



# RCMS NEWS

17  
2016

NAGOYA UNIVERSITY  
RESEARCH CENTER FOR MATERIALS SCIENCE

Reports and Communications of RCMS Activities  
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May 2016  
Issue #17



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# MEXT Project of Integrated Research on Chemical Synthesis 2015

In 2015, MEXT Project of Integrated Research on Chemical Synthesis, a pioneering synthesis of a new scientific base and nurturing the next generation of researchers (Hokkaido University Catalysis Research Center, Nagoya University Research Center for Materials Science, Kyoto University International Research Center for Elements Science Institute for Chemical Research, Kyushu University Institute for Materials Chemistry and Engineering) held the symposium below.

## The 6<sup>th</sup> Symposium on MEXT Project of Integrated Research on Chemical Synthesis

(Nagoya University, April 14, 2015)



Group photo with the guests



Poster



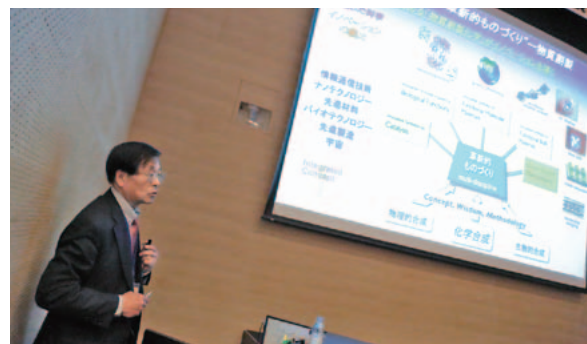
Invited lecture, Prof. Kawasaki



Assoc. Prof. Yamauchi



Prof. Takahashi



Designated Prof. Tatsumi

**The 6<sup>th</sup> Young Researchers Forum**  
(Kyusyu, July 3, 2015)



Group photo



**The 5<sup>th</sup> International Conference on MEXT Project of Integrated Research on Chemical Synthesis**  
(Nagoya University, January 29–30, 2016)



Opening, Prof. Awaga



Prof. DeBeer



Poster session



Discussion



Prof. Ruben



Lunch time



Group photo

# Core-to-Core Program

## The 19<sup>th</sup> Joint Seminars

The “Elements Function for Transformative Catalysis and Materials”, Core-to-Core program (2014 to 2018), has succeeded in sending young researchers to sites performing international joint research through cooperation with the University of Munster (Germany), the Berlin University of Technology (Germany), and Queen’s University (Canada). Further growth has been realized through the deployment of doctoral students and young researchers through the “Japanese-German Graduate Externship” (2005 to 2011) and “The Strategic Young Researcher Overseas Visit Program for Accelerating Brain Circulation” (2011 to 2013), results-producing projects in which the center and the Department of Chemistry at the Graduate School of Science have fulfilled a central role. The Core-to-Core Program has enabled the deployment of master’s students, and outstanding young researchers expected to perform globally in the future can now be refined through participation in international joint research performed overseas at an early stage.

### The 19<sup>th</sup> Core- to-Core Joint Seminar October 5–6, 2015, University of Münster, Germany



Prof. Yamaguchi



Group photo



Prof. Saito



Prof. Erker



Seminar room



Coffee break

# Integrative Graduate Education and Research Program in Green Natural Sciences (IGER)

Integrative Graduate Education and Research (IGER) Program in Green Natural Sciences was launched in 2011, and built on three pillars: (I) practicing cutting-edge fundamental natural science research, (II) completion of sufficient coursework to enable that research, and (III) graduate school literacy education (English training, studying abroad, skill seminars, etc.). Based on these, the program aims to nurture the “scientific ability and social skills to view situations from a broad perspective,” “developmental ability to extract practical results from fundamental research,” and “active international citizenship on a global scale,” along with fostering “corporate researchers cultivated as seeds in industry,” “academic researchers raised in the scholarly domain,” and “environmental coordinators and mentors active throughout global society” that will carry the environmental fields of the next generation.

[Environment of friendly competition] Since the number of students participating in this program is unlimited, the competition level is high. This creates an environment in which students who study different fields, and are in different academic years, can cooperate but also compete, during courses developed in collaboration with eight departments of the Graduate Schools of Science, Engineering and Bioagricultural Sciences, as well as various seminars coordinated by each school in the university, English training, and leadership training in North Carolina, USA. By presenting their academic achievements and research results, students can be stimulated and create a good network for exchange. Furthermore, this can benefit the students’ career path. Through this strategy, excellent human resources can be expected to develop.

