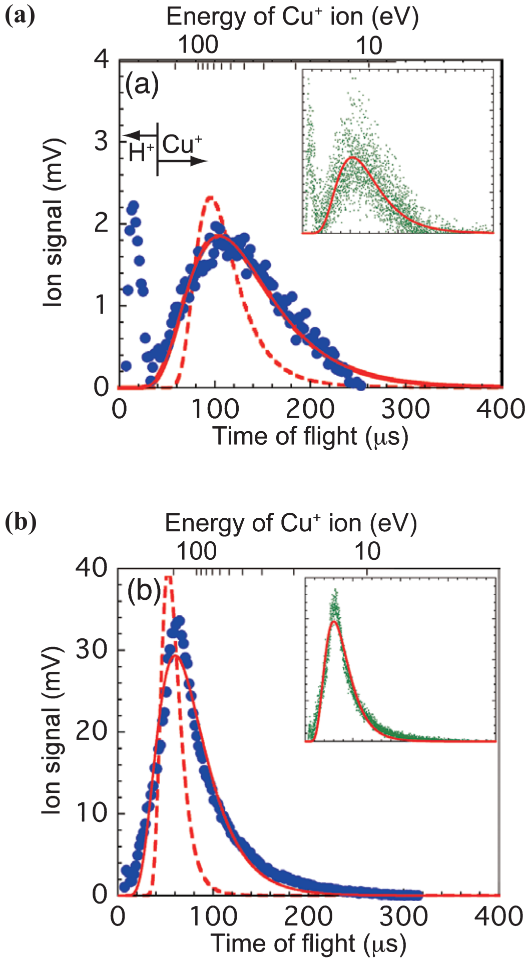


**Figure 2.** The TOF spectra for copper irradiated by femtosecond laser pulse ($F$=80mJ/cm$^2$, 170fs, 800nm). (a) Copper surface with mechanically polished and (b) Structured surface structure on copper with femtosecond laser pre-irradiation. Dashed lines and solid lines indicate the calculated SMB distribution and CEN distribution, respectively.

# Advanced Research Center for Beam Science
## – Electron Microscopy and Crystal Chemistry –

http://eels.kuicr.kyoto-u.ac.jp/Root/English


Prof
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KIYOMURA, Tsutomu


Res*
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## Students

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SAITO, Hikaru (D2)
ASO, Ryotaro (D2)
FUJIYOSHI, Yoshifumi (D1)
OGIMOTO, Mao (M2)
YAMAGUCHI, Atsushi (M1)
YAMAGUCHI, Hitomi (M1)

## Visitor

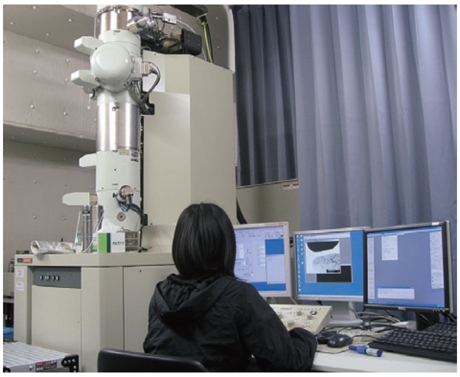
| | |
|---|---|
| Dr LO, Shen-Chuan | Industrial Technology Research Institute, Taiwan, 28 May–1 June, 15–19 October |

## Scope of Research

Crystallographic and electronic structures of materials and their transformations are studied through direct imaging of atoms or molecules by high-resolution electron spectromicroscopy which realizes energy-filtered imaging and electron energy-loss spectroscopy as well as high resolution imaging. By combining this with scanning probe microscopy, the following subjects are urging: direct structure analysis, electron crystallographic analysis, epitaxial growth of molecules, structure formation in solutions, and fabrication of low-dimensional functional assemblies.

**KEYWORDS**

TEM
STEM
Cryo-TEM
EELS
SPM



## Selected Publications

Kobayashi, T.; Ogawa, T.; Moriguchi, S.; Suga, T.; Yoshida, K.; Kurata, H.; Isoda, S., Inhomogeneous Substitution of Polyhalogenated Copper-phthalocyanine Studied by High-resolution Imaging and Electron Crystallography, *J. Electron Microsc.*, **52,** 85-90 (2003).

Minari, T.; Nemoto, T.; Isoda, S., Temperature and Electric-field Dependence of the Mobility of a Single-grain Pentacene Field-effect Transistor, *J. Appl. Phys.*, **99,** 034506 (2006).

Kiyomura, T.; Nemoto, T.; Ogawa, T.; Minari, T.; Yoshida, K.; Kurata, H.; Isoda, S., Thin-Film Phase of Pentacene Film Formed on KCl by Vacuum Deposition, *Jpn. J. Appl. Phys.*, **45,** 401-404 (2006).

Haruta, M.; Kurata, H.; Komatsu, H.; Shimakawa, Y.; Isoda, S., Site-resolved Oxygen K-edge ELNES of Layered Double Perovskite $La_2CuSnO_6$, *Physical Review B*, **80,** 165123 (2009).

Haruta, M.; Kurata, H., Direct Observation of Crystal Defects in an Organic Molecular Crystals of Copper Hexachlorophthalocyanine by STEM-EELS, *Sci. Rep.*, **2,** [252-1]-[252-4] (2012).

## Direct Observation of Crystal Defects in an Organic Molecular Crystals of Copper Hexachlorophthalocyanine by STEM-EELS

The structural analysis of crystal defects in organic thin films provides fundamental insights into their electronic properties for applications such as field effect transistors. Observation of crystal defects in organic thin films has previously been performed at rather low resolution by conventional transmission electron microscopy based on phase-contrast imaging. Herein, we apply for the first time annular dark-field imaging to the direct observation of grain boundaries in copper hexachlorophthalocyanine thin films at the atomic resolution level by using an aberration-corrected scanning transmission electron microscope combined with electron energy-loss spectroscopy. By using a low-dose technique and an optimized detection angle, we were able to visualize the contrast of light element (C and N) together with the heavier elements (Cl and Cu) within the molecular column. We were also able to identify unexpected molecular orientations in the grain boundaries along the {110} crystallographic planes giving rise to stacking faults.

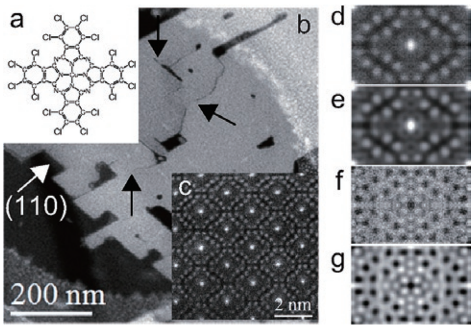


**Figure 1.** (a) Molecular structure of $Cl_{16}CuPc$. (b) Low-magnification image of $Cl_{16}CuPc$ molecular crystal projected along the c-axis. (c) High resolution LAADF-STEM raw image from a single crystal region. (d) Translationally averaged experimental and (e) noise-filtered LAADF-STEM images of one molecular column. (f) Translationally averaged experimental and (g) noise-filtered ABF-STEM images of one molecular column.

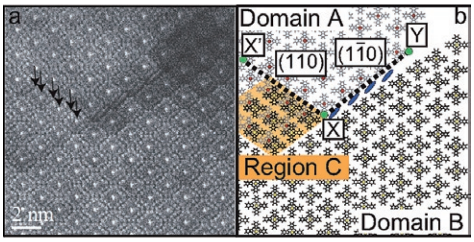


**Figure 2.** (a) LAADF-STEM image of complex defect region. The stacking fault was observed along the (110) plane and $Cl_{16}CuPc$ molecules with irregular orientation were identified in the grain boundary along the $(1\bar{1}0)$ plane as a line contrast. (b) Schematic diagram of molecular columns corresponding to (a). The two domains, A and B, can be seen as gray and black molecules, and molecules along the XY grain boundary are shown as blue ellipses.

## Photoassisted Scanning Tunneling Microscopy Investigation on the ZnO(0001)-Zn Surface Treated by Alkaline Solution

In this study, the surface geometric structures of epitaxial (0001) ZnO films treated by NaOH solution are investigated using photoassisted scanning tunneling microscopy (STM). By illuminating ultraviolet (UV) light on the epitaxial (0001) ZnO film, the tunneling current can be significantly enhanced to construct the well-defined STM images. Polarity identification of the epitaxial (0001) ZnO film by convergent-beam electron diffraction indicates that the epitaxial (0001) ZnO film exhibits the Zn-polar surface. Two types of topographic features, i.e., hexagonal pyramid and flat plane, are observed in the AFM images of the as-grown epitaxial (0001) ZnO film. UV-assisted STM images reveal the anisotropic etching behaviors of the epitaxial (0001) ZnO films in NaOH solution. The faceted and symmetrically layered hexagonal-pyramid feature gets asymmetrical and rounded with increasing etching time. On the other hand, few small hexagonal pits on the as-grown flat ZnO(0001)-Zn surface are developed to asymmetrically hexagonal cavities with flat terraces and steps after NaOH treatments. In addition, triangular reconstruction of the NaOH-treated ZnO(0001)-Zn surface and evidently layerstacking feature on a faceted ZnO surface with a step height resolved in the atomic scale are also demonstrated in ambience using the photoassisted STM.

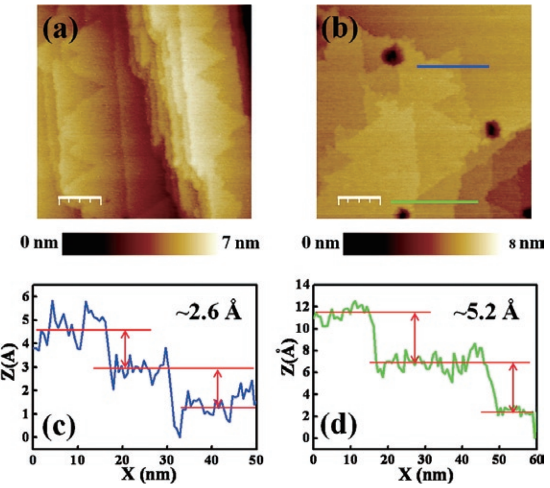


**Figure 3.** High-magnification UV-assisted STM images of ZnO films after NaOH treatments for (a) 20 s (scale bar = 30 nm) and (b) 50 s (scale bar = 32 nm). (c,d) Cross-sectional line profiles of the regions in (b) denoted by blue and green lines, respectively.

# Advanced Research Center for Beam Science
# – Structural Molecular Biology –

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Assist Prof *
YAMAUCHI, Takae
(D Agr)

* Advanced Research Center for Beam Science, Laboratory for Structual Proteomics

## Student

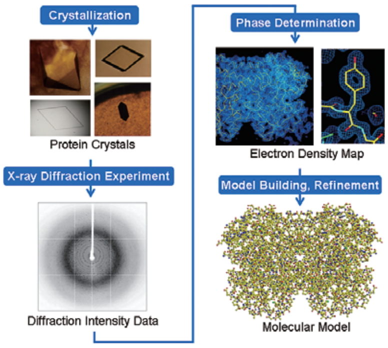
KOBAYASHI, Kazutaka (D1)

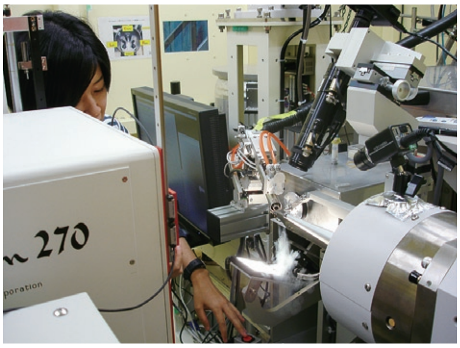
## Scope of Research

The research activities in this laboratory are performed for X-ray structural analyses of biological macromolecules and the investigation of the electronic state in materials as follows: The main subjects of the biomacromolecular crystallography are crystallographic studies on the reaction mechanism of enzymes, the relationship between the multiform conformation and the functional variety of proteins, and the mechanism of thermostabilization of proteins. In the investigation of the chemical state in materials, the characteristics of the chemical bonding in the atom and molecules are investigated in detail using a newly developed X-ray spectromator with a high-resolution in order to elucidate the property of materials. The theoretical analysis of the electronic states with DV-Xα and WIEN2k, and the development of new typed X-ray spectrometer with ultra high-resolution have also been carried out.

### KEYWORDS

Crystal
X-ray Crystallographic Analysis
Structural Biology
Protein Crystallography
Structure and Function





## Selected Publications

Fujii, T.; Maeda, M.; Mihara, H.; Kurihara, T.; Esaki, N.; Hata, Y., Structure of a NifS Homologue: X-ray Structure Analysis of CsdB, an *Escherichia coli* Counterpart of Mammalian Selenocysteine Lyase, *Biochemistry*, **39,** 1263-1273 (2000).

Fujii, T.; Sakai, H.; Kawata, Y.; Hata, Y., Crystal Structure of Thermostable Aspartase from *Bacillus* sp. YM55-1: Structure-based Exploration of Functional Sites in the Aspartase Family, *J. Mol. Biol.*, **328,** 635-654 (2003).

Hayashida, M.; Fujii, T.; Hamasu, M.; Ishiguro, M.; Hata, Y., Similarity between Protein-Protein and Protein-Carbohydrate Interactions, Revealed by Two Crystal Structures of Lectins from the Roots of Pokeweed, *J. Mol. Biol.*, **334,** 551-565 (2003).

Fujii, T.; Oikawa, T.; Muraoka, I.; Soda, K.; Hata, Y., Crystallization and Preliminary X-ray Diffraction Studies of Tetrameric Malate Dehydrogenase from the Novel Antarctic Psychrophile *Flavobacterium frigidimaris* KUC-1, *Acta Crystallogr. Sect. F Struct. Biol. Cryst. Commun.*, **63,** 983-986 (2007).

Fujii, T.; Goda, Y.; Yoshida, M.; Oikawa, T.; Hata, Y., Crystallization and Preliminary X-ray Diffraction Studies of Maleylacetate Reductase from *Rhizobium* sp. Strain MTP-10005, *Acta Crystallogr. Sect. F Struct. Biol. Cryst. Commun.*, **64,** 737-739 (2008).

## Crystal Structure Analysis of the Oxygenase Component (GraA) of a Resorcinol Hydroxylase

The resorcinol hydroxylase is involved in the first step of the resorcinol catabolic pathway and catalyzes hydroxylation of resorcinol to hydroxyquinol. The enzyme belongs to the two-component flavin-diffusible monooxygenae (TC-FDM) family and consists of two components: an oxygenase and a flavin reductase. It uses molecular oxygen and reduced flavin for hydroxylation and NAD(P)H for flavin reduction. The small component, flavin reductase, generates reduced flavin for the oxygenase component to oxygenate the substrate. Thus, the enzymatic reaction is separated into two steps. However, hydroxylation activity is exhibited in the cooperative presence of both the components. To understand the structural basis for the catalytic mechanism, we first performed the crystal structure analysis of the oxygenase component (GraA) from *Rhizobium* sp. strain MTP-10005. GraA is an oligomer and its subunit consists of 409 amino acid residues with the mass of 43,305 Da.

The N-terminal His-tagged GraA was used for crystallization. Tetragonal-bipyramidal crystals with typical size of 0.17 × 0.30 × 0.025 $\mathrm{mm}^3$ were obtained in about 6 days by a vapor diffusion method using PEG3350 as a precipitating agent. They belonged to the tetragonal space group $I4_122$ with unit cell dimensions of $a = b = 101.1$ Å, $c = 319.4$ Å and contained one GraA subunit in asymmetric unit. Diffraction data were collected up to 2.3 Å resolution under cryogenic conditions at beamline BL5A, PF, Tsukuba, Japan. The structure was determined by molecular replacement and refined at 2.3 Å resolution up to $R = 0.179$ and $R_{\mathrm{free}} = 0.217$. The current structure of GraA subunit contains 376 of 409 residues (residue number 17–166, 171–270, 284 – 409) and 247 water molecules.

GraA is a tetramer of four identical subunits related to one another by three molecular two-fold axes which are identical to crystallographic two-fold axes. A given pair of two subunits in the molecule form a close dimer with C-terminal $\alpha$-helical domains crossed together around a crystallographic two-fold axis. Then, two of the close dimers form a loose dimer around another crystallographic two-fold axis crossing perpendicular to the former two-fold axis. Finally, the GraA tetrameric molecule adopts the structure of a dimer of dimers with three molecular two-fold axes perpendicular to one another. The subunit consists of three domains. The N-terminal domain (residues Met1–Ala121) has an $\alpha$-structure mainly of antiparallel $\alpha$-helices, the central domain has a $\beta$-structure of two $\beta$-sheets stacked together, and the C-terminal domain (residues Phe218–Tyr409) has a four-helix-bundle structure of long antiparallel $\alpha$-helices involved in tetramer formation. The space that is encompassed by these three domains is enough to adopt both of the coenzyme, $\mathrm{FADH_2}$, and the substrate, resorcinol.

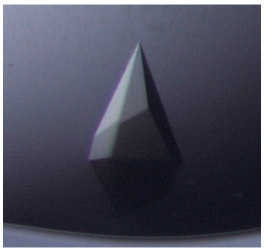


**Figure 1.** Crystal of the oxygenase component (GraA) of a resorcinol hydroxylase from *Rhizobium* sp. strain MTP-10005.

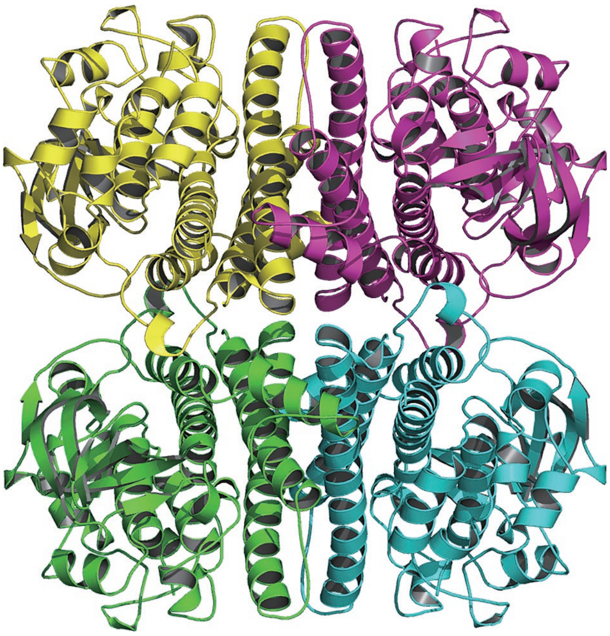


**Figure 2.** Tetrameric molecular structure of the oxygenase component (GraA) of a resorcinol hydroxylase from *Rhizobium* sp. strain MTP-10005.

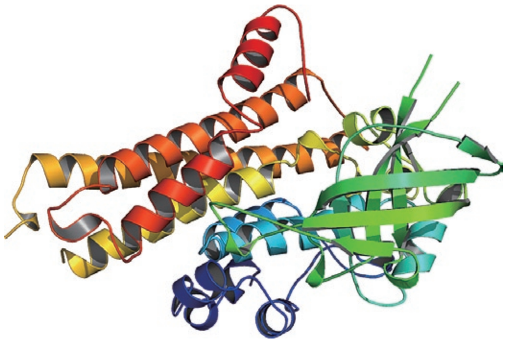


**Figure 3.** Subunit structure of the oxygenase component (GraA) of a resorcinol hydroxylase from *Rhizobium* sp. strain MTP-10005.

# International Research Center for Elements Science
# – Organic Main Group Chemistry –

**http://es.kuicr.kyoto-u.ac.jp/index_en.html**

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## Researcher

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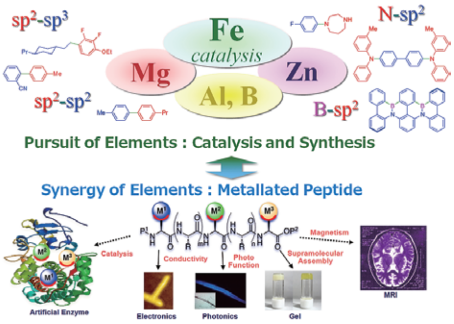
YOKOI, Tomoya (M2)
KAWABATA, Tatsuya (M2)
NAKAJIMA, Sho (M1)
MOCHIZUKI, Ayaka (M1)
YOSHIDA, Ryota (M1)
AOKI, Yuma (UG)

## Visitors

| | |
|---|---|
| Prof Robin, B. Bedford | University of Bristol, U.K., 21 November |
| Prof Duncan, Wass | University of Bristol, U.K., 21 November |

## Scope of Research

Our research activity is focused on the development of molecular transformation reactions, which can provide new ways to exploit chemical resources, such as haloalkanes, alkenes, alcohol etc. The present research subjects are (1) metal-catalyzed C–C and C–N bond forming reactions by using universal metals such as iron, magnesium and aluminum (2) development of smart materials based on synergistic effect of various metals on artificial peptides (3) synthesis of heteroatom-fused π-conjugated molecules toward optoelectronics (4) understanding of synergistic effects of multi-element center interactions for the catalysis with the help of quantum chemical methods and synchrotron X-ray absorption spectroscopy.



**KEYWORDS**

Carbon–Carbon Bond Formation
Iron Catalyst
Cross-Coupling Reaction
Metallated Peptide
π-Conjugated Molecule

## Selected Publications

Ghorai, S. K.; Jin, M.; Hatakeyama, T.; Nakamura, M., Cross-Coupling of Non-activated Chloroalkanes with Aryl Grignard Reagents in the Presence of Iron/*N*-Heterocyclic Carbene Catalysts, *Org. Lett.*, **14,** 1066-1069 (2012).

Hashimoto, T.; Hatakeyama, T.; Nakamura, M., Stereoselective Cross-Coupling between Alkenylboronates and Alkyl Halides Catalyzed by Iron-Bisphosphine Complexes, *J. Org. Chem.*, **77,** 1168-1173 (2012).

Isozaki, K.; Ogata, K.; Haga, Y.; Sasano, D.; Ogawa, T.; Kurata, H.; Nakamura, M.; Naota, T.; Takaya, H., Metal Array Fabrication through Self-assembly of Pt-complex-bound Amino Acids, *Chem. Commun.*, **48,** 3936-3988 (2012).

Hatakeyama, T.; Hashimoto, T.; Kathriarachchi, K. K. A. D. S.; Zenmyo, T.; Seike, H.; Nakamura, M., Iron-Catalyzed Alkyl-Alkyl Suzuki-Miyaura Coupling, *Angew. Chem. Int. Ed.*, **51,** 8834-8837 (2012).

Kawamura, S.; Kawabata, T.; Ishizuka, K.; Nakamura, M., Iron-Catalyzed Cross-Coupling of Halohydrins with Aryl Aluminium Reagents: a Protecting-group-free Strategy Attaining Remarkable Rate Enhancement and Diastereoinduction, *Chem. Commun.*, **48,** 9376-9378 (2012).

Hatakeyama, T.; Hashimoto, S.; Oba, T.; Nakamura, M., Azaboradibenzo[6]helicene: Carrier Inversion Induced by Helical Homochirality, *J. Am. Chem. Soc.*, **134,** 19600-19603 (2012).

# Topics

## Iron-Catalyzed Alkyl-Alkyl Suzuki-Miyaura Coupling

Suzuki-Miyaura coupling reaction is one of the most practical and reliable synthetic reactions for the production of functional molecules such as drug/agrochemical intermediates and organic electronic materials. We have developed an iron-catalyzed alkyl-alkyl Suzuki-Miyaura coupling of primary and secondary alkyl halides by using a Fe(acac)$_3$/Xantphos catalyst. The key to success is the use of *i*PrMgCl as an activator for trialkylboranes. The practicable functional-group compatibility and non-hazardous nature of the iron catalyst suggest that the present reaction is suitable for the facile synthesis of various functional molecules as illustrated by the synthesis of long-chain fatty acid derivatives.

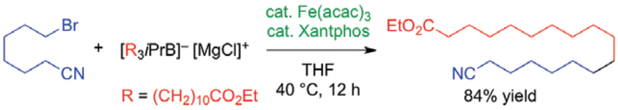


**Figure 1.** Iron-catalyzed alkyl-alkyl Suzuki-Miyaura coupling.

## Metal Array Fabrication through Self-assembly of Pt-complex-bound Amino Acids

Supramolecular self-assembly of amino acids and peptides constitutes a rational approach to fabricating nanostructures comprising highly ordered arrays of functional groups with tailored chemical and physical properties. Indeed, this approach has been widely exploited using various artificial amino acids and peptides which conjugate to photoactive as well as electrically and catalytically active functional groups. Thus, a supramolecular architecture with a well-oriented and highly periodic array of functionalities can be obtained, even with enhanced inherent functions. However, metal array fabrication using such conjugates still remains a largely untouched field. We reported a Pt complex-bound glutamic acid as a building block for a supramolecular β-sheet structure that supports a highly oriented Pt array.

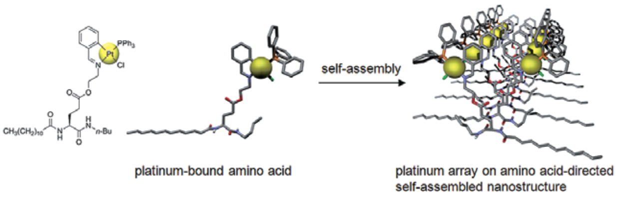


**Figure 2.** Metal array fabrication through self-assembly of Pt-complex-bound amino acids.

## Carrier Inversion of Azaboradibenzo[6]-helicene Induced by Helical Homochirality

Recently, the self-assembly of helicenes via unique π-π stacking interactions in solution, as well as in crystals, has been studied extensively, since these aggregates display intriguing properties such as liquid crystallinity, nonlinear optical susceptibility, and circularly polarized luminescence. So far, however, the electrical properties of these aggregates have not been investigated well, even though the π-π stacking interactions are expected to facilitate charge transport. We have synthesized azaboradibenzo[6]-helicene via a tandem bora-Friedel–Crafts-type reaction and revealed that the racemate and single enantiomer are p-type and n-type semiconductors, respectively. This unprecedented carrier inversion can be explained by changes in the packing structure of the respective hetero and homochiral crystals, as revealed by electronic coupling calculations.