[Seminars organized by graduate students] We provide opportunities to work out educational plans drawn up by students. Students have to carry out their plans by themselves, for instance, some groups of students have implemented a tutorial seminar to open up a new research field, a workshop to develop interdisciplinary fields, and a symposium to think about the challenges and future directions for various world issues as scientists. Through the implementations of their plans, students can acquire a range of practical and theoretical skills particularly in leadership, team building, negotiation, and problem-solving.

In 2015, over 250 graduate students enrolled in this program from graduate school of Science, Engineering and Agricultural Sciences. The program provided opportunity for 78 students to participate in international conferences held at outside Japan, and also provided opportunity of mid-term (2–3 months) foreign residency research for 17 students.

Ten students participated in the Leadership Program at North Carolina, US. All students not only attended lectures regarding Leadership, Entrepreneurship and Technology Transfer but also visited many laboratories in universities at North Carolina to build networks with PIs, postdocs and graduate students. In addition, all of them had opportunities to do presentations on their research to these researchers and have discussions. Furthermore, they visited some companies to learn some ideas of working in industry as a researcher and business environment in the USA from entrepreneurs and researchers.



Seminar organized by students



Poster awards ceremony



Leadership Program at North Carolina



# Research Topic

## (Inorganic Synthesis)

# Re-Analyzing Inorganic Reactions in Solution on the basis of Quantum Mechanics

Studies on (1) solvent exchange/ligand substitution reactions and (2) simple electron transfer reactions had been the central field of solution chemistry for decades, and it seemed only complicated reaction systems had been left untouched by the end of 1980's. However, credibility of the results for (1), namely the credibility of the categorization of reaction mechanisms to Dissociative, Interchange ( $I_a$  and  $I_d$ ), and Associative mechanisms, largely depended on the observed activation entropies and activation volumes both of which are sensitive to many factors such as solvation and de-solvation of chemical species. As a result, the observed activation entropies and activation volumes were almost identical for solvent exchange reactions of a metal ion in various solvents although solvent properties of each solvent are largely different. Therefore, it is certain that we have to re-analyze the results by using reliable physical principles, before concluding this research field. Results for such attempts are given in *The Review of High Pressure Science and Technology*, 8 (3), 193–208 (1998) and

*Inorganic Chemistry on the Basis of Quantum Theory* (Hideo D. Takagi, Nagoya Univ. Press, 2010), in which ligand exchange reactions were re-evaluated on the basis of the first- and second-order Jahn-Teller theory and the calculated ligand-field activation energies for each electronic configurations using effective nuclear charges.



As for the electron transfer reactions, most of experimental results were analyzed on the basis of the classical/ or semi-classical Marcus Theory, and such analyses were reliable because of the credibility of this physical theory. However, there is a factor overlooked by many researchers of this field: the adiabaticity of reactions. Many chemists believe that most electron transfer reactions are adiabatic as it has been known that reactions with transmission coefficient between  $10^{-3}$  and 1 may be considered adiabatic. However, it seems some reactions may not be adiabatic as (1) the distance between reactants are large and/or (2) the energy gap between the donor and acceptor orbitals is large. We investigated some copper (II)/(I) reaction systems and found that adiabaticity of electron transfer reactions varies with varying counter reagents: reactions are adiabatic and Marcusian for all self-exchange reactions and cross reactions with other copper complexes as counter reagents, while cross reactions with non-copper metal complexes as counter reagents are essentially non-adiabatic and controlled by the inner-sphere structural changes to induce either sequential transfer or super-exchange (*Inorg. Chem.*, 1999, **38**, 3352; *Chem. Phys. Lett.*, 1999, **306**, 291; *Inorg. Chim. Acta*, 2001, **324**, 252; *Chem. Phys. Lett.*, 2001, **344**, 441; *Inorg. Chem.*, 2007, **46**, 1419; *Dalton Trans*, **44**, 13979–13990 (2015)).

Relationship between solvent properties and reaction mechanisms is another important subject investigated in this research group. Thermal Z/E isomerization reactions of various azobenzenes in many solvents including various ionic liquids and supercritical carbon dioxide have been investigated (*Chem. Lett.*, 1159–1160 (1998); *J. Phys. Chem. A*, 103, 11250–11251 (1999); *Chem. A European Journal*, 2006, 12, 5328–8333). Currently, we are investigating solvent reorganization processes that accompany the redox process between photo-induced Zn-TPP and [Co(sepulchrate)<sup>3+</sup>] and the back electron transfer reaction between the  $\pi$ -cation radical and [Co(sepulchrate)<sup>2+</sup>] in various ionic liquids.

(Hideo TAKAGI)

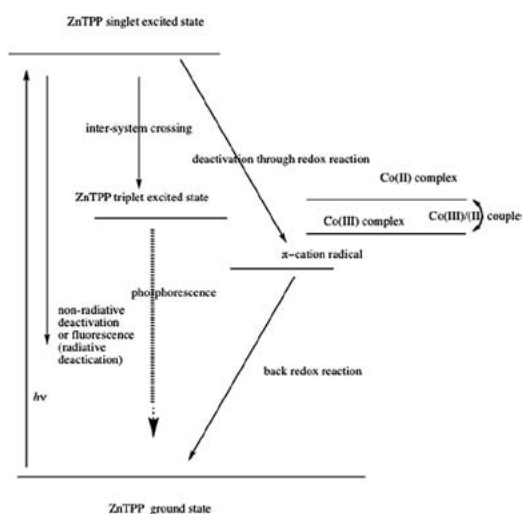


Figure 1. Photo-electron transfer reactions between ZnTPP – Co(sep)<sup>3+/2+</sup> in various ionic liquids.

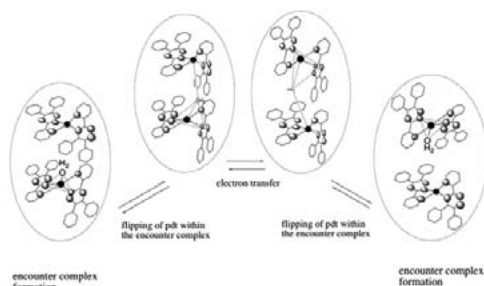


Figure 2. Electron self-exchange reaction for the [Cu(3-(2-pyridyl)-5,6-diphenyl-1,2,4-triazine)<sub>2</sub>]<sup>2+/+</sup> couple. The reaction involves flipping of coordinated triazine ring during the electron transfer process. However, the reaction is not Gated but concerted.

## Research Topic

(Functional Materials)

# Discovery of Novel Electrochemical Mechanism in a Metal-Organic Framework based Li-ion Battery

The Li-ion batteries are widely considered as a promising energy storage and power supplying devices for the portable electronics and electrical vehicles. To improve the performance of these batteries, such as storage density and output rate, material scientists are always motivated to develop novel electrode materials. With previous studies, our group has successfully illustrated the potential of molecular materials, including polynuclear metal clusters and metal-organic frameworks (MOFs). Although intriguing electrochemical characteristics have been observed for them, their insulating nature have significantly hindered a broad application of these molecular materials.

Since the preparation of conductive molecular materials is very challenging, the low conductive issue of molecular materials can't be simply solved by increasing their conductivity with proper design strategy. Nevertheless, we discovered a novel electrochemical scheme, namely "bipolar charging mechanism" with a lately ob-

tained redox active MOF,  $Mn_2(2,7-AQDC)_6(2,6-AQDC)(DMA)_6$  (AQDC = anthraquinone dicarboxylates, DMA = N,N-dimethylacetamide) as the cathode material of a Li-ion battery. Since the valence of manganese is Mn(II), they are oxidized to Mn(III) during the charge operation, and  $PF_6^-$  anions from the electrolyte are adsorbed to balance the charge of the framework. On the other hand, in the discharge step, the anions are firstly released and followed by the reduction of anthraquinones and the insertion of Li-ions. In other words, the electron storage process involves the movement of two type of ions from the electrolyte. With the contribution of two steps, this MOF exhibited a high capacity of 205 mAh/g and a stable cyclic performance that the capacity drop is less than 10% within 50 cycles. This newly discovered mechanism is the first mechanism that involves the insertion of two ion species, and significantly reduced the ionic traffic, and improved the efficiency of batteries.