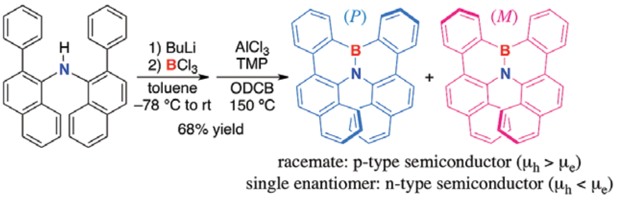


**Figure 3.** Synthesis and carrier inversion of azaboradibenzo[6]helicene.

# International Research Center for Elements Science
## – Advanced Solid State Chemistry –

http://www.scl.kyoto-u.ac.jp/~shimakgr/indexE.html


Prof
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Program-Specific Assist Prof
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PD
CHEN, Wei-tin
(Ph D)


PD
ZHANG, Shoubao
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MATSUMOTO, Kazuya (D3)
HIRAI, Kei (D1)
SHIMIZU, Takuya (M2)
NISHI, Hitomi (M2)
YAMADA, Marina (M2)
HADAME, Koji (M1)
HOSAKA, Yoshiteru (M1)
MURAKAMI, Noriaki (M1)

### Visitors

| | |
|---|---|
| Prof GREEDAN, John. E. | McMaster University, Hamilton, Canada, 12 November |
| Prof SARMA, D. D. | Indian Institute of Science, India, 28 September |
| Prof YU, Jaejun | Seoul National University, Korea, 8 August |
| Prof POEPPELMEIER, Ken | Northwestern University, U.S.A., 6 June |
| Prof LIU, Ru-Shi | National Taiwan University, Taiwan, 11–14 January |
| Prof ATTFIELD, J. Paul | University of Edinburgh, U.K., 11–14 January |

## Scope of Research

Transition metal oxides display a wide variety of interesting and useful functional properties, including electronic conduction, superconductivity, ferroelectricity, and ferromagnetism. In fact, some of these oxides have been used in current electronic devices. Our research mainly focuses on perovskite-structured transition metal oxides with novel functional properties due to complex couplings between their lattices, charges and spins. With advanced oxide-synthesis techniques such as high-pressure synthesis and epitaxial thin film growth, we are currently exploring such functional oxides.

**KEYWORDS**
Solid State Chemistry
Functional Transition Metal Oxides
Epitaxial Thin Film Growth
High Pressure Synthesis
Perovskite Structured Oxides

### Selected Publications

Chen, W. T.; Saito, T.; Hayashi, N.; Takano, M.; Shimakawa, Y., Ligand-hole Localization in Oxides with Unusual Valence Fe, *Sci. Rep.*, **2,** 449/1-6 (2012).

Azuma, M.; Chen, W. T.; Seki, H.; Czpski, M.; Olga, S.; Oka, K.; Mizumaki, M.; Watanuki, T.; Ishimatsu, N.; Kawamura, N.; Ishiwata, S.; Tucker, M. G.; Shimakawa, Y.; Attfield, J. P., Colossal Negative Thermal Expansion in $BiNiO_3$ Induced by Intermetallic Charge Transfer, *Nat. Comm.*, **2,** 347 (2011).

Inoue, S.; Kawai, M.; Ichikawa, N.; Kageyama, H.; Paulus, W.; Shimakawa, Y., Anisotropic Oxygen Diffusion at Low Temperature in Perovskite-Structure Iron Oxides, *Nat. Chem.*, **2,** 213-217 (2010).

Long, Y. W.; Hayashi, N.; Saito, T.; Azuma, M.; Muranaka, S.; Shimakawa, Y., Temperature-induced A-B Intersite Charge Transfer in an A-site-ordered $LaCu_3Fe_4O_{12}$ Perovskite, *Nature*, **458,** 60-63 (2009).

Kan, D.; Terashima, T.; Kanda, R.; Masuno, A.; Tanaka, K.; Chu, S.; Kan, H.; Ishizumi, A.; Kanemitsu, Y.; Shimakawa, Y.; Takano, M., Blue-light Emission at Room Temperature from $Ar^+$ -irradiated $SrTiO_3$, *Nat. Mater.*, **4,** 816-819 (2005).

## Ligand-hole Localization in Oxides with Unusual Valence Fe

Unusual high-valence states of iron are stabilized in a few oxides. A-site-ordered perovskite-structure oxides (Figure 1) contain such iron cations and exhibit distinct electronic behaviors at low temperatures, e.g. charge disproportionation (CD) ($4Fe^{4+} \rightarrow 2Fe^{3+} + 2Fe^{5+}$) in $CaCu_3Fe_4O_{12}$ and intersite charge transfer (CT) ($3Cu^{2+} + 4Fe^{3.75+} \rightarrow 3Cu^{3+} + 4Fe^{3+}$) in $LaCu_3Fe_4O_{12}$. We synthesized solid solutions of $CaCu_3Fe_4O_{12}$ and $LaCu_3Fe_4O_{12}$, and revealed how the instabilities of high-valence state of Fe in the oxides are relieved from extensive investigations of structural, electronic and magnetic properties in the wide temperature ranges from 5 to 500 K.

In Figure 2 shown is a compositional phase diagram of the $(Ca_{1-x}La_x)Cu_3Fe_4O_{12}$ solid solution, which is derived from all the experimental results. We see that the CD and CT phases coexist in the intermediate compositions and that the intersite CT transition temperatures ($T_{CT}$) increase with increasing La doping (i.e., with increasing $x$), while the CD transition temperatures ($T_{CD}$) do not change from that of $CaCu_3Fe_4O_{12}$. To explain the behaviors, we proposed a model that localization of ligand holes which are produced by the strong hybridization of iron $d$ and oxygen $p$ orbitals, plays a significant role on the distinct electronic behaviors. In the proposed ligand-hole picture, CD behavior is regarded as charge ordering of the ligand holes ($4d^5\underline{L} \rightarrow 2d^5 + 2d^5\underline{L}^2$). On the other hand, CT is regarded as a Mott transition of the ligand holes ($3d^9 + 4d^5\underline{L}^{0.75} \rightarrow 3d^9\underline{L} + 4d^5$). The difference between the CD and CT transitions is only the localization site of the ligand holes. This explains the coexistence of CT and CD in the solid solution. Our results demonstrate that the A-site-ordered perovskite-structure $Ca_{1-x}La_xCu_3Fe_4O_{12}$ solid solution is a novel example exhibiting interplay of the interactions mediated by the ligand holes.

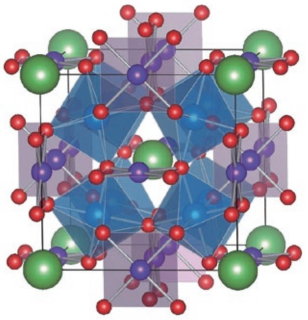

**Figure 1.** Crystal structure of the A-site-ordered double-perovskite.

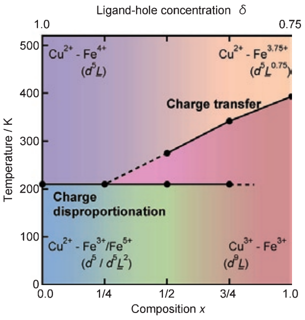

**Figure 2.** Compositional phase diagram for the $Ca_{1-x}La_xCu_3Fe_4O_{12}$ solid-solution.

## Thickness-Dependent Structure-Property Relationships in Strained (110) $SrRuO_3$ Thin Films

Recent advances in epitaxial thin films and heterostructures based on perovskite oxides have been some of the most exciting developments in functional materials. In particular, understanding of how the film accommodates epitaxial strain resulted from lattice mismatch between film and substrate is crucial as the strained films often show enhanced or modified functional properties as compared to the bulk counterpart. However, while it has been widely believed that the strain imposes new lattice constants on the film, what still remains unclear is how the perovskite lattice accommodates the increased elastic energy due to the epitaxial strain and how the strain accommodation affects physical properties of the film.

In this study, we investigated thickness-dependence of structure-property relationships in the strained $SrRuO_3$ (SRO) thin films. We found that, for the film thinner than 16 nm, the monoclinic structure with the $\sqrt{2}a_{pc} \times \sqrt{2}a_{pc} \times 2a_{pc}$ unit cell is epitaxially stabilized while the film thicker than 16 nm has the tetragonal structure with the cell-doubled $a_{pc} \times 2a_{pc} \times a_{pc}$ unit cell. The results of detailed structural characterizations indicate that the thickness-dependent structure change is ascribed to the substrate-induced modification in the $RuO_6$ octahedral rotation pattern in the strained film which has in-plane lattice parameters that are fixed by the substrate. We further demonstrate that physical properties are closely correlated with the film structure. The monoclinic film has the ferromagnetic transition temperature, $T_c$ which increases up to 130 K with increasing the thickness while the tetragonal film has $T_c$ ~100 K independent of the thickness. The magnetic anisotropy is also strongly affected by the film structures, indicating the importance of the magnetocrystalline effect in SRO. The results highlight that the epitaxial strain accommodation through the octahedral rotations in the strained SRO films plays a significant role in determining their structural phase and physical properties.

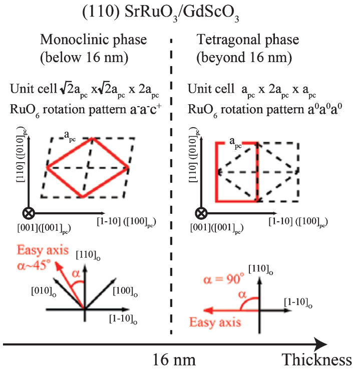

**Figure 3.** Thickness dependence of structure-property relationships in strained (110) $SrRuO_3$ thin films.

# International Research Center for Elements Science
# – Organotransition Metal Chemistry –

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## Scope of Research

This laboratory aims at establishment of new synthetic methodologies and new functional materials by designing well-defined catalysts based on transition metal chemistry. New concepts and ideas of molecular-based catalysts are accumulated by mechanistic investigations using experimental methods such as spectroscopy and kinetic techniques as well as theoretical methods. The research subjects include: (1) development of novel organotransition metal systems for catalysis based on precise ligand design, and (2) preparation of π-conjugated polymers by using direct arylation.

**KEYWORDS**

Transition Metal Complex
Homogeneous Catalyst
Reaction Mechanism
Low-coordinate Phosphorus Ligand
π-Conjugated Polymer

## Selected Publications

Wakioka, M.; Nakamura, Y.; Wang, Q.; Ozawa, F., Direct Arylation of 2-Methylthiophene with Isolated $[\mathrm{PdAr}(\mu\text{-}\mathrm{O_2CR})(\mathrm{PPh_3})]_n$ Complexes: Kinetics and Mechanism, *Organometallics*, **31,** 4810-4816 (2012).

Wang, Q.; Wakioka, M.; Ozawa, F., Synthesis of End-capped Regioregular Poly(3-hexylthiophene)s via Direct Arylation, *Macromol. Rapid Commun.*, **33,** 1203-1207 (2012).

Nakajima, Y.; Ozawa, F., Redox Chemistry of Bis(phosphaethenyl)pyridine Iron Complexes, *Organometallics*, **31,** 1203-1207 (2012).

## *N*-Alkylation of Amines with Alcohols Catalyzed by Bis(phosphaethenyl)pyridine Iridium and Ruthenium Complexes

Phosphaalkenes with P=C bonds exhibit strong π-accepting ability toward transition metals owing to their extremely low-lying π* orbitals. We recently demonstrated that PNP-pincer type phosphaalkene ligands, 2,6-bis(2-phosphaethenyl)pyridines (BPEP-Y; Y = Ph, H), successfully stabilize reactive complexes in a low oxidation state. In this study, we found that BPEP-Y complexes effectively catalyzed *N*-alkylation of amines with alcohols in high selectivity.

The Ir(I) complex [IrCl(BPEP-H)] (**1**), in conjunction with a strong base (CsOH), catalytically converted primary amines into secondary amines (eq 1). This catalysis was adaptable to substituted anilines and aliphatic amines and to several kinds of aliphatic alcohols. The formation of tertiary amines was not detected even in the presence of excess alcohols. In contrast, in the presence of $KH_2PO_4$ instead of CsOH, the same complex catalyzed *N*-alkylation of secondary amines to give tertiary amines (eq 2). Different from **1**, BPEP-Ph Ru(0) complex **2** predominantly catalyzed dehydrogenative coupling of alcohols and amines to form imines (eq 3).

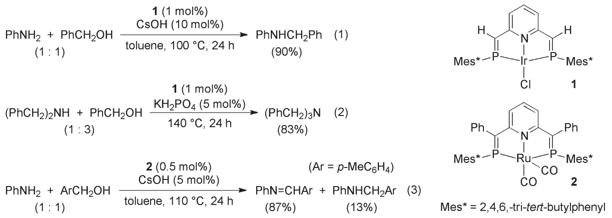
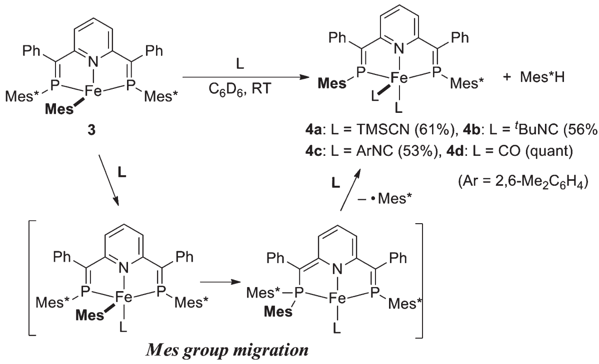


**Figure 1.** Structures and catalytic activities of **1** and **2**.

## Reactions of Bis(phosphaethenyl)pyridine Fe(I) Complexes with π-Acid Ligands

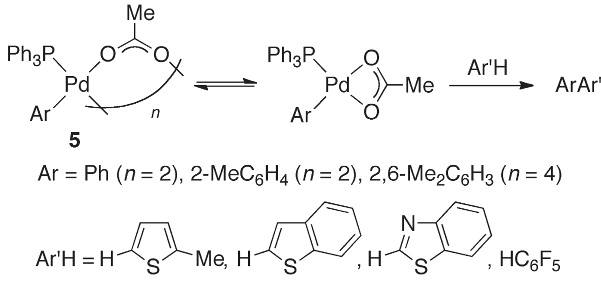
Low-coordinate Fe(I) complexes are rare for their instability, and their reactivity has been poorly understood. Recently, we have demonstrated that BPEP-Ph successfully stabilizes the Fe(I) mesityl complex **3**. In this study, we revealed unusual reaction behavior of **3** in the presence of π-acid ligands such as isocyanides and CO. Complex **3** underwent a structural rearrangement upon treatment with small excess π-acid ligands at ambient temperature, leading to the formation of Fe(0) complexes (**4a-d**). Interestingly, one Mes* group on the P=C bonds was replaced by the Mes group, which originally existed on the Fe center, probably via the migration of Mes group to the phosphorus atom (Scheme 1).



**Scheme 1**. Reaction of [FeMes(BPEP)] (**3**) with π-acid ligands.

## Direct Arylation of Heteroarenes with Isolated Arylpalladium Complexes

Dehydrohalogenative coupling of heteroarenes with aryl halides catalyzed by palladium complexes (so-called direct arylation) has attracted a great deal of attention as an alternative to conventional cross-coupling reactions. Recent theoretical studies have suggested that this catalysis involves an arylpalladium carboxylate intermediate, which undergoes C–H bond cleavage of aromatic compounds. However, isolated complexes that are reactive to C–H bond cleavage have been extremely limited. In this work, we found that arylpalladium complexes $[PdAr(\mu\text{-}O_2CMe)(PPh_3)]_n$ (**5**) react with various heteroarenes (Ar'H) to afford direct arylation products (ArAr') in high yields (Scheme 2). Kinetic and structural examinations indicate that **5** is interconverted with the monomeric complex $[PdAr(O_2CMe\text{-}\kappa^2O)(PPh_3)]$ in solution, which reacts with heteroarenes.



**Scheme 2**. Reaction of $[PdAr(\mu\text{-}O_2CMe)(PPh_3)]_n$ (**5**) with various heteroarenes (Ar'H).

# International Research Center for Elements Science
## – Photonic Elements Science –

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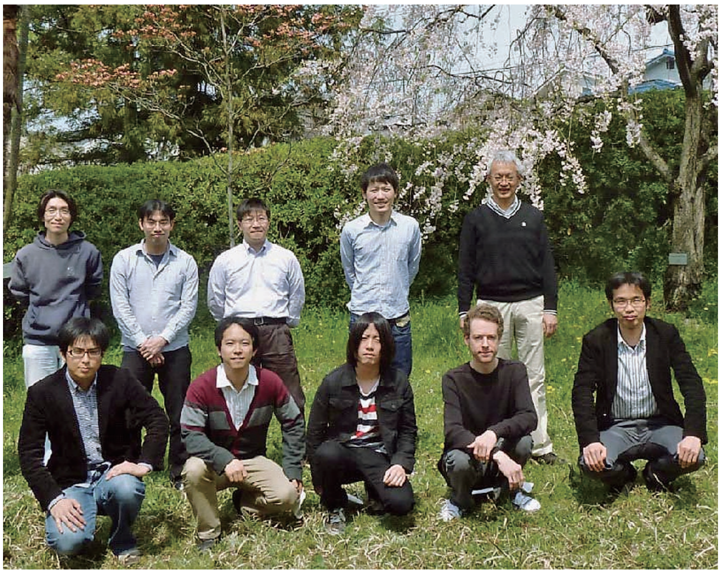
## Scope of Research

Our research interest is to understand optical and quantum properties of nanometer-structured materials and to establish opto-nanoscience for creation of innovative functional materials. Optical properties of semiconductor quantum nanostructures and strongly-correlated electron systems in low-dimensional materials are studied by means of space- and time-resolved laser spectroscopy. The main subjects are as follows: (1) Investigation of optical properties of single nanostructures through the development of high-resolution optical microscope, (2) Development of nanoparticle assemblies with new optical functionalities, and (3) Ultrafast optical spectroscopy of excited states of semiconductor nanostructures.

### KEYWORDS

Femtosecond Laser Spectroscopy
Carbon Nanotubes
Semiconductor Nanoparticles
Transition Metal Oxides
Semiconductor Nanostructures



### Selected Publications

Matsunaga, R.; Matsuda, K.; Kanemitsu, Y., Observation of Charged Excitons in Hole-doped Carbon Nanotubes Using Photoluminescence and Absorption Spectroscopy, *Phys. Rev. Lett.*, **106,** [037404-1]-[037404-4] (2011).

Yamada, Y.; Yasuda, H.; Tayagaki, T.; Kanemitsu, Y., Temperature Dependence of Photoluminescence Spectra of Undoped and Electron-doped $SrTiO_3$: Crossover from Auger Recombination to Single-carrier Trapping, *Phys. Rev. Lett.*, **102,** [247401-1]-[247401-4] (2009).

Matsunaga, R.; Matsuda, K.; Kanemitsu, Y., Evidence for Dark Excitons in a Single Carbon Nanotube Due to the Aharonov-Bohm Effect, *Phys. Rev. Lett.*, **101,** [147404-1]-[147404-4] (2008).

Hosoki, K.; Tayagaki, T.; Yamamoto, S.; Matsuda, K.; Kanemitsu, Y., Direct and Stepwise Energy Transfer from Excitons to Plasmons in Close-packed Metal and Semiconductor Nanoparticle Monolayer Films, *Phys. Rev. Lett.*, **100,** [207404-1]-[207404-4] (2008).

## Quantized Auger Recombination of Biexcitons in $Si_{1-x}Ge_x$ Nanocrystals

Fabrication and characterization of semiconductor nanocrystals (NCs) have been extensively studied due to interest both in the fundamental physics and potential applications in optoelectronic devices. We studied dynamics of quantized Auger recombination in $Si_{1-x}Ge_x$ NCs embedded in $SiO_2$ films by femtosecond intraband pump-probe spectroscopy. The temporal change of the electron-hole pair number under strong photoexcitation was well explained by the quantized Auger recombination model that considered the size distribution of NCs. On the basis of the dependence of the Auger decay rate on temperature and Ge composition, we confirmed the occurrence of breakdown of the *k*-conservation rule in quantized Auger recombination in Si and $Si_{1-x}Ge_x$ NCs.

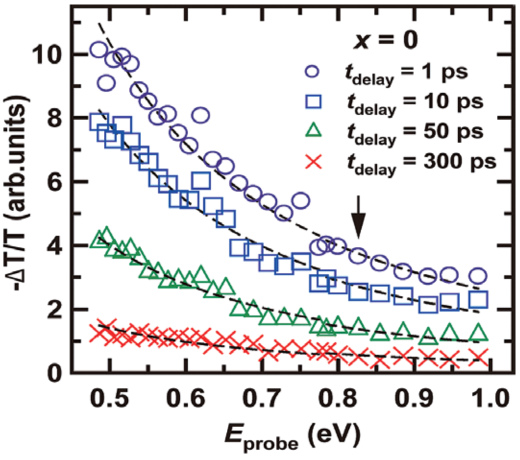


**Figure 1.** Time-resolved transmission spectra in Si nanocrystals.

## Dynamics of Exciton-hole Recombination in Hole-doped Carbon Nanotubes

Carbon nanotubes are one of the excellent materials for studying the optical properties of excitons, because of their unique band structures and large exciton binding energies. We studied the exciton decay dynamics in hole-doped single-walled carbon nanotubes (SWCNTs) by using femtosecond pump-probe transient absorption (TA) spectroscopy. By the doping of SWCNTs with holes, a fast decay component with the lifetime of a few picoseconds appears in TA signals, which corresponds to exciton decay through the Auger recombination between an exciton and a hole and the trion formation. We revealed that this exciton decay rate is quantized by the number of holes in a single SWCNT. The number of holes of a hole-doped SWCNT is successfully evaluated on the basis of TA decay dynamics.

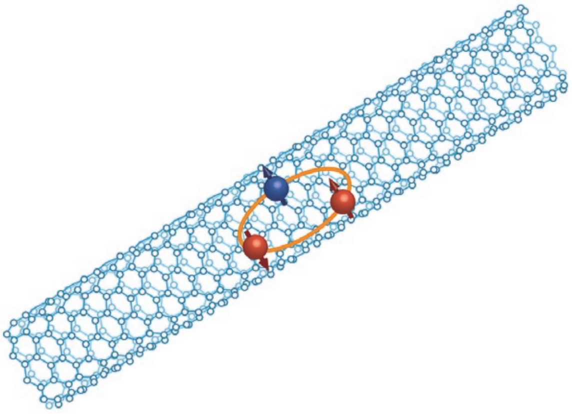


**Figure 2.** Schematic illustration of charged excitons in carbon nanotubes.

## Carrier Extraction from Ge/Si Quantum Dot Solar Cells

Quantum dots (QDs) have attracted attention because of their interesting physical properties and potential applications in optoelectronic devices such as light emitters and solar cells. In QDs, physical processes of generation, relaxation, and recombination of carriers are determined by their nanostructures and differ from those in bulk crystals. We report studies of the carrier extraction mechanism in Si solar cells with Ge QDs, which enable the optical absorption of photons with energies below the band gap of the host. Photocurrent measurements revealed that the photocurrent in the QD solar cells increased superlinearly with increasing excitation intensity under strong photoexcitation, which differed greatly from the behavior of Si solar cells without Ge QDs. This nonlinear photocurrent generation indicates that the carrier extraction efficiency from QDs is enhanced under strong photoexcitation by nonlinear carrier extraction processes, such as two-step photon absorption and hot carrier generation via Auger recombination.

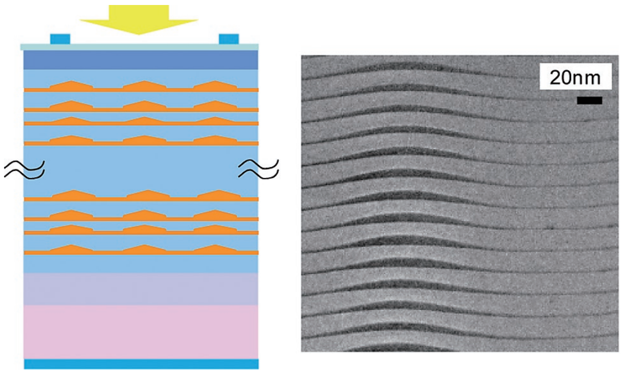


**Figure 3.** Schematic illustration of Ge/Si QDs (left). TEM image of Ge QD array (right).

# Bioinformatics Center
## – Chemical Life Science –

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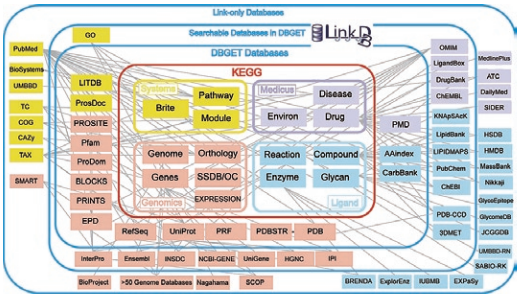
Dr TSAI, Yu-Shuen National Yang-Ming University, Taiwan, 7 October 2011–30 April 2012

## Scope of Research

The proteins responsible for biosynthesis, biodegradation, and transport of additional molecules, such as small metabolites, lipids and glycans, are encoded in the genome, which may indicate that all cellular functions are specified by the genomic DNA sequence. In practice, however, inferring higher-level systemic functions of the cell or the organism needs more than solely the genomic information. We are developing bioinformatics methods to integrate different types of data and knowledge on various aspects of the biological systems towards basic understanding of life as a molecular interaction/reaction system and also toward practical applications in medical and pharmaceutical sciences.


GenomeNet Top page



Databases available in the DBGET/LinkDB system of the GenomeNet service. Color of each database represents the type of its contents, yellow: systems information, purple: medical information, pink: genetic information, light blue: chemical information.

**KEYWORDS**
GenomeNet
(Meta)genomics
Pathway
Bioinformatics
Pharmacoinformatics

### Selected Publications

Takarabe, M.; Kotera, M.; Nishimura, Y.; Goto, S.; Yamanishi, Y., Drug Target Prediction Using Adversed Event Report Systems: A Pharmacogenomic Approach, *Bioinformatics*, **28,** i611-i618 (2012).

Mizutani, S.; Pauwels, E.; Stoven, V.; Goto, S.; Yamanishi, Y., Relating Drug-protein Interaction Network with Drug Side-effects, *Bioinformatics*, **28,** i522-i528 (2012).

Kotera, M.; Yamanishi, Y.; Moriya, Y.; Kanehisa, M.; Goto, S., GENIES: Gene Network Inference Engine Based on Supervised Analysis, *Nucleic Acids Res.*, **40,** W162-W167 (2012).

Kanehisa, M.; Goto, S.; Sato, Y.; Furumichi, M.; Tanabe, M., KEGG for Integration and Interpretation of Large-scale Molecular Datasets, *Nucleic Acids Res.*, **40,** D109-D114 (2012).

Takarabe, M.; Shigemizu, D.; Kotera, M.; Goto, S.; Kanehisa, M., Network-based Analysis and Characterization of Adverse Drug-drug Interactions, *J. Chem. Inf. Model.*, **51,** 2977-2985 (2011).