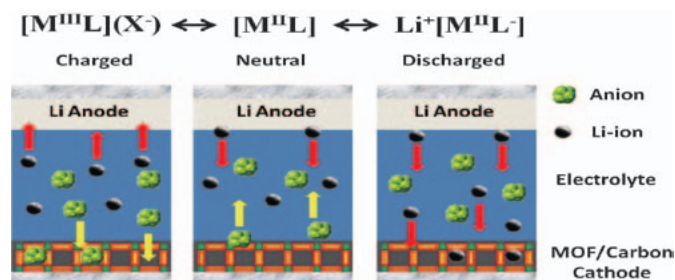


Figure 1. The scheme of bipolar charging mechanism.

### References

- [1] Z. Zhang, H. Yoshikawa, K. Awaga, *J. Am. Chem. Soc.*, **136**, 16112 (2014).
- [2] Z. Zhang, H. Yoshikawa, K. Awaga, *Chem. Mater.*, **28**, 1298 (2016).

(Zhongyue ZHANG)

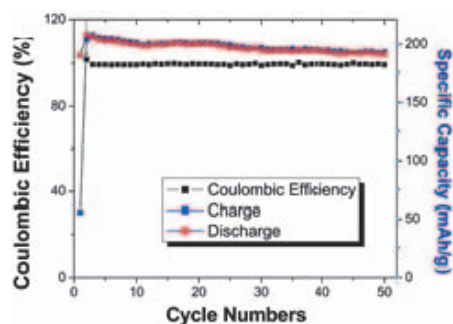


Figure 2. The cyclic performance of MOF-based battery.



# Research Topic

(Biomaterials Research)

## Translation with circular mRNA

Proteins possess divergent structures and functions and play the important roles in cells. This indicates that structural and functional analyses and production of proteins contribute to not only understanding of life phenomena but also the drug discoveries and industrial application. In addition, it is considered that artificial protein can be engineered by modification of the amino-acid sequence because the function and structure of protein depend on its amino-acid sequence.

The synthesis and engineering of protein will promote the industrial application of protein. Because of this, the artificial production of protein is one of the most crucial research for analyses and application of proteins. Conventionally, the target protein has been produced artificially in simple organism, such as *Escherichia coli*, yeast, and silkworm. Recently, the protein can be produced without living cell (Cell-free expression system). However, protein expression efficiency in cell-free expression system is less than it in conventional method.



To improve the protein expression in cell-free expression system, we focused on the late-limiting step of translation, the association and dissociation of ribosome and mRNA. To reduce the contribution of this step in protein synthesis, we have developed the rolling-cycle translation system (Figure 1). mRNA without stop codon was circularized by using enzymatic reaction and translated in cell-free expression system. As shown in Figure 2, the translation with circular mRNA produced higher amount of protein than that seen with linear mRNA. This result indicates that ribosome repeated the translation in the circular mRNA. In addition, we confirmed that it is possible to express protein by circular mRNA in the living eukaryote cell.

Furthermore, our group utilizes the biochemical, structural cellular-biological approaches into the analysis of biomolecules and our synthesized molecules.

(Fumiaki TOMOIKE)

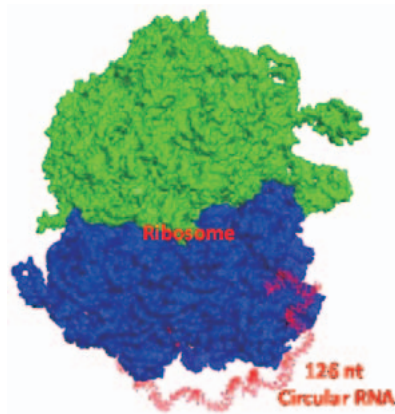


Figure 1. Translation with circular mRNA

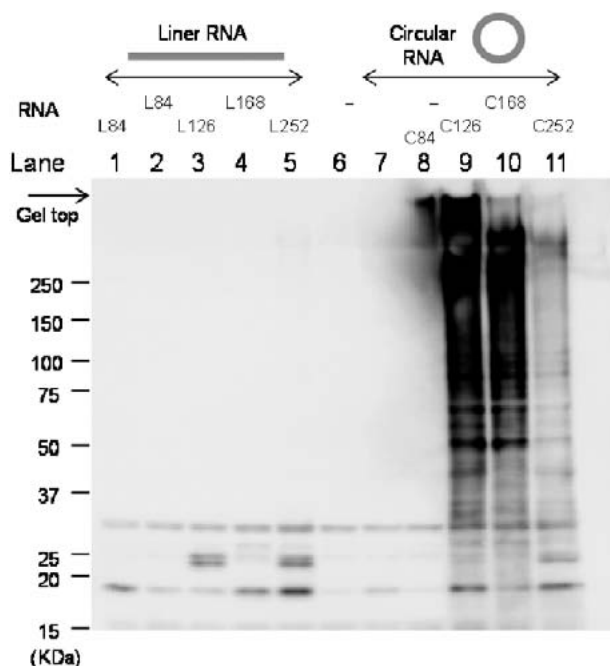


Figure 2. Comparison between translation with linear mRNA and circular mRNA.

## Research Topic (Molecular Catalysis)

# Development of Asymmetric Dehydrative Tsuji-Trost Allylation

Previously, we have designed and synthesized a new axially chiral PyCOOH-type ligand, R-Naph-PyCOOH (5-methyl-6-(2-R-naphthalen-1-yl)-pyridine-2-carboxylic acid). Complex of Cl-Naph-PyCOOH with [CpRu(II) (CH<sub>3</sub>CN)<sub>3</sub>]PF<sub>6</sub> (**1**) has been revealed to catalyze asymmetric dehydrative intramolecular O- and N-allylation with excellent reactivity and selectivity.<sup>[1,2]</sup>

The complex **1** captures an allylic alcohol substrate via “soft Ru/soft C=C double bond” interaction and “hard COOH/hard hydroxy oxygen atom” interaction to generate a catalyst/substrate complex **A**. Here, a donor-acceptor bifunctional catalyst mechanism operates to move **A** to the  $\pi$ -allyl complex. Such a cooperative mechanism is the origin of the reactivity toward the unlabile allylic alcohol.

Recently, we have extended this chemistry to alkenyl lactone synthesis. Optically active simple lactones with an allyloxycarbonyl moiety (alkenyl lactones) attract much attention from organic synthetic chemists because of their high functional convertibility. Among many excellent catalytic methods, intramolecular Tsuji-

Trost (T-T) allylation seems to be the most tangible, but it is limited to only a specific case. This may be due to the fact that the alkenyl lactone is an excellent  $\pi$ -allyl donor in the traditional Pd-catalyzed allylation using allyl esters under basic conditions. We have changed the situation by the reaction of  $\omega$ -carboxyl-substituted allylic alcohols to the lactones using catalyst **1**. The new method can be applied to the synthesis of various  $\gamma$ - and  $\delta$ -alkenyl substituted lactones. Introduction of a substituent at C(2) or C(3) of allylic alcohol moiety is acceptable. This new method should further enhance the utility of T-T-type asymmetric allylation, widening the scope of retrosynthetic analyses of natural and unnatural important chiral compounds.<sup>[3]</sup>

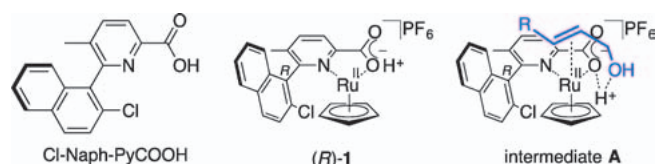
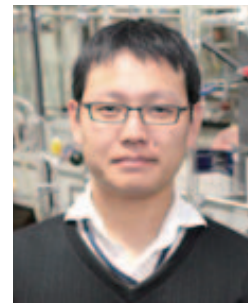


Figure 1. Dehydrative allylation catalyst

### References

- [1] S. Tanaka, T. Seki, M. Kitamura, *Angew. Chem. Int. Ed.* **2009**, *48*, 8948–8951.
- [2] T. Seki, S. Tanaka, M. Kitamura, *Org. Lett.* **2012**, *14*, 608–611.
- [3] Y. Suzuki, T. Seki, S. Tanaka, M. Kitamura, *J. Am. Chem. Soc.* **2015**, *137*, 9539–9542.