## Development of a Web-based Supervised Gene Network Inference Engine

Recent developments of biotechnologies, e.g., microarray and proteomics technologies, contribute to an increasing amount of high-throughput data for genes and proteins, which are useful sources to infer the biological networks on a large scale. We have developed GEne Network Inference Engine based on Supervised analysis (GENIES: http://www.genome.jp/tools/genies/), a web server to predict unknown part of gene network from various types of genome-wide data in the framework of supervised network inference (Kotera et al., 2012). The originality of the supervised network inference method lies in construction of a predictive model using partially known network information, and in the integration of heterogeneous data with kernel methods. The method is suitable for predicting potential interactions involving uncharacterized genes and their associations with known pathways. The GENIES server accepts any profiles of genes or proteins (such as gene expression profiles, protein subcellular localization profiles and phylogenetic profiles), or pre-calculated gene-gene similarity matrices (or kernels) in the tab-delimited file format. As a training data set to learn a predictive model, the users can choose either known molecular network information in the KEGG Pathway database, or their own gene network data. The server provides the list of newly predicted gene pairs, maps the predicted gene pairs onto the associated pathway diagrams in KEGG Pathway, and indicates candidate genes for missing enzymes in organism-specific metabolic pathways.

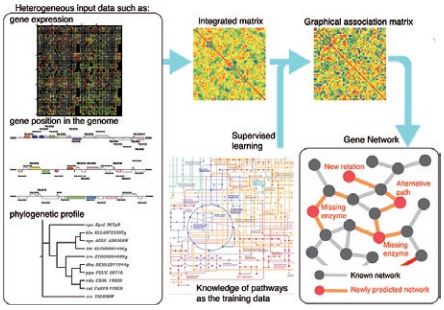


**Figure 1.** The workflow of GENIES.

## A Statistical Framework for Analyzing the Association between Drug Target Proteins and Drug Side-effects

Most drugs are small chemical compounds that target specific proteins to induce regulations of the overall protein networks, or pathways. This may result in expected therapeutic effects to the body, or occasionally undesired side-effects. Recently, several types of drug-related data have been accumulated in publicly available databases. Drug chemical structures, target proteins, and side-effects are such data types. Bioinformatics approaches are expected to be useful to retrieve important relationships between different types of data, which helps studies on the underlying mechanisms of drug-actions in a living system at different levels. Our lab has been focusing on storing such heterogeneous data in the form of relational database and developing related algorithms. Previously, we published a drug-drug interaction retrieval system in the KEGG DRUG database, which is a database-searching approach to comprehensively understand drug-drug interactions at the molecular scale (Takarabe et al., 2011). We took another approaches applying statistical methods, which link drug-protein interaction data at the molecular scale and their side-effects at the phenotypic scale. As one of our recent studies (Mizutani et al., 2012), we applied the sparse canonical correlation analysis (SCCA) to a drug-protein interaction data in a framework of predicting potential side-effects for a set of drugs (Figure 2). This resulted in an extraction of target proteins and side-effects in the form of correlated sets (Figure 3). A following pathway enrichment analysis using KEGG and Gene Ontology (GO) databases showed that proteins of similar biological processes were clustered together in the same extracted correlated sets, even if their molecular functions were different. In another study (Takarabe et al., 2012), we used similar approach to retrieve biologically relevant interpretations from the drug-target-side-effect associations. We believe our continuous efforts help promote discussions over the molecular mechanisms of drug side-effects and underlying biological knowledge.

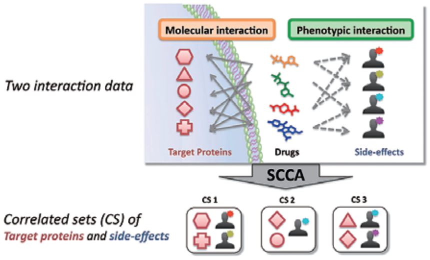


**Figure 2.** SCCA extracts correlated sets of target proteins and side-effects.

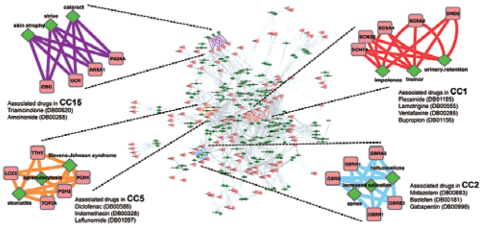


**Figure 3.** An illustration of the network of drug targeted proteins and side-effects in the extracted correlated sets (CSs).

# Bioinformatics Center
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MORI, Tomoya (D1)
RUAN, Peiying (D1)
UECHI, Risa (D1)
SHI, Dongyue (M2)
JIRA, Jindalertudomdee (M2)
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HWANG, Jaewook (M1)

## Visitor

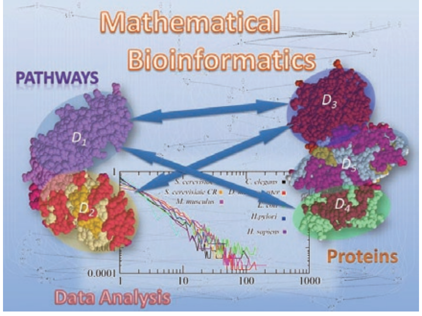
Ms JIANG, Hao The University of Hong Kong, China, P.R., 4 June–15 August

## Scope of Research

Due to rapid progress of the genome projects, whole genome sequences of organisms ranging from bacteria to human have become available. In order to understand the meaning behind the genetic code, we have been developing algorithms and software tools for analyzing biological data based on advanced information technologies such as theory of algorithms, artificial intelligence, and machine learning. We are recently studying the following topics: systems biology, scale-free networks, protein structure prediction, inference of biological networks, chemo-informatics, discrete and stochastic methods for bioinformatics.

### KEYWORDS

Scale-free Networks
Boolean Networks
Grammar-based Compression
RNA Secondary Structures
Chemical Graphs



## Selected Publications

Akutsu, T.; Kosub, S.; Melkman, A. A.; Tamura, T., Finding a Periodic Attractor of a Boolean Network, *IEEE/ACM Transactions on Computational Biology and Bioinformatics*, **9,** 1410-1421 (2012).

Akutsu, T.; Fukagawa, D.; Jansson, J.; Sadakane, K., Inferring a Graph from Path Frequency, *Discrete Applied Mathematics*, **160,** 1416-1428 (2012).

Nacher, J. C.; Akutsu, T., Dominating Scale-free Networks with Variable Scaling Exponent: Heterogeneous Networks Are Not Difficult to Control, *New Journal of Physics*, **14**, 073005 (2012).

Hayashida, M.; Ruan, P.; Akutsu, T., A Quadsection Algorithm for Grammar-Based Image Compression, *Integrated Computer-Aided Engineering*, **19,** 23-38 (2012).

Kato, Y.; Sato, K.; Asai, K.; Akutsu, T., Rtips: Fast and Accurate Tools for RNA 2D Structure Prediction Using Integer Programming, *Nucleic Acids Research*, **40,** W29-W34 (2012).

## Network Completion Using Dynamic Programming and Least-Squares Fitting

Analysis of biological networks is one of the central research topics in bioinformatics and computational systems biology. Recently, we proposed a concept of "Network Completion", which is to make the minimum amount of modifications to a given network so that the resulting network is most consistent with observed data. In our previous work, we studied the computational complexity of network completion under Boolean models.

In this work, we propose a novel method, DPLSQ, for completing genetic networks using gene expression time series data. Different from our previous work, we employ a model based on differential equations and assume that expression values of all nodes can be observed. DPLSQ is a combination of least-squares fitting and dynamic programming and one of its important features is that it can output an optimal solution (i.e., minimum squared sum) in polynomial time if the maximum indegree (i.e., the maximum number of input genes to a gene) is bounded by a constant. Although DPLSQ does not automatically find the minimum modification, it can be found by examining varying numbers of added/deleted edges, where the total number of such combinations is polynomially bounded. If a null network (i.e., a network having no edges) is given as an initial network, DPLSQ can work as an inference method for genetic networks. In order to examine the effectiveness of DPLSQ, computational experiments were conducted using both artificially generated and real gene expression time series data.

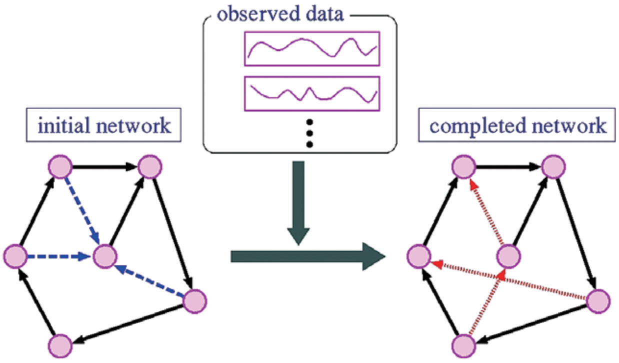


**Figure 1.** Network completion by addition and deletion of edges. Dashed edges and dotted edges denote deleted edges and added edges, respectively.

## Predicting Protein-RNA Residue-base Contacts Using Two-dimensional Conditional Random Field

To dissect the interactions between proteins and RNAs leads novel findings of molecular networks and functions in cellular systems. In terms of the interactions between amino acid residues in proteins, it is generally accepted that residues at interacting sites have coevolved with the corresponding residues in the partner protein to keep the interactions between proteins. In our previous work, based on this hypothesis, we calculated mutual information (MI) between residues from multiple sequence alignments of homologous proteins to identify residue-residue contact pairs in interacting proteins, and combined it with a discriminative random field (DRF) approach, which is a special type of conditional random fields (CRFs). Recently, the evolutionary correlation of the interactions between residues and DNA bases has also been found in certain transcription factors and the DNA-binding sites.

In this work, we employ CRFs to predict the interactions between protein residues and RNA bases. Furthermore, we introduce labels of amino acids and bases as features of a simple two-dimensional CRF instead of DRF. In addition, we examine the utility of L1-norm regularization (lasso) for CRF. To evaluate our method, we perform computational experiments of several interactions between the Pfam domains and Rfam entries, and calculate the average AUC (Area under ROC Curve) score. The results suggest that our CRF-based method using MI and labels with lasso is useful for further improving the performance, especially provided that the features of CRF are successfully reduced by the lasso approach.

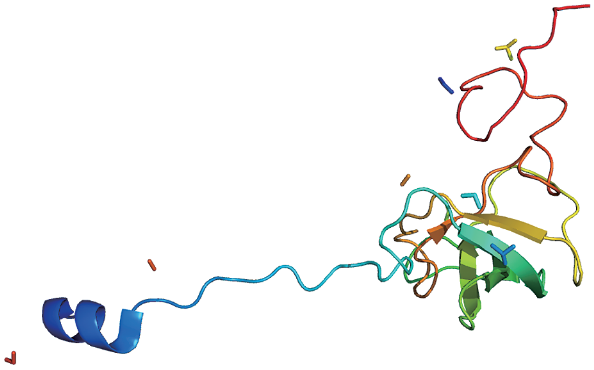


**Figure 2.** Protein RS12_THET8 of PDB code '1yl4' and the atoms of RNA M26923 within 3 Å of the protein.

# Bioinformatics Center
## – Bio-knowledge Engineering –

http://www.bic.kyoto-u.ac.jp/pathway/index.html


Prof
MAMITSUKA, Hiroshi
(D Sc)


Assist Prof
HANCOCK, Timothy Peter
(Ph D)


Assist Prof
KARASUYAMA, Masayuki
(D Eng)


PD
NGUYEN, Hao Canh
(Ph D)


Proj Res
NATSUME, Yayoi
(D Agr)

### Students

TAKAHASHI, Keiichiro (D2)    MOHAMED, Ahmed (D1)    CHEN, Zhuoxin (M1)

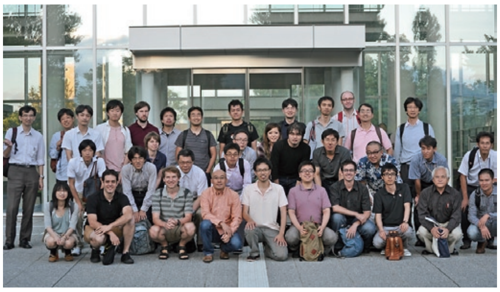
### Visitors

| | |
|---|---|
| Prof TULLIUS, Tom | Boston University, U.S.A., 11 January |
| Ms LEE, En-Shiun Annie | University of Waterloo, Canada, 1 February |
| Assoc Prof ZHU, Shanfeng | Fudan University, China, P.R., 24 March–23 August |
| Mr ZHENG, Xiaodong | Fudan University, China, P.R., 9 April–7 July |
| Mr JOHNSTON, Ian | Boston University, U.S.A., 15 May–15 August |
| Assist Prof CARVALHO, Luis | Boston University, U.S.A., 24 June–7 July |
| Mr DE LÉSÉLEUC, Sylvain | École Polytechnique, France, 19 July |
| Dr FUJIMAKI, Ryohei | NEC Labs America, U.S.A., 10 September |
| Prof WONG, Limsoon | National University of Singapore, Singapore, 1 November |

## Scope of Research

We are interested in graphs and networks in biology, chemistry and medical sciences, which include metabolic networks, protein-protein interactions and chemical compounds. We have developed original techniques in machine learning and data mining for analyzing these graphs and networks, occasionally combining with table-format datasets, such as gene expression and chemical properties. We have applied the developed techniques to real data to demonstrate the performance of the methods and further to find new scientific insights.

**KEYWORDS**
Bioinformatics
Data Mining
Systems Biology
Computational Genomics
Machine Learning



### Selected Publications

Hancock, T.; Mamitsuka, H., Boosted Network Classifiers for Local Feature Selection, *IEEE Transactions on Neural Networks and Learning Systems*, **23(11),** 1767-1778 (2012).

Hancock, T.; Wicker, N.; Takigawa, I.; Mamitsuka, H., Identifying Neighborhoods of Coordinated Gene Expression and Metabolite Profiles, *PLoS One*, **7(2)**, e31345 (2012).

Shiga, M.; Mamitsuka, H., A Variational Bayesian Framework for Clustering with Multiple Graphs, *IEEE Transactions on Knowledge and Data Engineering*, **24(4),** 577-590 (2012).

Nguyen, C. H.; Mamitsuka, H., Latent Feature Kernels for Link Prediction on Sparse Graphs, *IEEE Transactions on Neural Networks and Learning Systems*, **23(11),** 1793-1804 (2012).

Shiga, M.; Mamitsuka, H., Efficient Semi-Supervised Learning on Locally Informative Multiple Graphs, *Pattern Recognition*, **45(3),** 1035-1049 (2012).

## Imposing Network Structures for Feature Selection with Omic Data

Networks have become a common place to represent the relationship structure across many variables. For small numbers of variables, networks provide an intuitive model of the structure present within a dataset. However, as the size of the network model increases its representative power diminishes. In an effort to maintain the effectiveness of large network models, feature selection algorithms are employed to extract the relevant structure which is related to a specific phenomena. Currently, the requirement for accurate network feature selection algorithms is essential as the sizes and complexities of the known networks continue to grow.

Supervised classification algorithms are also commonly used as network feature selection methods. The size of the network structures has lead to the development of network regularization algorithms. These methods exploit a sparsity assumption to identify the minimum set of network nodes required to optimize classification performance. When the network structure is large and noisy the sparsity assumption made by these methods is appropriate it will enforce the selection of the minimal set of features required for accurate classification. However some networks in biology, such as metabolic networks, are known to possess highly coordinated responses to external phenomena. These responses potentially activate large sections of the network.

In highly correlated environments a related class of models, ensemble methods such as bagging and boosting, are known to perform well. Ensemble methods seek to represent the structure of a large complex dataset through a combination of small models which are built on a subset of important dataset features. In this research we observed an analogous idea to ensemble methods within factorized network probability distributions. Based upon this similarity we propose two novel optimization algorithms, Boosted Expectation Propagation (BEP) and Boosted Message Passing (BMP) (Hancock and Mamitsuka; 2010, 2012). Neither BEP nor BMP assume a sparse solution, but instead seek a weighted average of all network features where the weights are used to emphasize all features which are useful for classification. In this research we focus on applying BEP and BMP to real world networks. Furthermore, we investigate the similarity in selected features and performance between BEP and BMP and network regularized models. We compare model performances on two different types of biological networks, metabolic networks and protein-protein interaction (PPI) networks using microarray data. Our results on real world networks, presented in Figure 1, show that to extract features from correlated networks the assumption of sparsity will adversely effect classification accuracy and feature selection ability.

**References**

[1] Hancock, T.; Mamitsuka, H., Boosted Network Classifiers for Local Feature Selection, *IEEE Transactions on Neural Networks and Learning Systems*, **23(11),** 1767-1778(2012).

[2] Hancock, T.; Mamitsuka, H., Boosted Optimization for Network Classification, *Proceedings of the 13th International Conference on Artificial Intelligence and Statistics (AISTATS 2010) (JMLR: Workshop and Conference Proceedings)*, **9,** 305-312, Sardinia, Italy, May 2010, MIT Press.

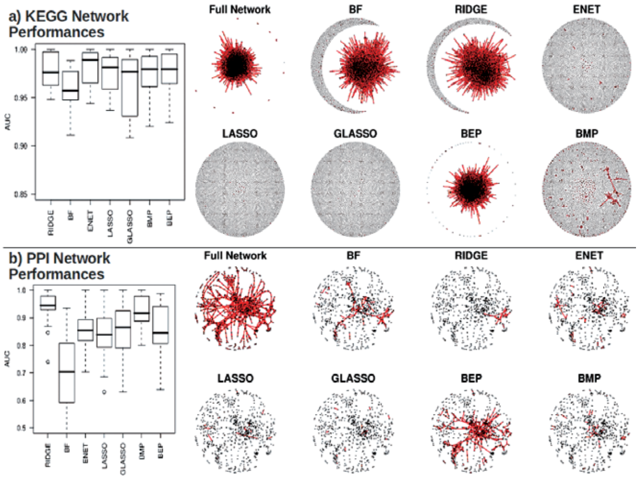


**Figure 1.** Imposing network structures for feature selection with omic data. The performance (in AUC) and the selected features of the proposed methods, BEP and BMP, and the comparison penalized approaches on the (a) KEGG metabolic network classifying heat stress in yeast, and (b) BIOGRID PPI network classifying tumor occurrence in humans. In the networks the selected features are represented as edges on the network. Good feature selection performance is assumed to highlight connected submodules.

# Endowed Research Section
## – Nano-Interface Photonics –
## (SEI Group CSR Foundation)

http://www.scl.kyoto-u.ac.jp/~opt-nano/NIP/index-eng.html

Program-Specific Assoc Prof
YAMADA, Yasuhiro
(D Sc)

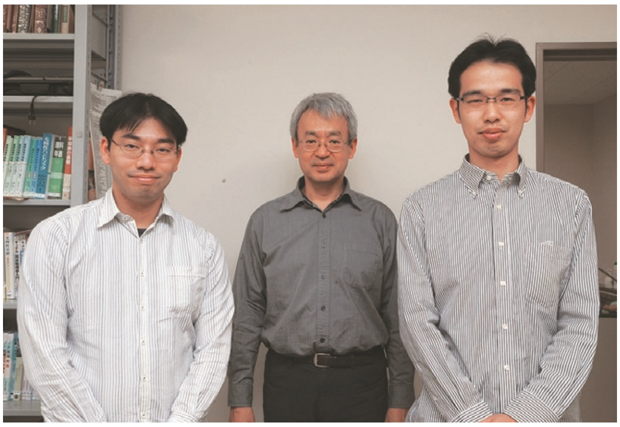
Program-Specific Assist Prof
OKANO, Makoto
(D Sc)

Prof (Supporting Faculty Member)
KANEMITSU, Yoshihiko
(D Eng)

## Scope of Research

Nanostructured materials are one class of the most promising candidates for future device materials because of their unique electronic and optical properties beyond the bulk crystals. Our research aim is to open up new research fields of nanomaterials science, by focusing on nano-interface as a platform to develop novel optical functionalities. We study optical properties of semiconductor nanomaterials by means of time- and space-resolved spectroscopy, leading to new solar energy conversion technologies. The main subjects are (1) photocarrier dynamics and photovoltaic effects in transition metal oxides and (2) ultrafast carrier dynamics and unique optical properties of one-dimensional materials.

**KEYWORDS**
Nano-interface
Photovoltaic Science
Nanocarbon Materials
Laser Spectroscopy
Solar Energy Conversion



### Selected Publications

Yamada, Y.; Kanemitsu, Y., Photoluminescence Spectra of Perovskite Oxide Semiconductors, *J. Lumin.*, **133,** 30-34 (2013).

Yamada, Y.; Kanemitsu, Y., Determination of Electron and Hole Lifetimes of Rutile and Anatase $TiO_2$ Single Crystals, *Appl. Phys. Lett.*, **101,** [133907-1]-[133907-4] (2012).

Okano, M.; Kanemitsu, Y.; Chen, S.; Mochizuki, T.; Yoshita, M.; Akiyama, H.; Pfeiffer, L. N.; West, K. W., Observation of High Rydberg States of One-dimensional Excitons in GaAs Quantum Wires by Magneto-photoluminescence Excitation Spectroscopy, *Phys. Rev. B*, **86,** [085312-1]-[085312-5] (2012).

Yamada, Y.; Kanemitsu, Y., Band-edge Luminescence from $SrTiO_3$: No Polaron Effect, *Thin Solid Films*, **520,** 3843-3846 (2012).

Okano, M.; Matsunaga, R.; Matsuda, K.; Masubuchi, S.; Machida, T.; Kanemitsu, Y., Raman Study on the Interlayer Interactions and the Band Structure of Bilayer Graphene Synthesized by Alcohol Chemical Vapor Deposition, *Appl. Phys. Lett.*, **99,** [151916-1]-[151916-3] (2011).

## Nanointerface as a Platform to Develop Novel Optical Functionalities

Solar energy conversion is a key technology to solve the world-wide and emergent energy problems, such as fossil fuel exhaustion and global warming. However, the conversion efficiency of practically used solar cell is still less than 30%, and thus there is a compelling need for the development of highly-efficient and cost-effective solar cells.

Nanostructured materials, such as nanoparticles, nanotubes, and nanowires, are the most promising candidates for the next-generation solar cells because of their unique electronic and optical properties beyond the bulk crystals. For example, plasmon resonance in metal nanoparticles enhances the light absorption efficiency, and carrier multiplication due to strong carrier confinement and Coulomb interactions in the semiconductor nanoparticles can improve the light conversion efficiencies.

To take more advantages of nanomaterials, it is significant to understand the role of their surface and interface. Nanomaterials have large surface-to-volume ratios, and thus their optoelectronic properties are strongly affected by the surrounding materials and interface states. This indicates that the novel optoelectronic properties can be developed by controlling the nano-interface. Moreover, in the practical nanomaterial-based devices, the energy and carrier transport processes are dominated by the characteristics of the interface between nanomaterials.

In our research group, we focus on such nano-interface as a platform to develop novel optical functionalities. Using advanced time- and space-resolved spectroscopy, we study the optical properties of unique nanomaterials and their nanocomposites. Through the studies on the nano-interface photonics, we aim to open up new research fields of nanomaterials science, leading to new solar energy conversion technology.

## Observation of High Rydberg States of One-dimensional Excitons in GaAs Quantum Wires by Magnetophotoluminescence Excitation Spectroscopy

We have studied the higher Rydberg states of the ground exciton in T-shaped GaAs quantum wires using magneto-photoluminescence excitation spectroscopy at low temperatures. Under strong magnetic field, a new peak appears at the onset of the one-dimensional (1D) continuum edge. The peak is assigned to the second even-parity Rydberg state on the basis of the polarization dependence measurements. By comparison with the ground exciton, it shows significantly low zero-field oscillator strength and a large diamagnetic shift. These characteristic features are attributed to the weakly bound wave function of the second Rydberg state intrinsic to 1D excitons.

## Determination of Electron and Hole Lifetimes of Rutile and Anatase $TiO_2$ Single Crystals

$TiO_2$ is one of the most important oxide semiconductors in terms of energy and environmental applications, such as dye-sensitized solar cells and photocatalysts. We investigated the photocarrier decay dynamics of rutile and anatase $TiO_2$ single crystals by combining the advantages of time-resolved photoluminescence, transient absorption, and photoconductivity spectroscopy analyses. Electrons and holes in rutile show exponential decays with the lifetime of a few tens of nanoseconds, while non-exponential decays are observed in anatase, indicating the presence of multiple carrier trapping processes. We revealed the generic features of the carrier recombination processes in rutile and anatase $TiO_2$.

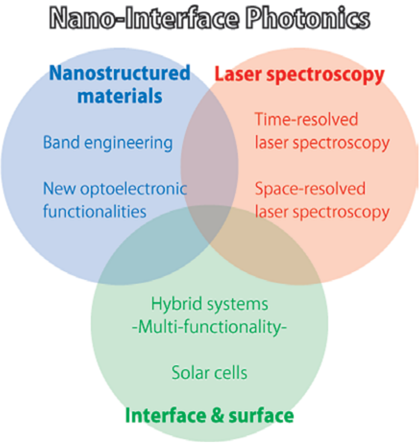


Figure 1.

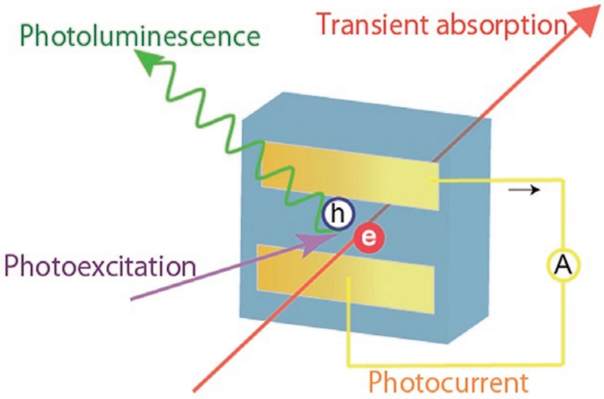


Figure 2.

# HAKUBI RESEARCHERS' ACTIVITIES IN ICR

## Hakubi Project: Fosterage and Support of Young Researchers, Kyoto University

## Research Topic

### Alternative Methods for Energy Conversion in the Solid State

Program-Specific Assoc Prof
NAUMOV, Panche
(D Sc)

Program-Specific Res
NATH, Naba Kamal
(Ph D)

**Host Laboratory** Laboratory of Molecular Aggregation Analysis and Laboratory of Organoelement Chemistry

**Host Professors** SATO, Naoki and TOKITOH, Norihiro

### Outline of Research

Panche's research interests are in the domain of solid-state structural chemistry. He employs a variety of analytical methods, including new techniques for X-ray diffraction, to study the molecular mechanisms involved in non-classical ways of energy conversion. He tries to understand the structural specifics affecting the transfer of energy throughout matter in these cases. His recent interests include bioluminescence – production of cold light by some organisms – as well as light-induced mechanical effects in molecular crystals.

## Research Topic

### Algorithmic Graph Theory with Applications to Bioinformatics

Program-Specific Assoc Prof
JANSSON, Jesper
(Ph D)

**Host Laboratory** Laboratory of Mathematical Bioinformatics

**Host Professor** AKUTSU, Tatsuya

### Outline of Research

During 2012, I worked on various projects related to Graph Algorithms and Bioinformatics. For example, the objective of one of the research projects (joint work with Professor Andrzej Lingas at Lund University, Sweden) is to develop fast methods for measuring the structural similarity between two input phylogenetic networks. We were able to show that if both of the input phylogenetic networks are so-called "galled trees" with n leaves each, then the rooted triplet distance can be computed in o(n^{2.687}) time. This upper bound was obtained by transforming the problem of computing the rooted triplet distance to that of counting monochromatic and almost-monochromatic triangles in an undirected, edge-colored graph. To count different types of colored triangles in a graph efficiently, we extended an existing technique based on matrix multiplication and obtained several new related results that may be of independent interest.

# ACTIVITIES OF JOINT USAGE/RESEARCH CENTER

# JURC Cooperative Research Subjects 2012

(1 April 2012 ~ 31 March 2013)

**STARTING-UP SUBJECTS**
**(IN SPECIFIC FIELDS CHOSEN BY JURC)**

Physics of THz Generation through the Interactions of Laser with Clusters
NAGASHIMA, Takeshi, Institute of Laser Engineering, Osaka University
**Host in JURC** HASHIDA, Masaki

Development of Beam Irradiation System with the Use of Electron Cooled Proton Beam and Its Application
SHIRAI, Toshiyuki, National Institute of Radiological Sciences
**Host in JURC** NODA, Akira

Development of Methods to Measure Four Wave-mixing Process in Vacuum
HONMA, Kensuke, Graduate School of Science, Hiroshima University
**Host in JURC** SAKABE, Shuji

Development of Catalytic Enantioselective Reactions Induced by Hydrophobic Chiral Interface around Two-dimensionally Arrayed Gold Nanoparticles
MIKI, Kazushi, Polymer Materials Unit, National Institute for Materials Science
**Host in JURC** NAKAMURA, Masaharu

Optical and Electrical Properties of Mixed Organic Semiconductors
NAITO, Hiroyoshi, The School of Engineering, Osaka Prefecture University
**Host in JURC** KANEMITSU, Yoshihiko

Development of Negative Thermal Expansion Material Based on a Perovskite $BiNiO_3$
AZUMA, Masaki, Materials and Structures Laboratory, Tokyo Institute of Technology
**Host in JURC** SHIMAKAWA, Yuichi

Synthesis of Sugar-Acetylenes by Iron-Catalyzed Cross-Coupling and Study on Their Stimulus-Response Luminescence
ORITA, Akihiro, Department of Applied Chemistry, Okayama University
**Host in JURC** NAKAMURA, Masaharu

Mechanistic Studies on the Iron Catalyze Carbon-carbon Bond Forming Reactions Based on the Solution-phase X-ray Absorption Spectroscopy
NAGASHIMA, Hideo, Institute for Materials Chemistry and Engineering, Kyushu University
**Host in JURC** NAKAMURA, Masaharu

Development of Ruthenium-Complex-Bound Amino Acids and Peptides and Their Application to Oxidative Degradation of Wooden Biomasses
WATANABE, Takashi, Research Institute for Sustainable Humanosphere, Kyoto University
**Host in JURC** NAKAMURA, Masaharu

Finding Frequent Similar Regions from Genome Sequences
NAKAMURA, Atsuyoshi, Graduate School of Information Science and Technology, Hokkaido University
**Host in JURC** MAMITSUKA, Hiroshi

Efficient Search Algorithms for Structured Data in Bioinformatics
TAKASU, Atsuhiro, National Institute of Informatics, Digital Content and Media Sciences Research Division
**Host in JURC** AKUTSU, Tatsuya

Probabilistic Methods for Analysis on Protein Interaction Networks
MARUYAMA, Osamu, Institute of Mathematics for Industry, Kyushu University
**Host in JURC** AKUTSU, Tatsuya

Development of Bioinformatic Method to Analyze MHC class II-binding Peptides
UDAKA, Keiko, Kochi Medical School
**Host in JURC** MAMITSUKA, Hiroshi

Co-clustering of Biological Datasets for Personalized Medicine
SHIGA, Motoki, Toyohashi University of Technology
**Host in JURC** MAMITSUKA, Hiroshi

Development of the Evaluation Method for Potential Functionome Harbored in the Genome and Metagenome
TAKAMI, Hideto, Institute of Biogeoscience, Japan Agency for Marine-Earth Science and Technology
**Host in JURC** GOTO, Susumu

Development of Novel 3-Dimensional $\pi$-Extended Molecules Directed toward Electronic Materials
SUGA, Seiji, Graduate School of Natural Science and Technology, Okayama University
**Host in JURC** MURATA, Yasujiro

Evaluation of EO Effect of High Orientation $Ba_2TiSi_2O_8$ Thin Film by Prepared Sol-gel Method
IHARA, Rie, Department of Applied Physics, Tohoku University
**Host in JURC** MASAI, Hirokazu

Investigation of Extraction Behaviors of Metal Ions in Liquid-liquid Extraction Systems Using a Novel Multidentate Ligand
MUKAI, Hiroshi, Faculty of Education, Kyoto University of Education
**Host in JURC** SOHRIN, Yoshiki

Role of Water in Motor Function of F1 Protein
IKEGUCHI, Mitsunori, Graduate School in Nanobioscience, Yokohama City University
**Host in JURC** MATUBAYASI, Nobuyuki

A Study on Intermolecular Atomic Contacts Involving Halogen and/or Chalcogen Atoms in Organic Crystals
TSUZUKI, Seiji, Nanosystem Research Institute, The National Institute of Advanced Industrial Science and Technology (AIST)
**Host in JURC** SATO, Naoki

Electronic Properties of Thin Films of Porphyrazine Derivative Compounds Containing Thiadiazole Rings

AWAGA, Kunio, Research Center for Materials Science, Nagoya University
**Host in JURC** SATO, Naoki

Induction of Membrane Curvature by Arginine-rich Peptides
SAKAMOTO, Kazutami, Faculty of Pharmacy, Chiba Institute of Science
**Host in JURC** FUTAKI, Shiroh

**EXPANDING SUBJECTS**
**(IN SPECIFIC FIELDS CHOSEN BY JURC)**

X-Ray Structure Analysis of Reaction Mechanism of Catabolic Enzymes
OIKAWA, Tadao, Faculty of Chemistry, Materials and Bioengineering, Kansai University
**Host in JURC** HATA, Yasuo

Efficiency Improvement of Multi-dimensional Doppler Laser Cooling for Ultra-low Temperature Beam Generation
OKAMOTO, Horomi, Graduate School of Advanced Sciences of Matter, Hiroshima University
**Host in JURC** NODA, Akira

X-Ray Structural Studies on Adaptation of Aspartate Rasemase to Enviromental Temperatures
GOGAMI, Yoshitaka, Kansai University High Technology Research Center
**Host in JURC** HATA, Yasuo

Photocarrier Recombination Dynamics in Nanodomain-structured Ferroelectrics
FUNAKUBO, Hiroshi, Interdisciplinary Graduate School of Science and Engineering, Tokyo Institute of Technology
**Host in JURC** KANEMITSU, Yoshihiko

Design and Synthesis of Metal Ligands Which Facilitate the Reductive Elimination Reaction and Their Application to the Synthesis of Cycloparaphenylenes
KORENAGA, Toshinobu, Graduate School of Natural Science and Technology, Okayama University
**Host in JURC** YAMAGO, Shigeru

Efficient Construction of Polyfunctionalized Molecules by Cooperative Effect of Transition Metals and Heteroatoms
SEGI, Masahito, School of Chemistry, College of Science and Engineering, Kanazawa University
**Host in JURC** TOSHIMITSU, Akio

Development of Methods for Discrimination and Syntheses of Chiral Molecules with Phosphoroselenoic Acid Derivatives Bearing a Binaphthyl Group
MURAI, Toshiaki, Faculty of Engineering, Gifu University
**Host in JURC** TOSHIMITSU, Akio

Development of Reversible Carbon–Carbon Bond Formation Reactions on Dynamic Tetrametallic Reaction Sites
OKAZAKI, Masaaki, Department of Frontier Materials Chemistry, Graduate School of Science and Technology, Hirosaki University
**Host in JURC** OZAWA, Fumiyuki

Synthesis of Cyclic $\pi$-Conjugated Molecules and Their Properties
SUZUKI, Toshiyasu, Institute for Molecular Science, National Institute of Natural Sciences
**Host in JURC** YAMAGO, Shigeru

Elucidation of the Mechanism of Encapsulation by Cycloparaphenylenes
HAINO, Takeharu, Graduate School of Science, Hiroshima University
**Host in JURC** YAMAGO, Shigeru

Cornea Regeneration by Small Molecule Fibronectin
KOIZUMI, Noriko, Department of Biomedical Engineering, Faculty of Life and Medical Sciences, Doshisha University
**Host in JURC** UESUGI, Motonari

Preparation of Organic-inorganic Hybrid Materials for Biosensor Application
FUJINO, Shigeru, Department of Chemical Engineering, Faculty of Engineering, Kyusyu University
**Host in JURC** YOKO, Toshinobu

Intracellular Gene Delivery Using Cell-penetrating Peptides
KOGURE, Kentaro, Department of Biophysical Chemistry, Kyoto Pharmaceutical University
**Host in JURC** FUTAKI,Shiroh

Elucidation of Excitation Relaxation Dynamics and Application of Fullerenes Directly Connected to an Organic Dye
OHKUBO, Kei, Department of Material and Life Science, Graduate School of Engineering, Osaka University
**Host in JURC** MURATA, Yasujiro

Synthesis, Structure and Electronic Properties of Carbazolophane-Polymers
TANI, Keita, Division of Natural Science, Osaka Kyoiku University
**Host in JURC** TSUJII, Yoshinobu

Making of the Vertical Cross Section of Bioactive Trace Metals in the Japan Sea
NAKAGUCHI, Yuzuru, Faculty of Science and Engineering, Kinki University
**Host in JURC** SOHRIN, Yoshiki

Elucidation of Dewetting Process in Polymer Blend Thin Films as Studied by Grazing-Incidence Small Angle X-ray Scattering
OGAWA, Hiroki, Japan Synchrotron Radiation Institute
**Host in JURC** KANAYA, Toshiji

Investigation of Effect of Loop/Bridge Conformation Ratio on Elastic Properties of the BAB Triblock Copolymer/AB Ring Diblock Copolymer Having Middle Block with Type-A Dipoles Aligned Parallel to the Chain Contour
TAKAHASHI, Yoshiaki, Institute for Materials Chemistry and Engineering, Kyushu University
**Host in JURC** WATANABE, Hiroshi

Study of Segmental Dynamics in Multi-Component Polymer Systems in Miscible State
URAKAWA, Osamu, Graduate School of Science, Osaka University
**Host in JURC** MATSUMIYA, Yumi

Elucidation of Correlation between Structural Formation Process and Relaxation Process during Applying Shear Flow
MATSUBA, Go, Department of Polymer Science and Engineering, Faculty of Science and Engineering, Yamagata University
**Host in JURC** KANAYA, Toshiji

Analysis of Molecular Adsorption of Water and Protein on a Stereo-Controlled Acrylamide Polymers
KATSUMOTO, Yukiteru, Graduate School of Science, Hiroshima University
**Host in JURC** HASEGAWA, Takeshi

## STARTING-UP SUBJECTS (ON-DEMAND FROM RELATED COMMUNITIES)

Study on the Regulatory Mechanism of Plant Epidermal Cell Differentiation
TOMINAGA, Rumi, Interdisciplinary Research Organization, University of Miyazaki
**Host in JURC** AOYAMA, Takashi

Overexpression of Miraculin Using *Arabidopsis thaliana*
INOUE, Hiroyasu, Faculty of Human Life and Environment, Nara Women's University
**Host in JURC** AOYAMA, Takashi

Small Molecules that Promote Differentiation into Pancreatic Beta Cells
KUME, Shouen, Institute of Molecular Embryology and Genetics, Kumamoto University
**Host in JURC** UESUGI, Motonari

Study for Tunnel Magnetoresistive Effect and Local Magnetism of Magnetic Tunnel Junctions Using $Co_2MnSn$ Heusler Alloy Electrodes Prepared by Atomically-controlled Alternate Deposition
TANAKA, Masaaki, Department of Engineering Physics, Electronics and Mechanics, Nagoya Institute of Technology
**Host in JURC** ONO, Teruo

Synthesis and Functions of Multi-Bridged Naphthalene Oligomers
KURAMOCHI, Koji, Graduate School of Life and Environmental Sciences, Kyoto Prefectural University
**Host in JURC** KAWABATA, Takeo

High-energy Ion Generation through the Interactions of Laser with Nano Particles
NAKAI, Mitsuo, Institute of Laser Engineering, Osaka University
**Host in JURC** SAKABE, Shuji

Identification and Functional Analysis of Bacterial Proteins Involved in Metal Metabolism
KURATA, Atsushi, Department of Applied Biological Chemistry, Faculty of Agriculture, Kinki University
**Host in JURC** KURIHARA, Tatsuo

Single-Electron Transistor Circuit Based on Nanoparticle
MAJIMA, Yutaka, Materials & Structures Laboratory, Tokyo Institute of Technology
**Host in JURC** TERANISHI, Toshiharu

Programmable Architecture of Metal Complex-metal Nanoparticle Composites
TANAKA, Kentaro, Graduate School of Science, Nagoya University
**Host in JURC** TERANISHI, Toshiharu

Preparation, Structure, and Electronic Properties of Thin Films of D(donor)–A(acceptor)–D and A–D–A Type Compounds
HAYASHI, Naoto, Graduate School of Science and Engineering for Research, University of Toyama
**Host in JURC** SATO, Naoki

## EXPANDING SUBJECTS (ON-DEMAND FROM RELATED COMMUNITIES)

Efficient Synthesis of π-Conjugated Polymers via Direct Arylation
KANBARA, Takaki, Graduate School of Pure and Applied Sciences, Tsukuba Research Center for Interdisciplinary Materials Science, University of Tsukuba
**Host in JURC** OZAWA, Fumiyuki

The Control of the Antiphase Boundary in Ferrimagnetic Spinel Ultrathin Films
NAGAHAMA, Taro, Laboratory of Advanced Materials Chemistry, Graduate School of Engineering, Hokkaido University
**Host in JURC** ONO, Teruo

Optical Functionalities of Silicon Photonic Crystals
TAKAHASHI, Yasushi, Reseach Organization for the 21st Century, Osaka Prefecture University
**Host in JURC** KANEMITSU, Yoshihiko

Search for Biologically Active Compounds from a Synthetic Library of Nitogen Heterocycles with Chiral Tetrasubstituted Carbon
ISHIBASHI, Masami, Graduate School of Pharmaceutical Sciences, Chiba University
**Host in JURC** KAWABATA, Takeo

Studies on the Transport and Metabolism of the Essential Trace Element Selenium in Mammals
MIHARA, Hisaaki, Department of Biotechnology, College of Life Sciences, Ritsumeikan University
**Host in JURC** KURIHARA, Tatsuo

Chemical Biology for Fine Analysis of Plant Hormone Signal Transduction Systems
HAYASHI, Ken-ichiro, Department of Biochemistry, Okayama University of Science
**Host in JURC** AOYAMA, Takashi

Synthesis and Properties of Well-Defined Poly(phenylene ethylene)s by Means of Organometalic Catalyst
KONISHI, Gen-ichi, Department of Organic and Polymeric Materials, Graduate School of Engineering, Tokyo Institute of Technology
**Host in JURC** NAKAJIMA, Yumiko

Dynamics of Spin-dependent Transport in Nanostructured Devices
KOBAYASHI, Kensuke, School of Science, Osaka University
**Host in JURC** ONO, Teruo

Electric and Magnetic Characteristics of New Ilmenite-type Iron Oxides
FUJII, Tatsuo, Faculty of Enginnering, Okayama University
**Host in JURC** SAITO, Takashi

Mechanistic Study of Calpain Modulation by Bioinformatics
ONO, Yasuko, Tokyo Metropolitan Institute of Medical Science
**Host in JURC** MAMITSUKA, Hiroshi

Bulk Hetero Junction Photovoltaic Devices Composed of Novel Donar Polymer and Novel Fullerene Derivatives
IE, Yutaka, The Institute of Scientific and Industrial Research, Department of Soft Nanomaterials, Nanoscience and Nanotechnology Center, Osaka University
**Host in JURC** MURATA, Yasujiro

Chemical Biology of GGsTop, a Compound Inducing Anti-oxidative Stress Response of Human Skin Cells
KOJIMA, Akiko, Department of Food and Human Health Sciences, Graduate School of Human Life Sciences, Osaka City University
**Host in JURC** HIRATAKE, Jun

## SUBJECTS FOCUSING OF JOINT USAGE OF JURC/ICR FACILITIES

Nano-electron Spectroscopic Study of Helium Bubbles in Si
MIYAMOTO, Mitsutaka, Interdisciplinary Faculty of Science and Engineering, Shimane University
**Host in JURC** KURATA, Hiroki

Systematic Syntheses and Properties of Polycyclic Aromatics Containing a Phosphorus Atom
OKUMA, Kentaro, Department of Chemistry, Faculty of Science, Fukuoka University
**Host in JURC** SASAMORI, Takahiro

Physicochemical Properties of Novel Aromatic Compounds with Heteroatoms
SAITO, Masaichi, Department of Chemistry, Graduate School of Science and Engineering, Saitama University
**Host in JURC** TOKITOH, Norihiro

Synthesis and Structure of Transition Metal Complexes with New Tripodal Tetradentate Ligand
UNNO, Masafumi, Graduate School of Engineering, Gunma University
**Host in JURC** TOKITOH, Norihiro

Synthesis and Structure of Main Group Element-Protected Metal Nanoparticles
FUJIHARA, Hisashi, Department of Chemistry, Fuculty of Science and Engineering, Kinki University
**Host in JURC** TOKITOH, Norihiro

Synthesis and Structure of Color-tunable Organotelluronium Salts
MINOURA, Mao, School of Science, Kitasato University
**Host in JURC** TOKITOH, Norihiro

Structural Features of Aromatic-rings-accumulated Molecules in Crystal
OKAMOTO, Akiko, Department of Organic and Polymer Materials Chemistry, Tokyo University of Agriculture & Technology
**Host in JURC** NAKAMURA, Masaharu

Solid-State NMR Analysis of Molecular Orientation in Organic LED Materials
ADACHI, Chihaya, OPERA, Kyushu University
**Host in JURC** KAJI, Hironori

NMR Characterization of Carbon Nitride
TAKARABE, Kenichi, Department of Applied Science, Okayama University of Science
**Host in JURC** KAJI, Hironori

Solid-state-NMR Study on Luminescence and Structure Characteristics of Organic Molecules
TOKUDOME, Yasuaki, Graduate School of Engineering, Osaka Prefecture University
**Host in JURC** KAJI, Hironori

## SUBJECTS ENCOURAGING JOINT PROGRAM

Elucidation of Electronic States, Local Structures, and Properties in Transition Metal Oxides Using Synchrotron Radiated X-rays
MIZUMAKI, Masaichiro, Japan Synchrotron Radiation Research Institute, SPring-8
**Host in JURC** ICHIKAWA, Noriya

The 8th International Workshop for East Asian Young Rheologists
TAKAHASHI, Yoshiaki, Institute for Materials Chemistry and Engineering, Kyushu University
**Host in JURC** WATANABE, Hiroshi

# JURC Publications

(until 31 May 2012)

**Dielectric and Viscoelastic Investigation of Segmental Dynamics of Polystyrene above Glass Transition Temperature: Cooperative Sequence Length and Relaxation Mode Distribution**
Matsumiya, Y.; Uno, A.; Watanabe, H., *Macromolecules*, **44,** 4355-4365 (2011).

**Abstract**

Atactic polystyrene (PS) has the type-B dipole perpendicular to the chain backbone so that its local, segmental motion activates the dielectric relaxation. For monodisperse oligostyrene (OS) and PS samples of various molecular weights $M$, details of this motion were examined at temperatures $T$ well above $T_g$ through comparison of the complex modulus, $G^* = G' + iG''$, and the complex dielectric permittivity, $\varepsilon^* = \varepsilon' - i\varepsilon''$, measured as functions of the angular frequency $\omega$. For the OS samples, $G^*(\omega)$ and $\varepsilon^*(\omega)$ fully relaxed through the segmental dynamics thereby exhibiting respective terminal relaxation tails (low-frequency tails), $G'(\omega) \propto \omega^2$, $G''(\omega) \propto \omega$, $\Delta\varepsilon'(\omega) \equiv \varepsilon'(0) - \varepsilon'(\omega) \propto \omega^2$, and $\varepsilon''(\omega) \propto \omega$, at $\omega$ below the segmental relaxation frequency $\omega_s$. For the PS samples, $G^*(\omega)$ relaxed partly through the segmental dynamics and then exhibited the polymeric full relaxation characterized by the Rouse-like behavior followed by the terminal flow behavior (with/without intermediate entanglement plateau depending on $M$). In contrast, $\varepsilon^*(\omega)$ of the PS samples still relaxed completely through the segmental dynamics. For respective samples, the $G^*(\omega)$ and $\varepsilon^*(\omega)$ data in the segmental relaxation zone exhibited very similar relaxation mode distribution and had the same time—temperature shift factor. Nevertheless, a ratio of the dielectrically and viscoelastically detected segmental relaxation times, $r(M) = \omega_{s,G}/\omega_{s,\varepsilon}$, and the dielectric relaxation intensity, $\Delta\varepsilon(M)$, decreased with increasing $M$ up to $M^* \cong 2 \times 10^3$ and then became insensitive to $M$ on a further increase of $M$. The viscoelastic segmental relaxation reflects the cooperative torsion of the repeating units along the molecular backbone (as noted from rheo-optical data), while the dielectric segmental relaxation detects reorientational motion of those units affected by both intra- and intermolecular cooperativity (as noted from the basic dielectric expression). The observed decreases of $r(M)$ and $\Delta\varepsilon(M)$ suggested that the dimension $\xi_m$ of the whole OS molecule (over which the cooperative torsion occurs) is smaller than the length scale $\xi_c$ for the intermolecular cooperative motion and that $\xi_m$ approaches $\xi_c$ on an increase of $M$ up to $M^*$. Consequently, the high-$M$ PS molecules having $\xi_m > \xi_c$ exhibited the $M$-insensitive $r(M)$ and $\Delta\varepsilon(M)$. Thus, the $M$ value for the crossover between these two regimes, $M^* \cong 2 \times 10^3$, can be taken as the molecular weight of the cooperative sequence along the PS backbone. Furthermore, the quantitative similarity of the viscoelastic and dielectric mode distributions suggests that the cooperative torsion of the repeating units along the molecular backbone is governed by the cross-correlation of the units belonging to different molecules.

**Directional Terahertz Emission from Air Plasma Generated by Linearly Polarized Intense Femtosecond Laser Pulses**
Jahangiri, F.; Hashida, M.; Tokita, S.; Nagashima, T.; Ohtani, K.; Hangyo, M.; Sakabe, S., *Applied Physics Express*, **5,** [026201-1]-[026201-3] (2012).

**Abstract**

Terahertz (THz) radiation from air plasma produced by linearly polarized intense femtosecond laser pulses was investigated. The laser energy dependence, directionality, and polarization properties of THz waves, measured in the present experiment, differed from those in previous reports and can be explained by parametric decay of laser light to R-waves in the presence of a spontaneous magnetic field.

**Colossal Negative Thermal Expansion in $BiNiO_3$ Induced by Intermetallic Charge Transfer**
Azuma, M.; Chen, W. T.; Seki, H.; Czapski, M.; Olga, S.; Oka, K.; Mizumaki, M.; Watanuki, T.; Ishimatsu, N.; Kawamura, N.; Ishiwata, S.; Tucker, M. G.; Shimakawa, Y.; Attfield, J. P., *Nature Communications*, [DOI: 10.1038/ncomms1361] (2011).

**Abstract**

The unusual property of negative thermal expansion is of fundamental interest and may be used to fabricate composites with zero or other controlled thermal expansion values. Here we report that colossal negative thermal expansion (defined as linear expansion $< -10^{-4}$ $K^{-1}$ over a temperature range ~100 K) is accessible in perovskite oxides showing charge-transfer transitions. $BiNiO_3$ shows a 2.6% volume reduction under pressure due to a Bi/Ni charge transfer that is shifted to ambient pressure through lanthanum substitution for Bi. Changing proportions of coexisting low- and high-temperature phases leads to smooth volume shrinkage on heating. The crystallographic linear expansion coefficient for $Bi_{0.95}La_{0.05}NiO_3$ is $-137 \times 10^{-6}$ $K^{-1}$ and a value of $-82 \times 10^{-6}$ $K^{-1}$ is observed between 320 and 380 K from a dilatometric measurement on a ceramic pellet. Colossal negative thermal expansion materials operating at ambient conditions may also be accessible through metal-insulator transitions driven by other phenomena such as ferroelectric orders.

**Preparation of $Co_2FeSn$ Heusler Alloy Films and Magnetoresistance of $Fe/MgO/Co_2FeSn$ Magnetic Tunnel Junctions**
Tanaka, M. A.; Ishikawa, Y.; Wada, Y.; Hori, S.; Murata, A.; Horii, S.; Yamanishi, Y.; Mibu, K.; Kondou, K.; Ono, T.; Kasai, S., *Journal of Applied Physics*, **111,** [053902-1]-[053902-4] (2012).

**Abstract**

To obtain magnetic tunnel junctions (MTJs) composed of nonequilibrium alloy, $Co_2FeSn$ films were prepared by atomically controlled alternate deposition at various substrate temperatures. X-ray diffraction patterns and Mössbauer spectra clarify that $Co_2FeSn$ films in the Heusler alloy phase can be realized by growing at a substrate temperature of 250 ℃ or below. Phase separation into cubic CoSn, hexagonal CoSn and cubic CoFe phases occurs in films grown at substrate temperatures 300 ℃ or greater. $Fe/MgO/Co_2FeSn$ MTJs were prepared with the $Co_2FeSn$ layer grown at various substrate temperatures. The MTJs with the ferromagnetic $Co_2FeSn$ layer grown at a substrate temperature of 250 ℃ showed tunnel magnetoresistance ratios of 72.2% and 43.5% at 2 K and 300 K, respectively.