(Shinji TANAKA)

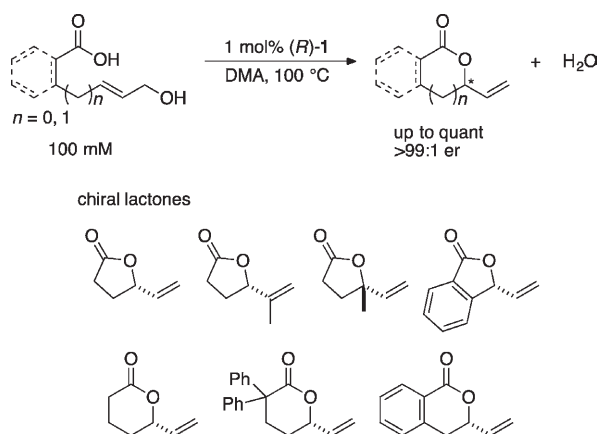


Figure 2. Optically active alkenyllactone synthesis via asymmetric dehydrative allylation.

# Visiting Professor 2015

## Prof. Fernando Palacio

Professor, University of Zaragoza



Period of Stay:

October 13, 2015

– December 12, 2015

Research Theme:

Development of novel molecular and nano magnets

Prof. Fernando Palacio from University of Zaragoza, Spain, stayed as a visiting professor in RCMS for two months from 13<sup>th</sup> October, 2015, to develop novel molecular- and nano-magnets. He is a solid-state physicist with strong expertise in these materials, and has been working in an interdisciplinary area between physics and chemistry, and between fundamental and applied research. His research into the ferromagnetic ordering of organic thiazyl radicals, and on the application of nanoparticles of iron oxides, are extremely famous. He is one of the pioneers of molecular magnetism, and has been leading this research field for a long time.

During his stay in Nagoya, he attended the group meetings of the Awaga group and gave his valuable advice to the students and young researchers. He was full of curiosity and had an interest in everything. In addition,

he gave us an IGER-RCMS seminar, “THERMOMETRY AT THE NANOSCALE USING FUNCTIONALIZED NANOPARTICLES” on Dec. 3<sup>rd</sup>. His contribution to RCMS was very significant in terms of both research and education.

Prof. Palacio is a great friend of Japan, and is a fan of Japanese foods, Japan-style hotels (Ryokan), and hot spring resorts. During his stay in Japan, his wife had an opportunity to come to Japan for two weeks, in which they enjoyed a weekend in Hakone. He also visited Nara with the exchange students from the University of Edinburgh. Since he has a great knowledge of the Japanese gardens, such as SHAKKEI, he was very happy to lecture the students from Edinburgh on Japanese culture.

With a lot of good memories from Japan, he returned to Spain on Dec. 12<sup>th</sup>



At the Seminar



Chemistry Gallery



Takayama trip



Making YUBA



At Yagoto Kosho-ji

# Report from the Chemical Instrumentation Facility

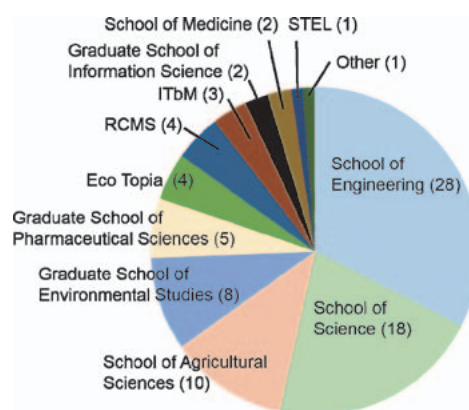
The Chemical Instrumentation Facility is a facility shared by the whole university that contains instrumental analysis equipment including a nuclear magnetic resonance (NMR) spectrometer, mass spectrometer, and spectroscopic analysis equipment for analyzing molecular structures. In the Chemical Instrumentation Facility, services are provided to users including teaching faculty, researchers, and students through maintenance of these measurement instruments, lectures on measurement methods, consultations for specific measurements, and entrusted measurement. During the 2015 fiscal year, as shown in "CIF Utilization Status", 86 research groups from the university registered to use the facility, and the number of teaching faculty, students, and researchers who registered to use the facility during the year was 800.