**Nanoparticles for *ex vivo* siRNA Delivery to Dendritic Cells for Cancer Vaccines: Programmed Endosomal Escape and Dissociation**
Akita, H.; Kogure, K.; Moriguchi, R.; Nakamura, Y.; Higashi, T.; Nakamura, T.; Serada, S.; Fujimoto, M.; Naka, T.; Futaki, S.; Harashima, H., *Journal of Controlled Release,* **143,** 311-317 (2010).

**Abstract**

We previously developed octaarginine (R8)-modified lipid envelope-type nanoparticles for siRNA delivery (R8-MEND). Herein, we report on their *ex vivo* siRNA delivery to primary mouse bone marrow-derived dendritic cells (BMDCs) for potential use as a cancer vaccine. Quantitative imaging analysis of the intracellular trafficking of siRNA revealed that the dissociation process, as well as the rate of endosomal escape limits the siRNA efficiency of the prototype R8-MEND, prepared by the hydration method (R8-MEND$_{\text{hydo}}$). Successful endosomal escape was achieved by using a pH-dependent fusogenic peptide (GALA) modified on a lipid mixture that was optimized for endosomal fusion. Furthermore, a modified protocol for the preparation of nanoparticles, mixing the siRNA/STR-R8 complex and small unilamellar vesicles (R8/GALA-MEND$_{\text{SUV}}$), results in a more homogenous, smaller particle size, and results in a more efficient intracellular dissociation. Gene knockdown of the suppressor of cytokine signaling 1 (SOCS1), a negativefeedback regulator of the immune response in BMDCs resulted in an enhanced phosphorylation of STAT1, and the production of proinflammatory cytokines. Moreover, SOCS1-silenced BMDCs were more potent in suppressing tumor growth. Collectively, these results show that siRNA loaded in R8/GALA-MEND$_{\text{SUV}}$ efficiently suppresses endogenous gene expression and consequently enhances dendritic cell-based vaccine potency *in vivo*.

# VISITING PROFESSORS' ACTIVITIES IN ICR

Vis Prof
NITTA, Junsaku
(D Eng)

Laboratory of Nanospintronics

Professor, Department of Materials Science, Tohoku University
(02 Aoba-yama, Aramaki, Aoba-ku, Sendai 980-8579)

**Lecture at *ICR***
Basic and Applied Research in Semiconductor Spintronics

Vis Prof
OSAWA, Masatoshi
(D Eng)

Laboratory of Solution and Interface Chemistry

Professor, Catalysis Research Center, Hokkaido University
(Kita-ku N21W10, Sapporo, Hokkaido 001-0021)

**Lecture at *ICR***
Chemical Reaction on Electrode Studied by Surface Enhanced Infrared Spectroscopy

Vis Prof
NODA, Koji
(D Eng)

Laboratory of Particle Beam Science

Director, Department of Accelerator and Medical Physics, Research Center for Charged Particle Therapy, National Institute of Radiological Sciences
(4-9-1 Anagawa, Inage-ku, Chiba-shi 263-8555)

**Lecture at *ICR***
Development of Heavy-Ion Radiotherapy Technology

Vis Prof
TOMITA, Masaru
(Ph D)

Laboratory of Bio-knowledge Engineering

Professor, Faculty of Environment and Information Studies, Keio University
(5322 Endo, Fujisawa, Kanagawa 252-8520)

**Lecture at *ICR***
Metabolome Analysis and Systems Biology

Vis Prof
LIKHTMAN, Alexey
(Ph D)

Laboratory of Molecular Rheology

Professor, Department of Mathematics, University of Reading
(Whiteknights, PO Box 217, Reading, RG6 6AH, UK)

**Lecture at *ICR***
Molecular Picture of Polymer Dynamics

Vis Assoc Prof
FURUBE, Akihiro
(D Eng)

Laboratory of Advanced Inorganic Synthesis

Senior Researcher, Research Institute of Instrumentation Frontier (RIIF), National Institute of Advanced Industrial Science and Technology (AIST)
(Tsukuba Central 5, 1-1-1 Higashi, Tsukuba, Ibaraki 305-8565)

**Lecture at *ICR***
Intersurface Electron Transfer at the Nanoparticles of Photoelectro Conversion Systems

Vis Assoc Prof
SATO, Moritoshi
(D Sc)

Laboratory of Molecular Biology

Associate Professor, Graduate School of Arts and Sciences, The University of Tokyo
(Komaba, Meguro-ku, Tokyo 153-0041)

**Lecture at *ICR***
Technologies for Visualizing and Operating Biomolecules

Vis Assoc Prof
TAKANO, Atsushi
(D Eng)

Laboratory of Molecular Rheology

Associate Professor, Laboratory of Physical Chemistry of Polymers, Department of Applied Chemistry, Graduate School of Engineering, Nagoya University
(Furo-cho, Chikusa-ku, Nagoya 464-8603)

Vis Assoc Prof
OHKI, Yasuhiro
(D Sc)

Laboratory of Organic Main Group Chemistry

Associate Professor, Graduate School of Science, and Research Center for Materials Science, Nagoya University
(Furo-cho, Chikusa-ku, Nagoya 464-8602)

**Lecture at *ICR***
Nitrogen Fixation with Metal Complexes

Prof Em KANEHISA, Minoru (D Sc)

Appointed as Res (pt) at ICR,
1 April 2012–31 March 2013

# PERSONAL

# Retirement

Professor NODA, Akira

Advanced Research Center for Beam Science

– Particle Beam Science –

On March 31, 2013, Dr. Akira Noda retired from Kyoto University after 22 years of service and was honored with the title of Professor Emeritus of Kyoto University.

Dr. Noda was born in Kyoto on August 28, 1948. He graduated from Faculty of Science, Kyoto University in 1971 and studied high energy physics under the supervision of Professor Emeritus Kozo Miyake in the Department of Physics, Graduate School of Science. In 1979, he received the doctoral degree of science for the thesis "Neutral Pion Photoproduction from Hydrogen at Forward Angles in the Energy Region between 450 MeV and 975 MeV". He was appointed Assistant Professor at Institute for Nuclear Study (INS), the University of Tokyo in 1976 and was appointed Professor at the Institute for Chemical Research, Kyoto University in 1991, directing the Accelerator Laboratory of Nuclear Science Research Facility. The laboratory was reorganized as Laboratory of Particle Beam Science in the Advanced Research Center for Beam Science in 2004, and he served as the first head of the center.

Throughout his academic career, Dr. Noda devoted himself to the development of the accelerators and the pursuit of high quality beams. At INS, he started his activity on accelerator and beam physics in a design work of a heavy ion synchrotron. He played a central role for designing of the synchrotron lattice and its magnets, which was really applied for the construction of Test Accumulation Ring for NUMATRON (TARN). After investigations on beam physics such as beam injection, accumulation and stochastic momentum cooling at TARN, he designed and constructed a heavy ion synchrotron-cooler ring, TARN II. Dr. Noda made an intense effort to construct a slow beam extraction system with 3rd order resonance at TARN II and invented a novel method of slow beam extraction with the use of RF knock out, which has been applied for real patient-treatments by synchronous irradiation with breathing at HIMAC in NIRS for the first time, which is now considered to be very important for a treatment of trunk of the body.

After he moved to ICR, he succeeded in the acceleration of proton by the 7 MeV linac and made important fundamental research in the accelerated beam properties. He also led the design and construction of the 100 MeV electron linac and an electron storage ring, Kyoto Storage Ring (KSR). He leaded activities in ICR by the Advanced Compact Accelerator Development Project by MEXT of Japanese Government on the construction of the Small Laser-equipped Storage Ring (S-LSR) and monochromization of laser-produced ions by RF phase rotation scheme. At S-LSR, great milestones of beam cooling, one-dimensional ordering of 7 MeV proton beam and efficient indirect transverse laser cooling by synchro-betatron resonant coupling were achieved.

Dr. Noda's educational contribution is also notable. In these years, he has supervised 14 graduate students 5 researchers for their doctor theses as a chief examiner. His students gained valuable experience concerning the whole system of the accelerator through the design and construction of the accelerator components and the experiments with the use of them under his dedicated supervision. His students assume important roles in many institutes in the accelerator society, such as KEK, JAEA, J-PARC, NIRS, JASRI and so on.

In addition to his own and collaboration research, his contribution to the accelerator and beam physics society was also significant. Dr. Noda promoted the launch of Beam Physics Division in the Physical Society of Japan as the chairman of the Japanese Beam Physics Club. He chaired the Scientific Programming Committee in the first International Particle Accelerator Conference (IPAC'10) held in Kyoto. His energetic commitment not only in the scientific program but also the hospitality led the conference to a great success as the largest accelerator conference ever held in Asia. He served as Editor in Chief of Japanese Journal of Applied Physics. Dr. Noda also improved international collaborations with BESSY, LNL, MPI-K, PAL, JINR and stimulated exchange of researchers between these institutes.

Dr. Noda's contribution to Kyoto University and the Institute through his scientific and educational activities is greatly acknowledged. His perpetual quest of the rule of nature will be remembered for a long time to come.

# Awards

## SASAMORI, Takahiro

**Sumitomo Chemical Award in Synthetic Organic Chemistry, Japan**

“Creation of a Novel Photocatalyst Based on Heavier Group 14 Elements with Controlled Coordination Numbers”

The Society of Synthetic Organic Chemistry, Japan

17 February 2012

## MIYAMOTO, Hisashi

**CSJ Student Presentation Award 2012**

The 92nd Annual Meeting of the Chemical Society, Japan

“Attempted Synthesis of Ansa-type Ferrocenyldigermene”

The Chemical Society of Japan

12 April 2012

## WAKAMIYA, Atsushi

**The Young Scientists’ Prize of the Commendation for Science and Technology**

“Studies on Functional π-Electronic Compounds Using Boron as a Key Element”

Ministry of Education, Culture, Sports, Science and Technology, Japan

17 April 2012

## KAWABATA, Takeo

**Molecular Chirality Award 2012**

“Creation of Memory of Chirality Concept and Application to Asymmetric Synthesis”

Molecular Chirality Research Organization (MCRO)

17 May 2012

## YOSHIMURA, Tomoyuki

**The Pharmaceutical Society of Japan, Kinki Branch Award for Young Scientists**

62nd Annual Meeting of the PSJ Kinki-Branch

“Aysmmetric Synthesis of Multisubstituted Beta-lactams via C-N Axially Chiral Enolate in Intramolecular Conjugate Addition”

The Pharmaceutical Society of Japan, Kinki-Branch

6 January 2012

## TOMOHARA, Keisuke

**Best Presentation Award**

The 132nd Annual Meeting of Pharmaceutical Society of Japan

“Asymmetric α-Arylation of α-Amino Acid Derivatives via Memory of Chirality”

The Pharmaceutical Society of Japan

31 March 2012

## KINOSHITA, Tomohiko

**Best Presentation Award**

The 132nd Annual Meeting of Pharmaceutical Society of Japan

“Development of Asymmetric Intermolecular Conjugate Addition Reaction via Memory of Chirality and Its Application in Total Synthesis of Manzacidin A”

The Pharmaceutical Society of Japan

31 March 2012

## SHIGETA, Takashi

**Best Presentation Award**

The 132nd Annual Meeting of Pharmaceutical Society of Japan

“Remote Asymmetric Desymmetrization of σ-Symmetric Long Chain Linear Diols by Organocatalytic Chiral Recognition”

The Pharmaceutical Society of Japan

31 March 2012

## HAMADA, Shohei

**Best Presentation Award**

10th Symposium on Organic Chemistry-The Next Generation

“Development of a Nitroxyl Radical Oxidation Catalyst by Electronic Tuning”

The Pharmaceutical Society of Japan, Division of Organic Chemistry

12 May 2012

## TANAKA, Daisuke

**CSJ Student Presentation Award 2012**

“Platonic Hexahedron Composed of Six Porphyrin Derivatives and Au Cluster”

The Chemical Society of Japan

12 April 2012

## YAMAGO, Shigeru

**SSOCJ DIC Award for Functional Material Chemistry 2011**

“Development of Highly Efficient Controlling Reagents for Living Radical Polymerization”

The Society of Synthetic Organic Chemistry, Japan

17 February 2012

**Ichimura Academic Award (Contribution Award)**

“Development and Application of New Living Radival Polymerization TERP”

The New Technology Development Foundation

27 April 2012

## MASAI, Hirokazu

**The 66th CerSJ Awards for Advancements in Ceramic Science and Technology**

“Fabrication of Rare Earth-Free Oxide Glass Phosphor”

The Ceramic Society of Japan

8 June 2012

**The Best Presentation Award**

7th Symposium of the Ceramic Society of Japan Kansai Branch

“Emission Property of Phosphate Glass Containing $Sn^{2+}$ Emission Center”

The Ceramic Society of Japan Kansai Branch

13 July 2012

## ONO, Teruo

**8th (FY2011) JSPS PRIZE**

“The Basic and Applied Research of Spin-Devices Based on Nano-Magnetic Materials”

Japan Society for the Promotion of Science

27 February 2012

## KOBAYASHI, Kensuke

**The 15th Marubun Award for Research Promotion**

“Development of Semiconductor Devices Based on Quantum Many-body Effects and their Dynamics”

Marubun Research Promotion Foundation

7 March 2012

## CHIBA, Daichi

**33rd Honda Memorial Young Researcher Award**

“Electric Field Control of Ferromagnetic Phase Transition in Semiconductors and Metals”

The Honda Memorial Foundation

30 May 2012

**Sir Martin Wood Prize**

“Electric Field Control of Ferromagnetism in Semiconductors and Metals”

Millennium Science Forum

14 November 2012

**ICR Award for Young Scientists**

“Electrical Control of the Ferromagnetic Phase Transition in Cobalt at Room Temperature”

Institute for Chemical Research, Kyoto University

7 December 2012

## SHIMAMURA, Kazutoshi

**JSAP Young Scientist Oral Presentation Award**

The 59th JSAP Spring Meeting, 2012

“Electrical Control of Magnetism in Co Ultra-Thin Film Using an Electric Double Layer”

The Japan Society of Applied Physics

11 September 2012

## IMANISHI, Miki

**The PSJ Award for Young Scientists**

“Design of Artificial DNA Binding Proteins toward Control and Elucidation of Cellular Functions”

The Pharmaceutical Society of Japan

28 March 2012

## KATAYAMA, Sayaka

**The Student Oral Presentation Award**

The 132nd Annual Meeting of the Pharmaceutical Society of Japan

“Development of Amphiphilic Arginine-rich Peptides for Mitochondria-target Delivery”

The Pharmaceutical Society of Japan

31 March 2012

## OKU, Akihiko

**The Student Oral Presentation Award**

The 132nd Annual Meeting of the Pharmaceutical Society of Japan

“A New Approach to the Preparation of Deubiquitinating-enzyme-resistant Ubiquitin Polymer”

The Pharmaceutical Society of Japan

31 March 2012

## KAWAGUCHI, Yoshimasa

**Best Discussion Award**

Bioorganic Research Insutitute Symposium

“Molecules for Analyzing Biological Function: Design and Synthesis of Unique Probes”

Suntory Foundation for Life Sciences

27 August 2012

## ITO, Yuki

**ICR Award for Graduate Students**

“Polarization Dependence of Raman Scattering from a Thin Film Involving Optical Anisotropy Theorized for Molecular Orientation Analysis”

Institute for Chemical Research, Kyoto University

7 December 2012

## WATANABE, Hiroshi

**The SRJ Award**

The 39th Annual Meeting of Society of Rheology, Japan

“Fundamental Findings in Softmatter Rheology on the Basis of Multiple Methods”

The Society of Rheology, Japan

10 May 2012

## YAMADA, Masako

**Takegoshi Award**

“Demonstration of Focusing Pulsed White VCN Beam Using Permanent Magnet Sextupole with Modulation Capability”

Faculty of Science, Kyoto University

26 June 2012

## INOUE, Shunsuke

**ICR Award for Graduate Students**

“Femtosecond Electron Deflectometry for Measuring Transient Fields Generated by Laser-accelerated Fast Electrons”

Institute for Chemical Research, Kyoto University

7 December 2012

## TAKAYA, Hikaru

**Thieme Chemistry Journal Award 2012**

Thieme Chemistry

22 January 2012

## HATAKEYAMA, Takuji

**The New Chemical Technology Research Encouragement Award**

“Synthesis and Integration of Heteroatom-fused Helically π-Conjugated Molecules toward Organic Photovoltaic Cell”

Japan Association for Chemical Innovation

25 May 2012

## SHIMAKAWA, Yuichi

**The Chemical Society of Japan (CSJ) Award for Creative Work**

The 29th Annual Meeting of the Chemical Society Japan

“Research on Synthesis, Structure Analysis, and Property Measurements of New Functional Oxide Materials”

The Chemical Society of Japan

26 March 2012

## KAN, Daisuke

**The Best Oral Presentation Award**

The 31st Autumn Meeting of the Japan Society of Applied Physics

"Structural Transition in $SrRuO_3$ Epitaxial Thin Films: Strain Effect in Nano-structure"

The Japan Society of Applied Physics

15 March 2012

## CHEN, Wei-tin

**ICR Award for Young Scientists (Foreign Researchers' Category)**

"Ligand-hole Localization in Oxides with Unusual Valence Fe"

Institute for Chemical Research, Kyoto University

7 December 2012

# Paper Awards

## CHIBA, Daichi, et. al.

**34th JSAP Outstanding Paper Award**

"Control of Multiple Magnetic Domain Walls by Current in a Co/Ni Nano-Wire"

Chiba, D.; Yamada, G.; Koyama, T.; Ueda, K.; Tanigawa, H.[1]; Fukami, S.[1]; Suzuki, T.[1]; Ohshima, N.[1]; Ishiwata, N.[1]; Nakatani, Y.[2]; Ono, T.

The Japan Society of Applied Physics

11 September 2012

[1] NEC Corporation, [2] University of Electro-communications

## INOUE, Shunsuke

**Presentation Award**

The 32nd Annual Meeting of the Laser Society of Japan

"Autocorrelation Method for Emission Duration Measurement of Femtosecond Laser Produced Fast Electrons"

The Laser Society of Japan

31 May 2012

## KARASUYAMA, Masayuki

**Seiichi Tejima Doctoral Dissertation Award**

"Parametric Optimization in Machine Learning"

Tokyo Institute of Technology

27 February 2012

# Poster Awards

## NAGATA, Koichi

**Poster Award**

The 59th Symposium on Organometallic Chemistry

"Trapping Reaction of a 1,2-Diarydialumene"

Division of Organometallic Chemistry, The Kinki Chemical Society, Japan

16 October 2012

## MIYAMOTO, Hisashi

**Best Poster Award**

The 4th Asian Silicon Symposium (ASIS-4)

"Synthetic Study on Novel Ferrocenophanes Bridged by a Dimetallene Unit"

Organizing Committee of ASIS-4

23 October 2012

## NISHIMURA, Hidetaka

**Poster Award**

23rd Symposium on Physical Organic Chemistry

"Development of Charge-transporting Materials Containing Oxygen-bridged Triarylamine Unit with Quasi-planar Structure"

The Society of Physical Organic Chemistry

21 September 2012

**Encouragement Award of Thin Film Solar Cells**

"Development of Charge-transporting Materials Containing Oxygen-bridged Triarylamine Unit"

Executive Committee of 4th Seminar on Thin Film Solar Cells

18 October 2012

## MISHIRO, Kenji

**Best Poster Award**

Symposium on Molecular Chirality ASIA 2012

"A Novel Chiral Structural Motif Consisting of a Cyclic Hydrogen Bonding Network"

Molecular Chirality Research Organization (MCRO)

18 May 2012

## TAKEUCHI, Hironori

**Best Poster Award**

The 47th Meeting on Organic Reaction for Young Scientists

"Efficient Total Syntheses of Naturally Occurring Glycosides"

Organizing Committee of the 47th Meeting on Organic Reaction for Young Scientists

3 August 2012

## KINOSHITA, Tomohiko

**Best Poster Award**

The 32nd Seminar on the Society of Synthetic Organic Chemistry, Japan, Kinki Branch

"Asymmetric Synthesis of Cyclic Amino Acid Derivatives with Tetrasubstituted Carbon Employing Dieckmann Condensation via Memory of Chirality"

The Society of Synthetic Organic Chemistry, Japan, Kinki Branch

22 November 2012

## SHIGETA, Takashi

**Best Poster Award**

The 29th Seminar on Synthetic Organic Chemistry

“Asymmetric Desymmetrization of σ-Symmetric Linear Diols by Organocatalytic Remote Chiral Recognition”

The Society of Synthetic Organic Chemistry, Japan, Tokai Branch

7 September 2012

## UEDA, Yoshihiro

**Excellent Poster Award**

The 6th Takeda Science Foundation Symposium on Pharma-Sciences

“Organocatalysis-based Enantioselective and Regioselective Total Synthesis of Natural Glycosides, Multifidoside A and B”

Organizing Committee of the 6th Takeda Science Foundation Symposium on PharmaSciences

14 September 2012

**Best Poster Award**

42nd Congress of Heterocyclic Chemistry

“Regioselective Acylation of a Cardiac Glycoside, Lanatoside C, by Organocatalysis”

Organizing Committee of 42nd Congress of Heterocyclic Chemistry

13 October 2012

## SAKAKIBARA, Keita

**The Best Poster Award**

The 3rd International Cellulose Conference

“Synthesis and Properties of Cellulose Derivatives with π-Conjugated Molecules”

The Cellulose Society of Japan

12 October 2012

## NAKANISHI, Yohei

**The Best Poster Award**

The 43rd Summer School of the Society of Fiber Science and Technology, Japan

“Development of Solid-State Dye-Sensitized Solar Cell by Effects of Polymer Brushes”

The Society of Fiber Science and Technology, Japan

9 August 2012

## WAKIUCHI, Araki

**The Best Poster Award**

The 2012 Annual Meeting of the Society of Fiber Science and Technology

“Synthesis of Well-Defined Fullerene-Terminated Polymers”

The Society of Fiber Science and Technology

7 June 2012

## OSAKI, Katsuhiro

**The Best Poster Prize**

The 49th Japanese Peptide Symposium

“Roles of Syndecan-4 and PKCα for Cellular Uptake of Arginine-rich Peptides”

The Japanese Peptide Society

8 November 2012

## FUKUCHI, Masashi

**The Young Poster Award**

12-1 NMR Conference of Research Group on Nuclear Magnetic Resonance in the Society of Polymer Science, Japan (SPSJ)

“Solid-State NMR Analysis of Phosphine Oxide Materials”

Research Group on Nuclear Magnetic Resonance in the Society of Polymer Science, Japan (SPSJ)

25 May 2012

## FUJIMURA, Subaru

**The Young Poster Award**

12-1 NMR Conference of Research Group on Nuclear Magnetic Resonance in the Society of Polymer Science, Japan (SPSJ)

"Solid-State NMR Analysis of Donor/Acceptor Interaction in P3HT : $C_{60}$ Blend Films"

Research Group on Nuclear Magnetic Resonance in the Society of Polymer Science, Japan (SPSJ)

25 May 2012

## SHINTANI, Megumi

**Student Presentation Award**

Membrane Symposium 2012

"Solution NMR-NOE Study on the Morphology of Aggregates Formed by Lipids with Different Chain Lengths"

The Membrane Society of Japan

7 November 2012

**Poster Presentation Award**

35th Symposium on Solution Chemistry of Japan

"Morphology Analysis of Mixture Aggregates of Phospholipids with Long and Short Chains through Solution-State $^1$H-NMR"

The Japan Association of Solution Chemistry

13 November 2012

## KAWAMOTO, Jun

**Poster Presentation Award**

The 9th International Congress on Extremophiles 2012

"Physiological Role of Eicosapentaenoic Acid in the Cold-adaptation Mechanism of an Antarctic Bacterium, *Shewanella livingstonensis* Ac10"

International Society for Extremophiles

13 September 2012

## SUGIURA, Miwa

**Best Presentation Award**

The 59th Annual Conference of the Japanese Biochemical Society, Kinki Branch

"Effect of the Absence of EPA on an Outer Membrane Protein in a Psychrotrophic Bacterium, *Shewanella livingstonensis* Ac10"

The Japanese Biochemical Society, Kinki Branch

19 May 2012

## ASO, Ryotaro;
## KAN, Daisuke;
## SHIMAKAWA, Yuichi;
## KURATA, Hiroki

**Poster Competition 1st PRIZE (Physical Sciences)**

15th European Microscopy Congress (EMC2012)

"Quantitative Strain Analysis of $BaTiO_3$ Epitaxial Thin Films Using Cs-TEM and STEM-EELS"

The International Federation of Societies for Microscopy

18 September 2012

## MUTO, Ai

**Koichi Suzuki Memorial Awards (Excellent Presentation Awards)**

The 85th Annual Meeting of the Japanese Biochemical Society

"Metabolic Pathway Evolution from the Aspect of Chemical Reaction Modules Conserved in the Global Metabolic Network"

Japanese Biochemical Society

16 December 2012

# Obituary

Professor Emeritus

Dr. OKA, Shinzaburo (1926–2012)

Dr. Shinzaburo Oka, Professor Emeritus of Kyoto University, passed away unexpectedly on March 12, 2012, in Osaka.

Dr. Shinzaburo Oka was born in Dalian, Manchuria (the present People's Republic of China) on March 21, 1926. He graduated from the Department of Chemistry, Faculty of Sciences, Kyoto University in 1947 and was employed in the Tuberculosis Research Institute, Kyoto University (the present Institute for Frontier Medical Sciences, Kyoto University) as a researcher, then in the Institute for Chemical Research, Kyoto University as a researcher in June, 1948 to continue his research on organic syntheses under the supervision of Professor Sango Kunichika. He was promoted to an Associate Professor in the Institute for Chemical Research, Kyoto University and received a doctoral degree from the Kyoto University for his studies on the dehydrogenation from aliphatic glycols in 1962. In 1971, Dr. Oka was promoted to a Full Professor of the Kyoto University to hold a chair of organic chemistry, or Laboratory of Organic Unit Reactions, the Institute for Chemical Research, Kyoto University. He retired from the Kyoto University on March 31, 1989 and was honored with the title of Professor Emeritus, Kyoto University on April 1, 1989.

Dr. Oka performed extensive researches in both fundamental and applied fields of organic chemistry such as alkylation of polyphenols, synthesis of crotonaldehyde by gas-phase condensation of acetaldehyde, preparation of lactones from aliphatic glycols, synthesis of acrolein from propylene or from formaldehyde and alkyl malonate, synthesis of methylene malonate from alkyl malonate and formaldehyde, and syntheses of cage-compounds.

He was also interested in organic syntheses mediated by organometallic compounds. The research in this field includes the carbon-carbon bond formation assisted by mercury or 8th group transition-metal elements, preparation of nitriles or halo compounds from halogenated compounds, dimerization of alkynes, preparation of ketones from acid chlorides, and preparation of nitriles from azides. His study in this field has been developed to the bio-inorganic chemistry of cytochrome P-450, which shed light on the mechanisms of certain biological reactions. His interest also concerned with organic syntheses by means of rare-earth metals such as of cerium. Dr. Oka's interest in organic syntheses did not stay in organic chemistry but further extended to the field of bio-organic chemistry including microbe-mediated syntheses of chiral building blocks.

Dr. Oka introduced sophisticated and modern technologies for elemental analyses to the Institute for Chemical Research, Kyoto University, and extended it very much.

Dr. Oka's superiority as a teacher, insight into science, and warm hospitality not only have attracted and stimulated many young and talented students but also have won him the respect and admiration of many friends and colleagues. Among his numerous professional activities, he has served as a executive board of a couple of scientific societies such as Chemical Society of Japan, Catalysis Society of Japan, and the Society of Synthetic Organic Chemistry, Japan.

# PUBLICATIONS
# INTERNATIONAL RESEARCH COLLABORATIONS
# SELECTED GRANTS
# THESES

# PUBLICATIONS

## DIVISION OF SYNTHETIC CHEMISTRY
### — Organoelement Chemistry —

Mizuhata, Y.; Sato, T.; Tokitoh, N., Reactions of an Overcrowded Silylene with Pyridines: Formation of a Novel 2*H*-1,2-Azasilepine and Its Further Cycloaddition, *Heterocycles*, **84,** 413-418 (2012).

Han, J. S.; Sasamori, T.; Mizuhata, Y.; Tokitoh, N., Evidence for a LiBr-Assisted Generation of a Silylene from a 1,2-Diaryl-1,2-dibromodisilene, *Chem. Asian J.*, **7,** 298-300 (2012).

Agou, T.; Sasamori, T.; Tokitoh, N., Synthesis of an Arylbromosilylene-Platinum Complex by Using a 1,2-Dibromodisilene as a Silylene Source, *Organometallics*, **31,** 1150-1154 (2012).

Hamaki, H.; Takeda, N.; Nabika, M.; Tokitoh, N., Catalytic Activities for Olefin Polymerization: Titanium(III), Titanium(IV), Zirconium(IV), and Hafnium(IV) β-Diketiminato, 1-Aza-1,3-butadienyl-imido, and 1-Aza-2-butenyl-imido Complexes Bearing an Extremely Bulky Substituent, the Tbt Group (Tbt=2,4,6-$[(Me_3Si)_2CH]_3C_6H_2$), *Macromolecules*, **45,** 1758-1769 (2012).

Sugamata, K.; Sasamori, T.; Tokitoh, N., Generation of an Organotellurium(II) Cation, *Eur. J. Inorg. Chem.*, 775-778 (2012).

Agou, T.; Sugiyama, Y.; Sasamori, T.; Sakai, H.; Furukawa, Y.; Takagi, N.; Guo, J. D.; Nagase, S.; Hashizume, D.; Tokitoh, N., Synthesis of Kinetically Stabilized 1,2-Dihydrodisilenes, *J. Am. Chem. Soc.*, **134,** 4120-4123 (2012).

Miyake, H.; Sasamori, T.; Tokitoh, N., Synthesis and Properties of 4,5,6-Triphospha[3]radialene, *Angew. Chem. Int. Ed.*, **51,** 3458-3461 (2012).

Agou, T.; Nagata, K.; Sakai, H.; Furukawa, Y.; Tokitoh, N., Synthesis, Structure, and Properties of a Stable 1,2-Dibromodialumane(4) Bearing a Bulky Aryl Substituent, *Organometallics*, **31,** 3806-3809 (2012).

Sasamori, T.; Miyamoto, H.; Sakai, H.; Furukawa, Y.; Tokitoh, N., 1,2-Bis(ferrocenyl)digermene: A d-π Electron System Containing a Ge=Ge Unit, *Organometallics*, **31,** 3904-3910 (2012).

Sasamori, T.; Sakagami, M.; Niwa, M.; Sakai, H.; Furukawa, Y.; Tokitoh, N., Synthesis of a Stable 1,2-Bis(ferrocenyl)diphosphene, *Chem. Commun.*, **48,** 8562-8564 (2012).

Miyake, H.; Sasamori, T.; Wu, J. I. C.; Schleyer, P. V. R.; Tokitoh, N., The 4,5,6-Triphospha[3]radialene Dianion: a Phosphorus Analogue of the Deltate Dianion. A $NICS(0)_{\pi zz}$ Examination of Their Aromaticity, *Chem. Commun.*, **48,** 11440-11442 (2012).

Azuma, E.; Nakamura, N.; Kuramochi, K.; Sasamori, T.; Tokitoh, N.; Sagami, I.; Tsubaki, K., Exhaustive Syntheses of Naphthofluoresceins and Their Functions, *J. Org. Chem.*, **77,** 3492-3500 (2012).

Watanabe, H.; Yoshimura, T.; Kawakami, S.; Sasamori, T.; Tokitoh, N.; Kawabata, T., Asymmetric Aldol Reaction via Memory of Chirality, *Chem. Commun.*, **48,** 5346-5348 (2012).

Azuma, S.; Nishio, K.; Kubo, K.; Sasamori, T.; Tokitoh, N.; Kuramochi, K.; Tsubaki, K., Three Different Dimerizations of 2-Bromo-3-methyl-1,4-naphthoquinones, *J. Org. Chem.*, **77,** 4812-4820 (2012).

### — Structural Organic Chemistry —

Troselj, P.; Bris, A.; Murata, Y.; Margetic, D., Structural Evidence for the Arc-shaped Topology of Hetero[5]polynorbornanes, *Struct. Chem.*, **23,** 791-799 (2012).

Li, Y.; Chen, J.; Lei, X.; Lawler, R.; Murata, Y.; Komatsu, K.; Turro, N., Comparison of Nuclear Spin Relaxation of $H_2O@C_{60}$ and $H_2@C_{60}$ and Their Nitroxide Derivatives, *J. Phys. Chem. Lett.*, **3,** 1165-1168 (2012).

Horsewill, A. J.; Panesar, K. S.; Rols, S.; Ollivier, J.; Johnson, M. R.; Carravetta, M.; Mamone, S.; Levitt, M. H.; Murata, Y.; Komatsu, K.; Chen, J. Y.-C.; Johnson, J. A.; Lei, X.; Turro, N. J., Inelastic Neutron Scattering Investigations of the Quantum Molecular Dynamics of a $H_2$ Molecule Entrapped inside a Fullerene Cage, *Phys. Rev. B*, **85,** [205440-1]-[205440-12] (2012).

Zoleo, A.; Lawler, R.; Lei, X.; Li, Y.; Murata, Y.; Komatsu, K.; Valentin, M. D.; Ruzzi, M.; Turro, N. J., ENDOR Evidence of Electron-$H_2$ Interaction in a Fulleride Embedding $H_2$, *J. Am. Chem. Soc.*, **134,** 12881-12884 (2012).

Beduz, C.; Carravetta, M.; Chen, J. Y.-C.; Concistre, M.; Denning, M.; Frunzi, M.; Horsewill, A. J.; Johannessen, O. G.; Lawler, R.; Lei, X.; Levitt, M. H.; Li, Y.; Mamone, S.; Murata, Y.; Nagel, U.; Nishida, T.; Ollivier, J.; Rols, S.; Room, T.; Sarker, R.; Turro, N. J.; Yang, Y., Quantum Rotation of *Ortho* and *Para*-water Encapsulated in a Fullerene Cage, *Proc. Natl. Acad. Sci. USA*, **109,** 12894-12898 (2012).

Li, Y.; Lei, X.; Lawler, R. G.; Murata, Y.; Komatsu, K.; Turro, N. J., Synthesis, Isomer Count, and Nuclear Spin Relaxation of $H_2O@Open-C_{60}$ Nitroxide Derivatives, *Org. Lett.*, **14,** 3822-3825 (2012).

Kushida, T.; Zhou, Z.; Wakamiya, A.; Yamaguchi, S., Planarized B-Phenylborataanthracene Anion: Structural and Electronic Impacts of Coplanar-Constraint, *Chem. Commun.*, **48,** 10715-10717 (2012).

Araki, T.; Wakamiya, A.; Mori, K.; Yamaguchi, S., Elucidation of π-Conjugation Modes in Diarene-Fused 1,2-Dihydro-1,2-diborin Dianions, *Chem. Asian J.*, **7,** 1594-1603 (2012).

Neue, B.; Fröhlich, R.; Wibbeling, B.; Fukazawa, A.; Wakamiya, A.; Yamaguchi, S.; Würthwein, E.-U., Synthesis and Photophysical Properties of Aryl Substituted 2-Borylbenzaldimines and Their Extended π-Conjugated Congeners, *J. Org. Chem.*, **77,** 2176-2184 (2012).

Nambo, M.; Wakamiya, A.; Itami, K., Palladium-catalyzed Tetraallylation of $C_{60}$ with Allyl Chloride and Allylstannane: Mechanism, Regioselectivity, and Enantioselectivity, *Chem. Sci.*, **3,** 3474-3481 (2012).

Ookubo, Y.; Wakamiya, A.; Yorimitsu, H.; Osuka, A., Synthesis of a Library of Fluorescent 2-Aryl-3-trifluoromethylnaphthofurans from Naphthols by Using a Sequential Pummerer-annulation/Cross-coupling Strategy and Their Photophysical Properties, *Chem. Eur. J.*, **18,** 12690-12697 (2012).

Zhou, Z.; Wakamiya, A.; Kushida, T.; Yamaguchi, S., Planarized Triarylboranes: Stabilization by Structural Constraint and Their Plane-to-bowl Conversion, *J. Am. Chem. Soc.*, **134,** 4529-4532 (2012).

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Murata, Y., New World of Fullerene Derivatives, *Chemistry & Chemical Industry*, **65,** 113-114 (2012) (in Japanese).

Murata, Y., Single Molecule of Water Encapsulated in Fullerene $C_{60}$, *Japanese Scientists in Science*, 44 (2012) (in Japanese).

Wakamiya, A., Developments of Highly Emissive Organic Solid Using Boron As a Key Element, *Photochemistry*, **43,** 35-38 (2012) (in Japanese).

### — Synthetic Organic Chemistry —

Furuta, T.; Kawabata, T., Desymmetrization of Meso Anhydride, *Comprehensive Chirality (Carreira, E. M. and Yamamoto, H. Ed.), Elsevier*, **5,** 581-599 (2012).

Yoshida, K.; Mishiro, K.; Ueda, Y.; Shigeta, T.; Furuta, T.; Kawabata, T., Nonenzymatic Geometry-selective Acylation of Tri- and Tetrasubstituted α,α'-alkenediols, *Adv. Syn. Catal.*, **354,** 3291-3298 (2012).

Schedel, H.; Kan, K.; Ueda, Y.; Mishiro, K.; Yoshida, K.; Furuta, T.; Kawabata, T., Asymmetric Desymmetrization of Meso-diols by $C_2$-symmetric 4-pyrrolidinopyridines, *Beil. J. Org. Chem.*, **8,** 1778-1787 (2012).

Ueda, Y.; Mishiro, K.; Yoshida, K.; Furuta, T.; Kawabata, T., Regioselective Diversification of a Cardiac Glycoside, Lanatoside C, by Organocatalysis, *J. Org. Chem.*, **77,** 7850-7857 (2012).

Yoshida, K.; Shigeta, T.; Furuta, T.; Kawabata, T., Catalyst-controlled Reversal of Chemoselectivity in Acylation of 2-Aminopentane1,5-diol Derivatives, *Chem. Commun.*, **48,** 6981-6983 (2012).

Furuta, T.; Kawabata, T., Chiral DMAP-type Catalysts for Acyl-transfer Reactions, *Science of Synthesis: Asymmetric Organicatalysis 1(List, B. Ed.), Georg Thieme Verlag KG (Stuttgart•New York)*, 497-546 (2012).

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Mabuchi, R.; Kurita, A.; Miyoshi, N.; Yokoyama, A.; Furuta, T.; Goda, T.; Suwa, Y.; Kan, T.; Amagai, T.; Ohshima, H., Analysis of $N^{\varepsilon}$-ethyllysine in Human Plasma Proteins by Gas Chromatography-Negative Ion Chemical Ionization/Mass Spectrometry as a Biomarker for Exposure to Acetaldehyde and Alcohol, *Alcohol.: Clin. Exp. Res.*, **36,** 496-508 (2012).

Monguchi, D.; Yoshimura, T.; Irie, K.; Hayashi, K.; Majumdar, S.; Sasamori, T.; Tokitoh, N.; Kawabata, T., Asymmetric Intramolecular Conjugate Addition of α-Amino Acid Derivatives via Racemization-Free Equilibrium of Intermediary Chiral Enolates, *Heterocycles*, **86,** 1483-1494 (2012).

Yoshimura, T.; Takuwa, M.; Tomohara, K.; Uyama, M.; Hayashi, K.; Yang, P.; Hyakutake, R.; Sasamori, T.; Tokitoh, N.; Kawabata, T., Protonation-Assisted Conjugate Addition of Axially Chiral Enolates: Asymmetric Synthesis of Multisubstituted β-Lactams from α-Amino Acids, *Chem. Eur. J.*, **18,** 15330-15336 (2012).

Azuma, Y.; Imai, H.; Yoshimura, T.; Kawabata, T.; Imanishi, M.; Futaki, S., Dipicolylamine as a Unique Structural Switching Element for Helical Peptides, *Org. Biomol. Chem.*, **10,** 6062-6068 (2012).

Watanabe, H.; Yoshimura, T.; Kawakami, S.; Sasamori, T.; Tokitoh, N.; Kawabata, T., Asymmetric Aldol Reaction via Memory of Chirality, *Chem. Commun.*, **48,** 5346-5348 (2012).

### — Advanced Inorganic Synthesis —

Sakamoto, M; Tanaka, D.; Tsunoyama, H.; Tsukuda, T.; Minagawa, Y.; Majima, Y.; Teranishi, T., Platonic Hexahedron Composed of Six Organic Faces with an Inscribed Au Cluster, *J. Am. Chem. Soc.*, **134,** 816-819 (2012).

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Hattori, S.; Kano, S.; Azuma, Y.; Tanaka, D.; Sakamoto, M.; Teranishi, T.; Majima, Y., Coulomb Blockade Behaviors in Individual Au Nanoparticles as Observed through Noncontact Atomic Force Spectroscopy at Room Temperature, *Nanotechnology*, **23, [**185704-1]- **[**185704-9] (2012).

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## DIVISION OF MATERIALS CHEMISTRY

### — Chemistry of Polymer Materials —

Nomura, A.; Ohno, K.; Fukuda, T.; Sato, T.; Tsujii, Y., Lubrication Mechanism of Concentrated Polymer Brushes in Solvents: Effect of Solvent Viscosity, *Polym. Chem.*, **3,** 148-153 (2012).

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Kondo, T.; Nomura, K.; Murou, M.; Gemmei-Ide, M.; Kitano, H.; Noguchi, H.; Uosaki, K.; Ohno, K.; Saruwatari, Y., Structure of Water in the Vicinity of a Zwitterionic Polymer Brush as Examined by Sum Frequency Generation Method, *Colloids Surf. B: Biointerfaces*, **100,** 126-132 (2012).

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# INTERNATIONAL RESEARCH COLLABORATIONS

**[Australia]**
Australian National University, Research School of Earth Sciences

Central Queensland University, Centre for Molecular Architecture

Monash University, Department of Biochemistry and Molecular Biology

**[Austria]**
University of Natural Resources and Life Sciences, Department of Chemistry

**[Belgium]**
Université Catholique de Louvain, Institute on Condensed Matter and Nano-science

**[Canada]**
University of Calgary, Department of Chemistry

**[China, P.R.]**
Chinese Academy of Sciences, Tianjin Institute of Industrial Biotechnology

Fudan University, School of Computer Science

Fudan University, Shanghai Key Lab of Intelligent Information Processing

Hunan University, College of Chemistry and Chemical Engineering

Normal University, Shenyang, College of Chemistry and Life Science

Peking University, College of Life Science

Shanghai Jiao Tong University, State Key Laboratory of Metal Matrix Composites

Sichuan University, Analytical and Testing Center

The University of Hong Kong, Department of Mathematics

University of Science and Technology of China, Department of Chemistry

University of Science and Technology of China, Department of Modern Mechanics, CAS Key Laboratory of Mechanical Behavior and Design of Materials

**[Croatia]**
Ruđer Bošković Institute, Division of Organic Chemistry and Biochemistry

**[Czech R.]**
Academy of Sciences of the Czech Republic, Institute of Organic Chemistry and Biochemistry

**[Estonia]**
National Institute of Chemical Physics and Biophysics

**[France]**
IFREMER, Centre de Brest

Mines ParisTech, Centre for Computational Biology

Pasteur Institute, Bioinformatique Structurale

Université de Rennes, Sciences Chimiques de Rennes

University of Strasbourg, Institute of Genetics and Molecular and Cellular Biology (IGBMC)

University of Toulouse, Laboratoire d'Etude en Géophysique et Océanographie Spatiales

**[Germany]**
Friedrich-Alexander-Universität, Interdisciplinary Center for Molecular Materials

Max Planck-Institute for Chemistry, Department of Geochemistry

University of Konstanz, Department of Computer and Information Science

**[Greece]**
FORTH, Institute of Electronic Structure & Laser

**[Israel]**
Ben-Gurion University of the Negev, Department of Computer Science

University of Haifa, Department of Biology & Environment

**[Italy]**
Università "Federico II", Dipartimento di Ingegneria Chimica

**[Korea, R.]**
Konkuk University, Konkuk University-Fraunhofer ISE Next Generation Solar Cell Research Center (KFnSC)

Pusan National University, Department of Chemistry, and Chemistry Institute for Functional Materials

**[New Zealand]**
University of Otago, Department of Chemistry

**[Sweden]**
Stockholm University, Department of Biochemistry and Biophysics

**[Taiwan]**
Academia Sinica, Research Center for Applied Sciences

National Cheng Kung University, Department of Chemical Engineering

National Sun Yat-Sen University, Department of Materials Science and Opto-electronic Engineering

National Tsing-Hua University, Department of Physics and Institute of Nanoengineering and Microsystems

**[U.K.]**
Imperial College London, Department of Earth Science and Engineering

Newcastle University, School of Chemistry

Southampton University, School of Chemistry

The University of Edinburgh, Centre for Science at Extreme Conditions (CSEC) and School of Chemistry

University of Bristol, School of Earth Sciences

University of Cambridge, Cavendish Laboratory

University of Oxford, Department of Materials

**[U.S.A.]**
Baylor College of Medicine, Verna and Marrs McLean Department of Biochemistry and Molecular Biology

Bermuda Institute of Ocean Sciences

Brown University, Department of Chemistry

California Institute of Technology, Division of Geological and Planetary Sciences

Columbia University, Department of Chemistry

Indiana University-Purdue University Indianapolis (IUPUI), Department of Chemistry & Chemical Biology

Marine Biological Laboratory, Bay Paul Center for Comparative Molecular Biology and Evolution

Massachusetts Institute of Technology, Earth, Atmospheric and Planetary Sciences

Temple University, Department of Chemistry

University of California, Institute for Marine Science

University of Hawaii, School of Ocean and Earth Science and Technology

University of Miami, Department of Chemistry

University of Pennsylvania, Department of Materials Science and Engineering and Laboratory for Research on the Structure of Matter

University of South Carolina, Department of Earth and Ocean Sciences

Woods Hole Oceanographic Institution, Department of Marine Chemistry and Geochemistry

Yale University, Department of Molecular, Cellular and Developmental Biology

*The list shows the institutions with which papers are co-authored.

# SELECTED GRANTS

## DIVISION OF SYNTHETIC CHEMISTRY

### — Organoelement Chemistry —

Tokitoh, N.
Creation of Novel Catalysts Centered on the Coordination Diversity of Heavy Typical Elements
Grants-in-Aid for Scientific Research on Innovative Area "Stimuli-responsive Chemical Species for the Creation of Functional Molecules"
28 June 2012–31 March 2017

Tokitoh, N.
Development of Pt–Silylyne Complexes and Their Application to Synergetic and Tandem Activation of Small Molecules
Grants-in-Aid for Challenging Exploratory Research
1 April 2012–31 March 2014

Tokitoh, N.
Construction of Polycyclic Aromatic Compounds Containing Heavier Group 14 Elements and Development of Their Functions by Utilizing the Features of Main Group Elements
Grants-in-Aid for Scientific Research (B)
1 April 2010–31 March 2013

Sasamori, T.
Construction of Novel d-π Conjugated Systems Containing Heavier Main Group Elements and Their Functions
Grants-in-Aid for Young Scientists (A)
1 April 2011–31 March 2014

Mizuhata, Y.
Construction of Novel Silicon–Silicon Double-Bond Compounds Bearing Alkynyl Substituents
Grants-in-Aid for Young Scientists (B)
1 April 2009–31 March 2012

Mizuhata, Y.
Synthesis of Phthalocyanine Derivatives Bearing Phosphorus Atoms as Skeletal Elements and Their Properties
Grants-in-Aid for Scientific Research on Innovative Area "π-Space"
1 April 2011–31 March 2013

Agou, T.
Bottom-up Syntheses of Electron-Deficient Aluminum Clusters and Elucidation of Their Properties
Grants-in-Aid for Scientific Research (C)
1 April 2012–31 March 2015

Kawashima, T.; Kobayashi, J.; Agou, T.
Development of Dimensionally Extended Hetero-π-conjugated Molecules
Grants-in-Aid for Scientific Research (B)
1 April 2009–31 March 2012

### — Structural Organic Chemistry —

Murata, Y.
Synthesis of Tailor-made Nanocarbons and Their Application to Electronic Devices
Grants-in-Aid for Scientific Research (A)
1 April 2011–31 March 2016

Murata, Y.
Molecular Interface Science of π-Conjugated Carbon Complexes on Non-Equilibrated States
PRESTO (Precursory Research for Embryonic Science and Technology), Japan Science and Technology Agency
1 October 2012–31 March 2016

Murata, Y.
Creation and Function of Spherical π-Space Encapsulating an Active Small Molecule
Grants-in-Aid for Scientific Research on Innovative Areas "π-Space"
1 December 2008–31 March 2013

Wakamiya, A.; Murata, Y.
Development of Dye-sesitized Solor Cells Using Organic Dyes Derived from Natural Products
ALCA (Advanced Low Carbon Technology Research and Development Program), Japan Science and Technology Agency
1 October 2011–31 March 2017

Wakamiya, A.
Development of Organic Dyes Based on Fine Tuning of π-Orbitals Using DFT Calculations
PRESTO (Precursory Research for Embryonic Science and Technology), Japan Science and Technology Agency
1 October 2010–31 March 2016

Murata, M.
Synthesis of Electron-Accepting π-Systems Containing Fulvalene as a Key Structural Unit
Grant-in-Aid for Scientific Research (B)
1 April 2012–31 March 2015

### — Synthetic Organic Chemistry —

Kawabata, T.
Fine Organic Synthesis Based on Catalytic Regioselective Functionalization
Grants-in-Aid for Scientific Research (A)
1 April 2009–31 March 2013

Kawabata, T.
Regioselective Molecular Transformation Based on Organocatalytic Molecular Recognition
Grants-in-Aid for Scientific Research on Innovative Area
1 October 2011–31 March 2015

Furuta, T.
Development of Regio- and Stereoselective Reactions of Polyfunctionalized Molecules by Axially Chiral Catalysts
Grants-in-Aid for Scientific Research (C)
28 April 2011–31 March 2014

Yoshimura, T.
Synthesis of Novel Amino Acids and Natural Products Derived from Amino Acids via Memory of Chirality
Grant-in-Aid for Young Scientists (B)
28 April 2011–31 March 2013

## — Advanced Inorganic Synthesis —

Teranishi, T.
Development of Structure-Specific Energy-Related Functional Materials Using Heterostructured Nanoparticles
Grants-in-Aid for Scientific Research (A)
1 April 2011–31 March 2014

Teranishi, T.
Study on Correlation between Structure and Hydrogen Storing Properties of Palladium Nanoparticles
Grants-in-Aid for Challenging Exploratory Research
1 April 2012–31 March 2014

Teranishi, T.
Synthesis of Macrocyclic π-Conjugated Ligand-Protected Gold Clusters and Fabrication of Nano-Gap Single Electron Devices
CREST (Core Research for Evolutional Science and Technology), Japan Science and Technology Agency
1 October 2008–31 March 2014

Teranishi, T.
Establishment of Deeply Penetrating Photoacoustic Imaging Technology Based on Fucntional Probes: Design and Synthesis of Activatable Probes and Development of in Vivo Imaging Technology
Industry-Academia Collaborative R&D Programs, Japan Science and Technology Agency
1 December 2011–31 March 2017

Teranishi, T.
Synthesis of Magnetic Nanoparticles for Creating Novel Nanocomposite Magnetic Materials
Elements Strategy Intiative, Ministry of Education, Culture, Sports, Science and Technology
1 July 2012–31 March 2022

Teranishi, T.
Research on Nanoscale Phase-Controlled Nanocomposite Magnets
Mirai Kaitaku Jitsugen Project, METI
1 October 2012–31 March 2022

Sakamoto, M.
Fabrication of Nanocrystal Superstructure toward Novel Artificial Photosynthesis
PREST (Precursory Research for Embryonic Science and Technology), Japan Science and Technology Agency
1 April 2012–31 March 2015

Sakamoto, M.
Research for the Photochemical Functions of Porphyrin Face-coordinated Metal Nanoparticles
Grants-in-Aid for Young Scientists (B)
1 April 2011–31 March 2013

# DIVISION OF MATERIALS CHEMISTRY

## — Chemistry of Polymer Materials —

Tsujii, Y.
Development of Novel Nanosystem by Hierarchically Assembling Concentrated Polymer Brushes
CREST (Core Research for Evolutional Science and Technology), Japan Science and Technology Agency
1 October 2009–31 March 2015

Tsujii, Y.
Super Lubrication of Novel Nano-Brushes
Advanced Environmental Materials of Green Network of Excellence (GRENE) Program, Ministry of Education, Culture, Sports, Science and Technology
6 December 2011–31 March 2016

Tsujii, Y.
Development of High-Performance Li-ion Batteries Using High-capacity, Low-cost Oxide Electrodes
Industrial Technology Research Grant Program, NEDO
1 October 2012–31 March 2017

Ohno, K.
Development of Next-Generation MRI Contrast Agent
Industrial Technology Research Grant Program, NEDO
1 July 2009–30 June 2013

Ohno, K.
Pharmacokinetics of Well-Defined Polymer Brush-Afforded Fine Particles
Grants-in-Aid for Young Scientists (A)
1 April 2011–31 March 2014

Ohno, K.
Development of Molecular Targeted MRI Contrast Agent
A-STEP (Adaptable and Seamless Technology Transfer Program through Target-Driven R&D), Japan Society and Technology Agency
1 October 2012–30 September 2015

Sakakibara, K.
Construction of Photoresponsive Cellulosic Nanostructures via Polysaccharide-Based Hierarchic Assembly
Grants-in-Aid for Young Scientist (B)
1 April 2012–31 March 2014

## — Polymer Controlled Synthesis —

Yamago, S.
Creation of Hoop-shaped π-Conjugated Molecules through the Supramolecular Chemical Approach and Elucidation of Their Properties
CREST (Core Research for Evolutional Science and Technology), Japan Science and Technology Agency
1 October 2010–31 March 2016

## — Inorganic Photonics Materials —

Yoko, T.
Organic-inorganic Material for Biosensor Application
Grants-in-Aid for Challenging Exploratory Research
1 April 2011–31 March 2014

Tokuda, Y.
Self-organization Synthesis of Nano-tube for Biosensor Application
Grant for Basic Science Research Projects, Sumitomo Foundation
1 November 2011–31 March 2013

Masai, H.
Fabrication of Amorphous Glass Phosphor Containing $ns^2$-Type Emission Center
Research Institute for Production Development
1 August 2012–31 August 2013

### — Nanospintronics —

Ono, T.
Development of Novel Spin Dynamics Devices
Grants-in-Aid for Scientific Research (S)
1 April 2011–31 March 2016

Chiba, D.
Nanosystem and Function Emergence
PRESTO (Precursory Research for Embryonic Science and Technology), Japan Science and Technology Agency
1 October 2010–31 March 2014

## DIVISION OF BIOCHEMISTRY
### — Biofunctional Design-Chemistry —

Futaki, S.
Novel Methods for Delivering Nucleic Acids Therapeutics
Strategic Japanese-Swedish Cooperative Programme on "Multidisciplinary BIO", Japan Science and Technology Agency
1 July 2009–30 June 2012

Imanishi, M.
Construction of Rhythmic Gene Expression Systems Based on the Cellular Clock
Grants-in-Aid for Scientific Research on Innovative Areas
1 April 2012–31 March 2014

Nakase, I.
Development of Mitochondria-Targeted Cell-Penetrating Peptides and Delivery of Bioactive Molecules
Grants-in-Aid for Young Scientists (B)
1 April 2011–31 March 2013

### — Chemistry of Molecular Biocatalysts —

Hiratake, J.
Applications of Cellular Collagen Biosynthesis Induced by Novel γ-Glutamyl Transpeptidase (GGT) Inhibitors
A-STEP (Adaptable and Seamless Technology Transfer Program through Target-Driven R & D), Japan Society and Technology Agency
1 December 2009–31 March 2012

Hiratake, J.
Drug Development Based on Asparagine Synthetase Inhibitors
Grants-in-Aid for Scientific Research (C)
1 April 2011–31 March 2014

Koeduka, T.
Biochemical Characterization of Reductase Responsible for the Diversity of Floral Scent in Petunia
Grants-in-Aid for Scientific Research (C)
1 April 2012–31 March 2015

### — Molecular Biology —

Aoyama, T.
Regulatory Mechanisms for Functional Morphologies of Plants
Bilateral Program for Joint Research between JSPS and NSFC
1 April 2012–31 March 2015

Aoyama, T.
Growth Strategy of Plants through Morphological Changes of Roots
Grants-in-Aid for Scientific Research on Innovative Area
1 April 2011–31 March 2013

Tsuge, T.
Regulatory Mechanism of Plant Morphogenesis by the Regulator of mRNA Metabolism SAP130
Grants-in-Aid for Scientific Research (C)
1 April 2010–31 March 2013

Tsuge, T.
Regulatory Mechanism of Environmental Stimuli Response that Integrates mRNA Metabolism and Protein Degradation in the Cell
Grants-in-Aid for Scientific Research on Innovative Area
1 April 2011–31 March 2013

## DIVISION OF ENVIRONMENTAL CHEMISTRY
### — Molecular Materials Chemistry —

Kaji, H.
Fabrication of High-Performance Polymer EL Devices Having Covalently-Bonded Interfaces
Grants-in-Aid for Scientific Research (A)
1 April 2009–31 March 2012

Goto, A.
Dual Control Living Polymerizations with Organic Catalysts
Grants-in-Aid for Young Scientists (A)
1 April 2011–31 March 2014

Goto, A.
High Performance Color Material by Living Radical Polymerization with Organic Catalysts
A-STEP (Adaptable and Seamless Technology Transfer Program through Target-Driven R&D), Japan Society and Technology Agency
1 November 2011–31 March 2015

### — Hydrospheric Environment Analytical Chemistry —

Sohrin, Y.
Ocean Section Study in the Pacific Ocean, Indian Ocean and Japan Sea Using Multielemental Analysis of Trace Metals
Grants-in-Aid for Scientific Research (A)
1 April 2012–31 March 2015

Sohrin, Y.
Development of a New Automated System for Preconcentration of Heavy Metals to Assess the Influence of Biology and Its Application to Oceanographic Study
Steel Foundation for Environmental Protection Technology
1 November 2011–31 October 2013

Murayama, M. (Investigator: Sohrin, Y.)
Reconstruction of Redox Conditions in Meedee Lake, Mediterranean, Sediment Core Using Molybdenum/Tungsten Ration
Grants-in-Aid for Scientific Research (C)
1 April 2010–31 March 2013

**— Solution and Interface Chemistry —**

Hasegawa, T.
Structural Analysis and Control of an Organic Thin Film of Solar Cell Using MAIR Spectroscopy
Grant for Basic Science Research Projects, Sumitomo Foundation
1 November 2012–30 November 2013

Hasegawa, T.
Operando Analysis of Concentration and Diffusion of Negatively-Adsorptive Chemical Species in A Monolayer Formed at an Air/Water Interface
Grants-in-Aid for Scientific Research on Innovative Areas “Molecular Sciences of Soft Interface”
1 April 2011–31 March 2013

Matubayasi, N.
Free-Energy Analysis of ATP hydrolysis
Grants-in-Aid for Scientific Research on Innovative Areas “Hydration and ATP Energy”
1 December 2008–31 March 2013

**— Molecular Microbial Science —**

Kurihara, T.
Functional Analysis and Application of Phospholipids Containing Polyunsaturated Fatty Acids in Bacterial Cell Membrane
Grants-in-Aid for Scientific Research (B)
1 April 2012–31 March 2015

Kurihara, T.
Exploration of Cold-Adapted Microorganisms for Development of New Low-Temperature Biotechnological Processes
Grants-in-Aid for Scientific Research (B)
1 April 2010–31 March 2013

Kurihara, T.
Development of Biocatalysts for Remediation of Environments Polluted with Persistent Organohalogen Compounds
Grants-in-Aid for Challenging Exploratory Research
1 April 2012–31 March 2014

Kawamoto, J.
Exploration of Functional Metal-Nanoparticle-Producing Bacteria from Extreme Environments
Grants-in-Aid for Scientific Research (B)
1 April 2012–31 March 2015

Kawamoto, J.
Synthesis of Functional Metal Nanoparticles by Using Metal-Metabolizing Bacteria
Grants-in-Aid for Challenging Exploratory Research
1 April 2011–31 March 2013

## DIVISION OF MULTIDISCIPLINARY CHEMISTRY

**— Polymer Materials Science —**

Kanaya, T.
Non-equilibrium Intermediate States and Polymer Crystallization–Towards Establishment of Basis for Industrial Application
Grants-in-Aid for Scientific Research (A)
1 April 2012–31 March 2017

Nishida, K.
Property Control of Water-soluble Cellulose Derivatives
Grants-in-Aid for Scientific Research (C)
1 April 2011–31 March 2014

**— Molecular Rheology —**

Watanabe, H.
Nonlinear Feedback between Phase Growth and Chain Dynamics in Polymer Blends
Grants-in-Aid for Scientific Research (A)
1 April 2012–31 March 2015

Masubuchi, Y.
Relaxation of Polymer Chain under Flow
Grants-in-Aid for Scientific Research (B)
1 April 2011–31 March 2014

Matsumiya, Y.
Molecular Interpretation of Cooperative Length of Polymer Segment
Grants-in-Aid for Scientific Research (C)
1 April 2012–31 March 2015

**— Molecular Aggregation Analysis —**

Yoshida, H.
Inverse-Photoemission Spectroscopy with Zero Kinetic Energy Electrons for Measuring the Unoccupied Electronic States of Organic Semiconductors
PRESTO (Precursory Research for Embryonic Science and Technology), Japan Science and Technology Agency
1 October 2009–31 March 2013

## ADVANCED RESEARCH CENTER FOR BEAM SCIENCE

**— Laser Matter Interaction Science —**

Sakabe, S.
Demonstration of Ultra-fast Electron Diffraction Using Fast Electrons Accelerated in Plasmas by an Intense Femtosecond Laser
Grants-in-Aid for Scientific Research (S)
1 April 2011–31 March 2016

Sakabe, S.
High Energy Electron Gun of a Fine Wire Driven by an Intense Femtosecond Laser
Grants-in-Aid for Challenging Exploratory Research
1 April 2010–31 March 2012

Sakabe, S.
Development of Single-shot Ultrafast Electron Diffraction Using Femtosecond Electron Pulses Generated by an Ultra Intense Short Pulse Laser
The Mitsubishi Foundation
1 October 2012–30 September 2013

Sakabe, S.
Demonstration of Ultra-fast Electron Diffraction Using Fast Plasma Electrons Produced by an Intense Femtosecond Laser
Yamada Science Foundation
1 April 2010–31 March 2012

Hashida, M.
Amorphous Metal Thin Film with the Surface of Periodic Nano-Structures Self-Formed by Femtosecond Laser Pulses
Grants-in-Aid for Scientific Research (C)
1 April 2010–31 March 2013

Tokita, S.
Ultrafast Observation of Relativistic Laser-plasma Interactions Using Femtosecond Electron Beams
Grants-in-Aid for Scientific Research (C)
1 April 2012–31 March 2015

Tokita, S.
Development of Short-pulse Intense Laser Technology in Mid-Infrared Fluoride Fiber Lasers
Grants-in-Aid for Young Scientists (B)
1 April 2010–31 March 2012

### — Electron Microscopy and Crystal Chemistry —

Kurata, H.
Advanced Characterization Nanotechnology Platform at Kyoto University
Nanotechnology Platform Project, Ministry of Education, Culture, Sports, Science and Technology
2 July 2012–31 March 2022

## INTERNATIONAL RESEARCH CENTER FOR ELEMENTS SCIENCE

### — Organic Main Group Chemistry —

Nakamura, M.
Development of Selective Organic Synthesis Based on Iron Catalysis
Funding Program for Next Generation World-Leading Researchers (NEXT Program)
1 March 2011–31 March 2014

Takaya, H.
A Comprehensive Research on Iron- and Nickel-Catalyzed Organic Reactions: Development of New Catalyst, New Reactions, New Spectroscopic Methods
CREST (Core Research for Evolutional Science and Technology), Japan Science and Technology Agency
1 April 2011–31 March 2016

Takaya, H.
New Catalyst toward Biorefinery of Lignins Based on Metal-Conjugate Amino Acids and Peptides
CREST (Core Research for Evolutional Science and Technology), Japan Science and Technology Agency
1 April 2011–31 March 2016

Hatakeyama, T.
Synthesis of Helical π-Conjugated Molecules toward Next Generation Semiconductors
PRESTO (Precursory Research for Embryonic Science and Technology), Japan Science and Technology Agency
1 October 2011–31 March 2015

Hatakeyama, T.
Synthesis of Heterographene Derivatives by Tandem Hetero-Friedel-Crafts Reactions
Grants-in-Aid for Young Scientists (A)
1 April 2011–31 March 2014

### — Advanced Solid State Chemistry —

Shimakawa, Y.
Exploring for New Functional Materials with Unusual Ionic States and Coordinations
Creation of Innovative Functions of Intelligent Materials on the Basis of the Element Strategy
1 April 2011–31 March 2016

### — Organotransition Metal Chemistry —

Ozawa, F.
Synthesis and Catalytic Properties of Stimulus-responsible Transition Metal Complexes Bearing Low-coordinate Phosphorus Ligands
Grants-in-Aid for Scientific Research on Innovative Areas “Stimuli-responsive Chemical Species for the Creation of Functional Molecules”
1 April 2012–31 March 2017

Ozawa, F.
Development of Highly Efficient Catalysts for the Synthesis of π-Conjugated Polymers via Direct Arylation
ACT-C (Advanced Catalytic Transformation Program for Carbon Utilization), Japan Science and Technology Agency
1 October 2012–31 March 2018

Wakioka, M.
Development of Living Polymerization Based on Direct Arylation
Grants-in-Aid for Young Scientists (B)
1 April 2012–31 March 2015

### — Photonic Elements Science —

Kanemitsu, Y.
Microscopic Spectroscopy of Highly Excited State in Semiconductor Nanostructures and Exploring Novel Optical Functionality
Grants-in-Aid for Scientific Research on Innovative Areas “Optical Science of Dynamically Correlated Electrons”
13 November 2008–31 March 2013

Kanemitsu, Y.
Evaluation of Nonradiative Carrier Recombination Loss in Concentrator Heterostructure Solar Cells
CREST (Core Research for Evolutional Science and Technology), Japan Science and Technology Agency
1 October 2011–31 March 2017

Tayagaki, T.
Controlling of the Many-body Interaction between Photoexcited Carriers toward Hot Carrier Solar Cells
PRESTO (Precursory Research for Embryonic Science and Technology), Japan Science and Technology Agency
1 October 2009–31 March 2013

## BIOINFORMATICS CENTER

### — Chemical Life Science —

Goto, S.
Key Technology Development for Data Integration and Application to Emerging Fileds
Life Science Database Integration Project, Japan Science and Technology Agency
1 April 2011–31 March 2014

Kanehisa, M.
Genome-based Integrated Resource of Diseases, Drugs, and Environmental Substances
Life Science Database Integration Project, Japan Science and Technology Agency
1 April 2011–31 March 2014

### — Mathematical Bioinformatics —

Akutsu, T.; Kawabata, T.; Nagamochi, H.; Hayashida, M.
An Approach to Novel Structural Design by Combining Discrete Methods and Kernel Methods
Grants-in-Aid for Scientific Research (A)
1 April 2010–31 March 2015

Akutsu, T.
Discrete Model-Based Methods for Control of Complex Biological Systems
Grants-in-Aid for Challenging Exploratory Research
1 April 2010–31 March 2013

### — Bio-knowledge Engineering —

Mamitsuka, H.
Estimating Data Structures from Various Semi-Structured Data
Grants-in-Aid for Scientific Research (B)
1 April 2012–31 March 2015

Natsume, Y.
In Silico Analysis of Histone Modification Dynamics that Regulate Developmental Processes
PRESTO (Precursory Research for Embryonic Science and Technology), Japan Science and Technology Agency
1 October 2010–31 March 2015

## ENDOWED RESEARCH SECTION

### — Nano-Interface Photonics (SEI Group CSR Foundation) —

Yamada, Y.
Study of Photovoltaic Effects and Photocarrier Recombination Dynamics Driven by Spontaneous Polarization in Ferroelectric Semiconductors
Grants-in-Aid for Young Scientists (B)
1 April 2012–31 March 2014

# THESES

ASAKAWA, Harutoshi
D Eng, Kyoto University
"Formation of Giant Single Crystals of Isotactic Propylene via Mesophase"
Supervisor: Prof KANAYA, Toshiji
26 March 2012

AZUMA, Yusuke
D Pharm Sc, Kyoto University
"Introducing a Metal-switchable Function into Proteins Using Terdentate Ligands"
Supervisor: Prof FUTAKI, Shiroh
26 March 2012

CID, Abigail Parcasio
D Sc, Kyoto University
"Stoichiometry among Bioactive Trace Metals in the Bering Sea and the Arctic Ocean"
Supervisor: Prof SOHRIN, Yoshiki
26 March 2012

DAI, Xianzhu
D Agr, Kyoto University
"Studies on the Folding of an Outer Membrane Protein from a Psychrotrophic Bacterium, *Shewanella livingstonensis* Ac10"
Supervisor: Prof KURIHARA, Tatsuo
26 March 2012

duVERLE, David
D Pharm Sc, Kyoto University
"Building a Machine-Learning Framework for Protein Interactions: Calpain Cleavage Prediction and Gene Regulatory Network Inference"
Supervisor: Prof MAMITSUKA, Hiroshi
26 March 2012

HASHIMOTO, Toru
D Eng, Kyoto University
"Development of Iron-Catalyzed Suzuki-Miyaura Coupling Reaction"
Supervisor: Prof NAKAMURA, Masaharu
26 June 2012

HIROSE, Hisaaki
D Pharm Sc, Kyoto University
"Study on the Efficient Internalization Pathways of Arginine-rich Cell-penetrating Peptides"
Supervisor: Prof FUTAKI, Shiroh
26 March 2012

IKEUCHI, Hideyuki
D Agr, Kyoto University
"Studies on Human Asparagine Synthetase Inhibitors"
Supervisor: Prof HIRATAKE, Jun
23 May 2012

JAHANGIRI, Fazel
D Sc, Kyoto University
"Terahertz Emission from Gas and Atomic Cluster Plasmas Induced by Intense Femtosecond Laser Pulses"
Supervisor: Prof SAKABE, Shuji
26 March 2012

JITSUMORI, Keiji
D Agr, Kyoto University
"Studies on Dehalogenase that Catalyzes Defluorination of Fluoroacetate and Related Enzyme"
Supervisor: Prof KURIHARA, Tatsuo
26 March 2012

KOYAMA, Tomohiro
D Sc, Kyoto University
"Investigation of Current-induced Magnetic Domain Wall Motion in Ferromagnetic Nano-wire"
Supervisor: Prof ONO, Teruo
23 March 2012

MISHIMA, Eri
D Eng, Kyoto University
"Organoheteroatom-Mediated Living Vinyl Polymerization under Acidic Condition"
Supervisor: Prof YAMAGO, Shigeru
26 March 2012

NAKANO, Kunihiro
D Sc, Kyoto University
"Investigation of Current-driven Vortex Oscillations in Ferromagnetic Disks"
Supervisor: Prof ONO, Teruo
23 March 2012

NOSHIRO, Daisuke
D Pharm Sc, Kyoto University
"Creation of Channel Peptides whose Assemblies are Controllable by External Stimuli"
Supervisor: Prof FUTAKI, Shiroh
26 March 2012

OGATA, Kazuki
D Eng, Kyoto University
"Syntheses and Functions of Metalated Amino Acids and Peptides"
Supervisor: Prof NAKAMURA, Masaharu
19 March 2012

PARK, Jungha
D Agr, Kyoto University
"Studies of Cold-Inducible Inner Membrane Proteins of a Psychrotrophic Bacterium, *Shewanella livingstonensis* Ac10"
Supervisor: Prof KURIHARA, Tatsuo
26 March 2012

SATO, Sho
D Agr, Kyoto University
"Chemical Studies on Physiological Roles of Eicosapentaenoic Acid in Bacterial Membrane"
Supervisor: Prof KURIHARA, Tatsuo
26 March 2012

SATO, Takahiro
D Sc, Kyoto University
"Studies on Disilenes Bearing Alkynyl Groups and Unusual Reactivity of Overcrowded Silylene with Pyridines"
Supervisor: Prof TOKITOH, Norihiro
26 March 2012

SUGAMATA, Koh
D Sc, Kyoto University
"Studies on the Synthesis and Properties of Low-coordinated Chalcogen(II) Cations"
Supervisor: Prof TOKITOH, Norihiro
26 March 2012

TANAKA, Hidenori
D Eng, Kyoto University
"Conformational Characteristics of Radiation-Modified Polysilanes in Their Self-Assemblies"
Supervisor: Prof KANAYA, Toshiji
26 March 2012

TOMOHARA, Keisuke
D Pharm Sc, Kyoto University
"New Aspects in Chemistry of Axially Chiral Enolates: Development of Asymmetric Reactions via C–O Axially Chiral Enolates and $\alpha$-arylation of Amino Acid Derivatives"
Supervisor: Prof KAWABATA, Takeo
26 March 2012

VASUDEVAN, Anoop
D Agr, Kyoto University
"Studies on the Metabolism of 2-Chloroacrylate in *Burkholderia* sp. WS"
Supervisor: Prof KURIHARA, Tatsuo
26 March 2012

YAMAMOTO, Junya
D Pharm Sc, Kyoto University
"Synthesis of Novel Axially Chiral Amino Acids and Their Application to Organocatalytic Reaction"
Supervisor: Prof KAWABATA, Takeo
26 March 2012

YU, Hao-Hsin
D Pharm Sc, Kyoto University
"Development of Novel Systems Promoting Intracellular Protein Delivery"
Supervisor: Prof FUTAKI, Shiroh
26 March 2012

# THE 112TH ICR ANNUAL SYMPOSIUM

# SEMINARS

# MEETINGS AND SYMPOSIA

# THE 112TH ICR ANNUAL SYMPOSIUM

(7 December 2012)

## ORAL PRESENTATION

FUJII, Tomomi et al. (Structural Molecular Biology)
"Structural Insights into Action of Enzymes for Resorcinol Catabolism"

TSUGE, Tomohiko (Molecular Biology)
"Molecular Mechanisms Regulating Gene Expression Involved in Morphogenesis"

SAKAMOTO, Masanori et al. (Advanced Inorganic Synthesis)
"Platonic Hexahedron Composed of Six Organic Faces with an Inscribed Au Cluster"

KAYAHARA, Eiichi et al. (Polymer Controlled Synthesis)
"Synthesis of Cycloparaphenylene (CPP) Analog and Highly Strained CPP by Using Cyclic Platinum Complexes"

GOTO, Atsushi et al. (Molecular Materials Chemistry)
"A New Family of Controlled Radical Polymerization with Organic Catalysts"

HASEGAWA, Takeshi (Solution and Interface Chemistry)
"Analysis of Correlation between Molecular Assembled Structure and Hydration in a Langmuir-adsorbed Monolayer at the Air/water Interface"

SHIMIZU, Masahiro et al. (Laser Matter Interaction Science)
"Self-organization of Nanostructure on Metal Surface under Femtosecond Laser Pulse Irradiation"

–ICR Award for Young Scientists–
CHIBA, Daichi (Nanospintronics)
"Electrical Control of the Ferromagnetic Phase Transition in Cobalt at Room Temperature"

– ICR Award for Young Scientists (Foreign Researchers' Category) –
CHEN, Wei-tin (Advanced Solid State Chemistry)
"Ligand-hole Localization in Oxides with Unusual Valence Fe"

−ICR Award for Graduate Students−
ITO, Yuki (Solution and Interface Chemistry)
"Polarization Dependence of Raman Scattering from a Thin Film Involving Optical Anisotropy Theorized for Molecular Orientation Analysis"

−ICR Award for Graduate Students−
INOUE, Shunsuke (Laser Matter Interaction Science)
"Femtosecond Electron Deflectometry for Measuring Transient Fields Generated by Laser-accelerated Fast Electrons"

## POSTER PRESENTATIONS

LW : Laboratory Whole Presentation
LT : Laboratory Topic
GE : General Presentation

### — Organoelement Chemistry —

LW "Studies on the Synthesis and Properties of Novel Organic Compounds Containing Heavier Elements"

GE MIYAMOTO, Hisashi; SASAMORI, Takahiro; TOKITOH, Norihiro
"Generation of a Novel Ferrocenophane Bridged by a Ge=Ge Unit"

### — Structural Organic Chemistry —

LW "Research Activities in Structural Organic Chemistry Laboratory"

GE SHIMOGAWA, Hiroyuki; WAKAMIYA, Atsushi; MURATA, Yasujiro
"Synthesis and Properties of Thieno-fused BODIPY Derivatives"

GE YOSHIKAWA, Osamu; WAKAMIYA, Atsushi; MURATA, Yasujiro
"Chromic Properties of Boryl-substituted Dithienylbenzothiadiazole Derivatives"

### — Synthetic Organic Chemistry —

LW "Asymmetric Synthesis via Enolates with Dynamic Chirality"

LW "Regioselective Molecular Transformation by Organo Catalysis"

### — Advanced Inorganic Synthesis —

LW "Research Activities in Advanced Inorganic Synthesis"

GE YOSHINAGA, Taizo; FRUBE, Akihiro; KANEHARA, Masayuki; TERANISHI, Toshiharu
"Evaluation of the Electric Field Enhancement Factor in Plasmonic Indium Tin Oxide Nanoparticle Film by Femtosecond Transient Absorption in the Near IR Region"

GE TANAKA, Daisuke; SAKAMOTO, Masanori; TERANISHI, Toshiharu
"Interfacial Interaction between Au Cluster and Porphyrin in Porphyrin Face-coordinated Au Cluster"

GE SATO, Ryota; ITO, Shin-ichi; TOMISHIGE, Keiichi; TERANISHI, Toshiharu
"Designed Synthesis of Monodisperse Metal/Pt Core/Shell Nanoparticles with Precisely-Tuned Pt Atomic Layers and Their CO Adsorption Properties"

GE Wu, Hsin-Lun; EGUCHI, Miharu; MITSUI, Daisuke; TERANISHI, Toshiharu
"Seed-Mediated Synthesis of Rhombic Dodecahedral Au Nanocrystals and Their 3D-FDTD Simulations"

### — Chemistry of Polymer Materials —

GE NAKANISHI, Yohei; KAWANO, Yuko; SAKAKIBARA, Keita; OHNO, Kohji; MORINAGA, Takashi; SATO, Takaya; TSUJII, Yoshinobu
"Fabrication of Novel Ionics-materials by Higher-order Structural Control of Ionic Liquid/polymer Composites"

GE HSU, Shu-Yao; AKIMOTO, Shuhei; OHNO, Kohji; TSUJII, Yoshinobu
"Tribology Properties of Concentrated Polymer Brushes with Extraordinarily Large Thicknesses"

### — Polymer Controlled Synthesis —

LW "Research Activity of Polymer Controlled Synthesis"

GE ARIMA, Takahiro; NAKAMURA, Yasuyuki; YAMAGO, Shigeru
"Synthesis of End- and Mid-chain Functionalized Polymers by a Combination of TERP and Radical Coupling Reaction"

GE IWAMOTO, Takahiro; KURACHI, Daisuke; KAYAHARA, Eiichi; YAMAGO, Shigeru
"Synthesis of [4]Cyclophenanthrene and [4]Cyclopyrene through Tetranuclear Platinum Complexes"

### — Inorganic Photonics Materials —

GE TANIMOTO, Toshiro; MASAI, Hirokazu; TOKUDA, Yomei; YOKO, Toshinobu
"Correlation between the Preparation Method and the Photoluminescent Property of SnO-ZnO-$P_2O_5$ Glasses"

GE OGAWA, Tadahiro; TOKUDA, Yomei; MASAI, Hirokazu; YOKO, Toshinobu
"Adsorption of Proteins on Organic-inorganic Hybrid Thin Films Prepared by Sol-gel Method"

### — Nanospintronics —

GE MATSUO, Sadashige
"Quantum Transport Effect in $Bi_2Se_3$ Thin Film"

GE UEDA, Kohei
"Current Induced Magnetic Domain Wall in Co/Ni Nanowires"

GE ARAKAWA, Tomonori
"Real-time Measurement of Quantum Transport by Single Electron Transistor"

### — Biofunctional Design-Chemistry —

LW "Research Activities in Biofunctional Design Chemistry Laboratory"

GE TANAKA, Gen; NAKASE, Ikuhiko; KAWAGUCHI, Yoshimasa; FUTAKI, Shiroh
"Importance of CXCR4 in Efficient Cellular Internalization of Cell-penetrating R12 Peptide"

### — Chemistry of Molecular Biocatalysts —

LW "Research Activities of Laboratory of Chemistry of Molecular Biocatalysts"

GE KIRIKAE, Hiroaki; KOEDUKA, Takao; WATANABE, Bunta; HIRATAKE, Jun
"Synthesis and Evaluation of 4-Coumarate:CoA Ligase Inhibitors"

### — Molecular Biology —

LW "Studies Promoted by the Laboratory of Molecular Biology"

### — Chemical Biology —

GE HIRATA, Nao; UESUGI, Motonari
"Fluorescent Chemical Probes for Human Stem Cells"

### — Molecular Materials Chemistry —

LW "Research Activities in Molecular Materials Chemistry Laboratory"

GE FUKUSHIMA, Tatsuya; FUJIMURA, Subaru; KAJI, Hironori
"Solid-state NMR Analysis of Donor/Acceptor Structures in Organic Solar Cells"

GE OHTSUKI, Akimichi; GOTO, Atsushi; KAJI, Hironori
"Photo-Induced Controlled Radical Polymerization with Organic Catalysts"

### — Hydrospheric Environment Analytical Chemistry —

GE TAKANO, Shotaro; SOHRIN, Yoshiki; HIRATA, Takafumi; TANIMIZU, Masaharu
"Development of a Simple Pretreatment Method Using NOBIAS CHELATE-PA1 Resin for Measurment of Copper Isotopic Composition in Seawater"

GE NORISUYE, Kazuhiro; YAMAMOTO, Jun; TAKANO, Shotaro; SOHRIN, Yoshiki
"The Distribution of Bismuth in the Western North Pacific"

### — Solution and Interface Chemistry —

GE SHIMOAKA, Takafumi; ITOH, Yuki; HASEGAWA, Takeshi
"Dynamic Rearrangement of Stearic Acid Molecules Adsorbed on a Gold Surface Induced by Ambient Water Molecules Studied by Infrared Spectroscopy"

### — Molecular Microbial Science —

LW "Research Activities of Molecular Microbial Science Laboratory"

GE SUGIURA, Miwa; KAWAMOTO, Jun; ESAKI, Nobuyoshi; KURIHARA, Tatsuo
"Control of the Production of Outer Membrane Proteins by Eicosapentaenoic Acid in a Psychrotrophic Bacterium, *Shewanella livingstonensis* Ac10"

**— Polymer Materials Science —**

LW "Research Topics in Polymer Material Science Laboratory"

GE JIN, Ling; DENG, Cong; POLEC, Inga; INOUE, Rintaro; NISHIDA, Koji; KANAYA, Toshiji
"Influence of Atactic Polystyrene on the Shear-induced Precursor in Isotactic Polystyrene"

GE HARA, Ayana; INOUE, Rintaro; NISHIDA, Koji; KANAYA, Toshiji
"The Observation of Multiple Structure Formed of Introduced Phase Separation of Epoxy"

GE SAKAI, Tatsuya; INOUE, Rintaro; NISHIDA, Koji; KANAYA, Toshiji
"Studies on Carbon Nanotube/poly(vinyl alcohol) Gel Composite by Light Scattering and Small Angle X-ray Scattering"

GE KATAYAMA, Yutaka; NISHIDA, Koji; INOUE, Rintaro; KANAYA, Toshiji
"Structure Formation of Methylcellulose Aqueous Solution in Sol Region"

**— Molecular Rheology —**

GE KAWASAKI, Yohji; WATANABE, Hiroshi; UMEKI, Yuka; NISHIKAWA, Makiya
"Viscoelastic Properties of DNA Hydrogel"

**— Molecular Aggregation Analysis —**

GE MURDEY, Richard; SATO, Naoki
"Growth Morphology and Photoconductivity of Lead Phthalocyanine Thin Films"

GE ASAMI, Koji
"Low-frequency Dielectric Dispersion of Lipophilic-ion-doped Biological Cells"

**— Interdisciplinary Chemistry for Innovation —**

LW "Research Activities of Interdisciplinary Chemistry for Innovation"

**— Particle Beam Science —**

GE NASU, Yuji; IKEDA, Hideki; KITAHARA, Ryunosuke; FUWA, Yasuhiro; TONGU, Hiromu; IWASHITA, Yoshihisa; ICHIKAWA, Masahiro
"Development of Very Small ECR $H^+$ Ion Source with Permanent Magnets"

GE FUWA, Yasuhiro; IKEDA, Hideki; KITAHARA, Ryunosuke; NASU, Yuji; TONGU, Hiromu; IWASHITA, Yoshihisa; MATSUMOTO, Toshihiro; MICHIZONO, Shinichiro; FUKUDA, Shigeki
"Klystron Beam Focusing Magnet Composed of Anisotropic Ferrite Magnets"

GE SOUDA, Hikaru; NAKAO, Masao; TONGU, Hiromu; NODA, Akira; JIMBO, Kouichi; OSAKI, Kazuya; OKAMOTO, Hiromi; YURI, Yosuke; HE, Zhengqi; GRIESER, Manfred; MADSEN, Niels
"Efficient Indirect Transverse Laser Cooling of Mg Ion Beam by Reducing Particle Numbers with Scraper"

GE IMAJO, Sohei; IWASHITA, Yoshihisa; SHIMIZU, Hirohiko M.; YOSHIOKA, Tamaki; KITAGUCHI, Masaaki; ARIMOTO, Yasushi; SEKI, Yoshichika; and NOP Collaboration
"The R&D of the UCN Accelerator for Neutron EDM Experiment at J-PARC"

**— Laser Matter Interaction Science —**

GE NAKAJIMA, Hiroaki; TOKITA, Shigeki; INOUE, Shunsuke; HASHIDA, Masaki; SAKABE, Shuji
"Long-distance Guidance of Fast Electrons along a Metal Wire Irradiated by an Intense Femtosecond Laser Pulse"

GE MIYASAKA, Yasuhiro; HASHIDA, Masaki; SHIMIZU, Masahiro; TOKITA, Shigeki; SAKABE, Shuji
"Mechanism of Femtosecond Laser Nano Ablation for Metals ~Nonthermal Ion Emission from Nano Structures on Surface~"

**— Electron Microscopy and Crystal Chemistry —**

LW "Research Activities in Laboratory of Electron Microscopy and Crystal Chemistry"

GE SAITO, Hikaru; KURATA, Hiroki
"Optical Property of Nanomaterial Using Angular Resolved EELS"

GE ASO, Ryotaro; KAN, Daisuke; SHIMAKAWA, Yuichi; KURATA, Hiroki
"Quantitative Strain Analysis of Epitaxial Perovskite Oxide Thin Films Using Cs-TEM and Cs-STEM"

**— Structural Molecular Biology —**

LW "Research Activities at Laboratory of Structural Molecular Biology"

**— Organic Main Group Chemistry —**

LW "Activities in Organic Main Group Chemistry"

GE HASHIMOTO, Sigma; OBA, Tsuyoshi; HATAKEYAMA, Takuji; NAKAMURA, Masaharu
"Synthesis and Physical Properties of BN-fused Helical $\pi$-Conjugated Molecules"

GE IMAYOSHI, Ryuji; YOSHIMOTO, Yuya; GHORAI, Sujit K.; HATAKEYAMA, Takuji; NAKAMURA, Masaharu
"Synthesis of Arylamines Based on Iron-Catalyzed Aromatic Amination"

GE YOKOI, Tomoya; ISOZAKI, Katsuhiro; OGATA, Kazuki; SASANO, Daisuke; SEIKE, Hirofumi; TAKAYA, Hikaru; NAKAMURA, Masaharu
"Synthesis and Functions of ONO-Pincer Ru-Complex-Bound Norvalines"

### — Advanced Solid State Chemistry —

LW “Introduction of Advanced Solid State Chemistry Laboratory”

GE MATSUMOTO, Kazuya; SHIMAKAWA, Yuichi
“Oxygen Incorporation into Infinite-layer Structure $AFeO_2$ (A=Sr, Ca)”

### — Organotransition Metal Chemistry —

LW “Activity Report: Organotransition Metal Chemistry Laboratory”

GE WAKIOKA, Masayuki; KITANO, Yutaro; TAKETANI, Tomoyoshi; NAKAMURA, Yuki; HIHARA, Yoshihiro; OZAWA, Fumiyuki
“A New Synthetic Route to π-Conjugated Polymers via Palladium-catalyzed Direct Arylation”

GE NAKAJIMA, Yumiko; LIN, Ya-Fan; MINAMI, Ataru
“Synthesis and Properties of 3d Metal Complexes Bearing a Low-coordinate Phosphorus Ligand”

### — Photonic Elements Science —

LW “Research Topics in Photonic Elements Science Group”

### — Chemical Life Science —

LW “Recent Update of GenomeNet Including Reaction Ontology”

GE MUTO, Ai; KOTERA, Masaaki; TOKIMATSU,Toshiaki; NAKAGAWA, Zenichi; GOTO, Susumu; KANEHISA, Minoru
“Metabolic Pathway Evolution from the Aspect of Chemical Reaction Modules Conserved in the Global Metabolic Network”

### — Mathematical Bioinformatics —

LW “Research Topics of Laboratory of Mathematical Bioinformatics”

### — Bio-knowledge Engineering —

GE HANCOCK, Timothy; MAMITSUKA, Hiroshi
“Multi-omic Metabolic Network Analysis”

### — Nano-Interface Photonics (SEI Group CSR Foundation) —

LW “Research Topics in Nano-interface Photonics Group”

### — Research Center for Low Temperature and Materials Sciences —

GE TERASHIMA, Takahito
“Properties of Heavy-fermion $Ce_{1-x}Yb_xCoIn_5$ System by MBE”

# SEMINARS

Dr AKAIKE, Kouki
Functional Soft Matter Research Group, RIKEN, Saitama, Japan
"Correlation between Characteristics of Organic Solar Cells and Their Interface Electronic Structures"
17 May 2012

Prof APELOIG, Yitzhak
Department of Chemistry, Technion, Israel Institute of Technology, Israel
"Novel Persistent and Stable Silyl Radicals and Radical Activation of SiH Bonds by Organozinc and Silylzinc Reagents"
16 October 2012

Dr BARUCH, Barzel
The Center for Complex Network Research at Northeastern University, the Dana Farber Cancer Center at Harvard Medical School Boston, Massachusetts, U.S.A.
"Scaling Theory of Network Dynamics: What Can Three Numbers Teach Us about a Complex System ?"
13 September 2012

Prof BORDEN, Weston Thatcher
Department of Chemistry, University of North Texas, U.S.A.
"Calculations on Tunneling by Carbon Tell Experimentalists Where to Look and What to Look for"
26 November 2012

Assist Prof CARVALHO, Luis
Mathematics and Computer Science Department, Boston University, U.S.A.
"Graph-regularized Centroid Estimation on a Hierarchical Bayesian Model for Genome-Wide Association Studies"
2 July 2012

Prof CATELLANI, Marta
Dipartimento di Chimica and CIRCC, Università di Parma, Parma, Italy
"The Role of Palladacyclesin Sequential Reactions"
8 November 2012

Dr CIPRIAN, Plostinar
Rutherford Appleton Laboratory, Romania
"Linac Studies for ISIS Upgrades"
15 October 2012

Prof CRUDDEN, Cathleen M
Department of Chemistry, Queen's University, Kingston, Canada
"Chirality Transfer in the Suzuki-Miyaura Reaction and in Mesoporous Materials"
1 March 2012

Prof DJUKIC, Jean-Pierre
Institut de Chimie, Université de Strasbourg, Strasbourg, France
"Non-Covalent Interactions in Transition Metal Chemistry: from Molecular Cohesion to Molecular Design"
28 February 2012

Prof DUNCAN, Wass
University of Bristol, U.K.
"Frustrated Lewis Pairs beyond the Main Group"
21 November 2012

Dr FERRIER, Meydi
Centre national de la Recherche Scientifique (CNRS), Orsay, France
"Probing the Dynamics of Andreev States in Coherent Normal/Superconducting Ring "
28 June 2012

Prof FUJII, Ikuo
Laboratory of Chemical Biology, Osaka Prefecture University, Japan
"Next-generation Antibody Drugs (Micro Antibody): Generation of Molecular Target Peptide from Sterically Controlled Peptide Library"
14 February 2012

Dr FUJIMAKI, Ryohei
NEC Laboratories, U.S.A.
"Factorized Asymptotic Bayesian Hidden Markov Models"
10 September 2012

Prof FUJITA, Makoto
Department of Applied Chemistry, The University of Tokyo, Japan
"Creation of Structure, Space, and Function by the Self-assembly Process"
2 November 2012

Assoc Prof FURUBE, Akihiro
National Institute of Advanced Industrial Science and Technology (AIST), Japan
"Intersurface Electron Transfer at the Nanoparticles of Photoelectro Conversion Systems"
29 October 2012

Prof GRÄSLUND, Astrid
Dept. of Biochemistry and Biophysics, Stockholm University, Stockholm, Sweden
"Cell Penetrating Peptides and Their Membrane Interactions: Biophysical Models for Mechanistic Insight"
23 January 2012

Prof GREEDAN, John. E.
Brockhouse Institute for Materials Research, McMaster University, Canada
"Oxygen Vacancy Order and Disorder in Defect Perovskites: Local and Average Structures and Magnetic Properties"
12 November 2012

Prof GRUSHUIN, Vladimir V.
Institute of Chemical Research of Catalonia (ICIQ), Tarragona, Spain
"Solving the Misteries of Catalyst Deactivation in Palladium-Catalyzed Cyanation of Haloarenes: An Illustration of How Mechanistic Understanding Can Benefit Practical Catalysis"
31 October 2012

Dr HADA, Masaki
Center for Free Electron Laser Science, University of Hamburg, Hamburg,Germany
"Femtosecond Electron Diffraction for "Molecular Movies"
9 November 2012

Prof HASSAGER, Ole
Department of Chemical and Biochemical Engineering, Technical University of Denmark, Denmark
"Filament Stretching Rheometry"
12 March 2012

Prof HAYASHI, Ken-ichiro
The Faculty of Science, Okayama University of Scinece, Okayama, Japan
"Chemical Biology for Analyzing Signal Transduction of Plant Hormones"
6 October 2012

Dr HINGAMP, Pascal
Aix-Marseille University, Marseille, France
"What Can Metagenomics Tell Us about Marine Large Eukaryotic Viruses? Preliminary Exploration of TARA -OCEANS Genomic Data"
14 February 2012

Assoc Prof HIRAYAMA, Tomoko
Department of Mechanical and Systems Engineering, Doshisha University, Kyoto, Japan
"Role of Adsorbed Additive Layers on Friction and Lubrication -From the View Point of Tribology-"
23 March 2012

Dr HO, Tung-Yuan
Associate Research Fellow, Research Center for Environmental Changes, Academia Sinica, Taiwan
"Trace Metal Biogeochemistry in the South China Sea"
"Ni Limitation of Nitrogen Fixation in *Trichodesmium*"
13 July 2012

Assoc Prof HOW, Sew Eng
School of Science & Technology, Universiti Malaysia Sabah, Sabah, Malaysia
"Solid Phase Synthesis of Dendrimers for Gene Delivery"
4 April 2012

Dr IKEDA, Kazuyoshi
EMBL-EBI, U.K.
"Overview of the ChEMBLdb: A Database of Drug, Lead and Target Data"
24 September 2012

Prof ISOBE, Hiroyuki
Department of Chemistry, Tohoku University, Sendai, Japan
"Development of Nano-carbon Structure Science"
10 November 2012

Assoc Prof JANSSON, Jesper
The Hakubi Project at Kyoto University, Kyoto, Japan
"Combinatorial Algorithms for Building a Phylogenetic Supertree"
16 April 2012

Dr KIHARA, Daisuke
Department of Biological Sciences/Computer Science, Purdue University, West Lafayette, U.S.A.
"Predictions of Structures of Protein Interactions"
28 May 2012

Dr KOMATSU, Katsuyoshi
National Institute for Material Science (NIMS), Japan
"Superconducting Proximity Effect from Zero Magnetic Field to Quantum Hall Regime in Graphene "
18 July 2012

Prof LEVITT, Malcolm
School of Chemistry, University of Southampton, U.K.
"A Singlet NMR"
31 October 2012

Prof LIPPOLIS, Vito
Department of Inorganic Chemistry, The University of Cagliari, Italy
"New [9]aneN$_3$ Derivatives for Selective Inorganic/organic Phosphate Binding and Sensing"
21 March 2012

Prof LODGE, Tim
Department of Chemical Engineering and Materials Science, University of Minnesota, U.S.A.
"Physical Gels from ABA and ABC Block Polymers in Water and Ionic Liquids"
10 December 2012

Dr LUTZ, Jean-François
Institut Charles Sadron, Strasbourg, France
"New Strategies for Controlling Monomer Sequences"
18 January 2012

Assoc Prof MAWATARI, Kazuma
Department of Applied Chemistry, The University of Tokyo, Tokyo, Japan
"Development of fL–aL Analysis System Using Extended Nanospace"
7 September 2012

Prof MCKENNA, Greg
Department of Chemical Engineering, Texas Tech University, U.S.A.
"Nanorheology of Ultrathin Polymer Films: Bubble Inflation and Liquid Dewetting"
12 November 2012

Prof MINDIOLA, Daniel J.
Department of Chemistry, Indiana University, Indiana, U.S.A.
"Titanium Alkylidynes. Methane Activation and Dehydrogenation of Volatile Paraffins"
18 May 2012

Prof MORI, Shigeyuki
Graduate School of Engineering, Iwate University, Iwate, Japan
"Tribological Control: In-Situ Observation of Contact Surface toward Better Lubricant"
5 November 2012

Prof MUÑIZ, Kilian
Institute of Chemical Research of Catalonia (ICIQ), Tarragona, Spain
"New Diamination Reactions of Alkenes: Palladium Catalysis and Iodine Reagents"
20 November 2012

Prof NICLES, Peter
Max-Born-Institute, Berlin, Germany, and APRI GIST, Korea, R.
"Energetic Photon from Short-pulse Laser Plasmas"
16 November 2012

Prof NIELS, Madsen
Swansea University, Department of Physics, U.K.
"Trapped Anti-hydrogen : A New Frontier in Fundamental Physics"
4 October 2012

Prof NISHIYAMA, Hisao
Graduate School of Engineering, Nagoya University, Nagoya, Japan
"Chiral NCN, NNN-Type Ligands; Metal Complexes and Asymmetric Catalytic Reactions –Rh, Ru, Fe, Co –"
11 May 2012

Prof NITTA, Junsaku
Tohoku University, Japan
"Electric Field Control of Persistent Spin Helix"
11 November 2012

Dr OGATA, Hiroyuki
Aix-Marseille University, Marseille, France
"Giant Viruses in Marine Environments"
14 February 2012

Assoc Prof OHKANDA, Junko
Institute of Scientific and Industrial Research (ISIR), Osaka University, Osaka, Japan
"Assembling Small Molecules for Disrupting and Detecting Protein-protein Interactions"
18 July 2012

Lect OHKUBO, Jun
Graduate School of Informatics, Kyoto University, Japan
"Counting Statistics and Related Topics"
23 May 2012

Prof PETEKIDIS, George
Department of Materials Science and Technology, University of Crete, Greece
"Flow of Colloidal Glasses and Gels"
30 November 2012

Prof POEPPELMEIER, Ken
Department of Chemistry, Northwestern University, U.S.A.
"Targeting Noncentrosymmetric Structures and Other New Materials"
6 June 2012

Prof ROBIN, B. Bedford
University of Bristol, U.K.
"Iron Cauldrons and Witches Brews"
21 November 2012

Dr ROGNAN, Didier
Centre National de la Recherche Scientifique (CNRS), France
"Fingerprinting Protein Cavities and Protein-ligand Complexes for Drug Design"
25 October 2012

Dr ROULLEAU, Preden
Commissariat à L'énergie Atomique (CEA), Saclay , France
"Photon-assisted Detection of the Noise of a Quantum Point Contact"
28 September 2012

Prof RUSSEL, Chris
School of Chemistry, University of Bristol, U.K.
"Novel Structure, Bonding, and Reactivity for Pnictogens in Low Coordinate Environments? Is Phosphorus a Carbon Copy?"
19 November 2012

Prof SARMA, D. D.
Solid State and Structural Chemistry Unit, Indian Institute of Science, India
"Probing Buried Layers"
28 September 2012

Assoc Prof SATO, Moritoshi
Graduate School of Arts and Sciences, University of Tokyo, Tokyo, Japan
"Technologies for Visualizing and Operating Biomolecules"
21 June 2012

Prof SAWADA, Kazuaki
Department of Electrical and Electronic Engineering, Toyohashi University of Technology, Aichi, Japan
"Electro-Cell Integrated System Using Ion-Imaging Sensors Technology"
10 September 2012

Prof SCHESCHKEWITZ, David
Department of Chemistry, Faculty 8: Natural Sciences and Technology III, Saarland-University at Saarbrücken, Germany
"The Chemistry of $Si_6R_6$ Isomers"
16-17 October 2012

Dr SCHUH, Tobias
Karlsruhe Institute of Technology (KIT), Germany
"Spin Dynamics of Atoms and Clusters on Surfaces "
27 August 2012

Prof SOO, Von-Wun
Department of Computer Science and Institute of Information Systems and Applications, National Tsing Hua University, Taiwan
"Identify Drug Co-target to Fight Drug Resistance Based on a Random Walk Model"
11 January 2012

Dr VIDAL, Virginie
ENSCP Chimie ParisTech, Paris, France
"Asymmetric Catalysis: From Laboratory Scale to Scale up Development"
29 October 2012

Prof WAGENER, Kenneth B.
University of Florida, Florida, U.S.A.
"Using Polymers to Treat Bone Cancer in Children"
17 May 2012

Prof WONG, Limsoon
School of Computing, National University of Singapore, Singapore
"A Novel Principle for Childhood ALL Relapse Prediction"
1 November 2012

Prof YAMADA, Masatoshi
Institute of Radiation Emergency Medicine, Hirosaki University, Japan
"Interdisciplinary Study on Environmental Transfer of Radionuclides from the Fukushima NPP Accident: Understanding the Distribution of Radioactive Materials in Sea and Seafloor Sediment"
13 December 2012

Prof ZETTERLUND, Per B.
The University of New South Wales, Australia
"Novel Approaches to Polymer/Particle Synthesis: (i) $CO_2$-Induced Miniemulsion Polymerization and (ii) Templated Polymerization within Nanoreactors"
20 December 2012

Dr ZHENG, Jian
Research Center for Radiation Protection, National Institute of Radiological Sciences, Japan
"Application of ICP-MS for the Determination of Artificial Radionuclides in Environmental Samples"
13 December 2012

# MEETINGS AND SYMPOSIA

**Japan-UK-Taiwan Meeting**
**“Synthesis and Properties of New Functional Materials”**
Organized by SHIMAKAWA, Yuichi
11-14 January 2012 (Uji, Japan)

**Asian Chemical Biology Initiative 2012 Hanoi Meeting**
Organized by UESUGI, Motonari
25-26 February 2012 (Hanoi, Vietnam)

**The Ceramic Society of Japan Annual Meeting 2012**
Organized by YOKO, Toshinobu
19-21 March 2012 (Kyoto, Japan)

**KUBIC-NII Joint Seminar on Bioinformatics 2012**
Organized by National Institute of Informatics and Institute for Chemical Research
26 April 2012 (Uji, Japan)

**The 10th International Conference on Heteroatom Chemistry**
Organized by TOKITOH, Norihiro; SASAMORI, Takahiro; MIZUHATA, Yoshiyuki; AGOU, Tomohiro
20-25 May 2012 (Uji, Japan)

**2012 Sapporo Workshop on Machine Learning and Applications to Biology (MLAB Sapporo 2012)**
Organized by MAMITSUKA, Hiroshi
6-7 August 2012 (Sapporo, Japan)

**The 5th MEXT Project of Integrated Research on Chemical Synthesis Forum**
**“Unique Peptide Assemblies with Biological Functions”**
Organized by FUTAKI, Shiroh
15 September 2012 (Uji, Japan)

**The 23rd Symposium on Physical Organic Chemistry**
Contributed by TOKITOH, Norihiro; SASAMORI, Takahiro; MIZUHATA, Yoshiyuki; AGOU, Tomohiro; MURATA, Yasujiro; WAKAMIYA, Atsushi; MURATA, Michihisa as Co-Organizer
19-21 September 2012 (Kyoto, Japan)

**MEXT Project of Stimuli-responsive Chemical Species for the Creation of Functional Molecules**
**“The 1st Symposium on Stimuli-responsive Chemical Species for the Creation of Functional Molecules”**
Organized by OZAWA, Fumiyuki
29 September 2012 (Uji, Japan)

**Wageningen University and Research Centre/Kyoto University Joint Workshop**
Organized by KURIHARA, Tatsuo
31 October 2012 (Uji, Japan)

**Kyoto University-Durham University Joint International Symposium 2012:**
***Emergence and Feedback in Physical and Social Systems***
Organized by WATANABE, Hiroshi
27-29 November 2011 (Uji, Japan)

**Catalysis Society of Japan and MEXT Project of Integrated Research on Chemical Synthesis**
**“The 40th Seminar on Organometallics (The 6th Forum on MEXT Project of Integrated Research on Chemical Synthesis)”**
Organized by OZAWA, Fumiyuki
30 November 2012 (Uji, Japan)

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