ESR (JESTE-200, JEOL)

## [CIF Utilization Status]

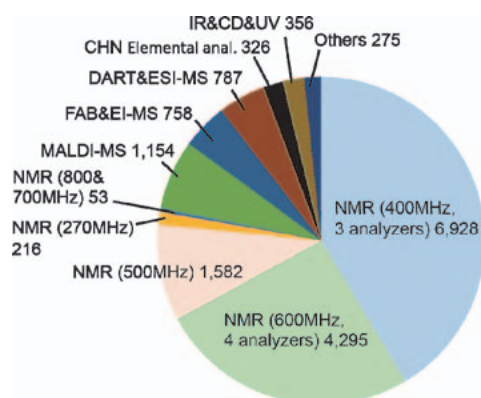
Utilization Status for the Academic Year 2015  
(April 2015 – April 2016)



Number of Uses/Measurements by Instrument



NMR room (ECS-400, JNM-A 600, JEOL)



Utilization Status by Department  
(Total: 86 Groups, 800 People)



FAB-MS (JMS 700, JEOL)

# RCMS Seminars

**April 1, 2015** Dr. Thanyada Rungrotmongkol  
(Department of Biochemistry, Faculty of Science,  
Chulalongkorn University Bangkok 10330, Thailand)  
"Molecular dynamics studies on infectious diseases of humans"

**IGER/RCMS Seminar**  
Theoretical Chemistry Colloquium

**April 1, 2015 (Wed), 16:00-17:00**  
RCMS, 2<sup>nd</sup> floor, Chemistry Gallery

**Molecular dynamics studies on infectious diseases of humans**

**Dr. Thanyada Rungrotmongkol**  
Department of Biochemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand

**Abstract:** We aimed at gaining insight into molecular details on the target proteins related to certain human diseases and health problems including influenza and cancer. The functional machinery of such proteins as well as drug inhibition, source of drug resistance and drug screening were studied using various computational techniques, i.e., homology modeling, combinatorial chemistry, molecular dynamics (MD) simulation, combined quantum-mechanics/molecular mechanics (QM/MM) and three-dimensional reference interaction site model (3D-RISM). As a result, several questions have been revealed, for example, why and how high pathogenicity of influenza H5N1 virus was experimentally better caused by substitution-like surface protein than the low pathogenic hemagglutinin; how available anti-influenza drugs can well inhibit the neuraminidase and/or M2 protein but less susceptibility against their mutants; and how protein is selectively transported through a M2 channel. The combinatorial chemistry and damped MD were successfully used to design and screen the potent compounds from available databases for inhibiting anti-influenza neuraminidase and hepatitis C NS5A protease, respectively. In addition, the release inhibition of NS5A by benzamide and telaprevir has been explored using the semi-empirical QM/MM MD simulations. As a result, the activation step is occurred in the concerted manner, with a consequence of inhibitor covalently bonded with enzyme formed in the last step of reaction.

Contact: Prof. Dr. Stephan Irie  
E-MAIL: irie@chem.nagoya-u.ac.jp Tel.: 8297

**IGER-ITbM-RCMS Seminar**

**Prof. Mark S. Taylor**  
University of Toronto

"Noncovalent and Reversible Covalent Interactions:  
Fundamental Studies and New Applications"

**May 11, 2015 (Mon) 16:00-17:30**  
Noyori Materials Science Laboratory 2F,  
Lecture Hall

Host: Shigehiro Yamaguchi (789-2291)

**May 11, 2015** Prof. Mark S. Taylor  
(University of Toronto)  
"Noncovalent and Reversible Covalent Interactions:  
Fundamental Studies and New Applications"

**May 12, 2015** Prof. Daniel T. Gryko  
(Polish Academy of Sciences)  
"From Pyrrolo[3,2-b]pyrroles to  $\Pi$ -expanded  
diketopyrrolopyrroles - the fluorophores for the future"

**IGER-ITbM-RCMS Seminar**

**Prof. Daniel T. Gryko**  
Polish Academy of Sciences

"From pyrrolo[3,2-b]pyrroles to  $\Pi$ -expanded diketopyrrolopyrroles  
- the fluorophores for the future"

**May 12, 2015 (Tue) 10:30-12:00**  
Noyori Materials Science Laboratory 2F,  
Lecture Hall

Host: Shigehiro Yamaguchi (789-2291)

**RCMS** Theoretical Chemistry Colloquium

**May 12, 2015 (Tue), 16:00-17:00**  
RCMS, 2<sup>nd</sup> floor, Chemistry Gallery

**Understanding and Designing  
Heterogeneous Catalysts from First  
Principles**

**Prof. Dr. Andreas Heyden**  
Associate Professor of Chemical Engineering  
University of South Carolina, Columbia, SC, USA

**Abstract:** In the last ~15 years computational catalysis started to significantly impact catalysis research by providing a new tool for testing experimental hypotheses and by screening a large number of materials in silico. In this seminar, I will present two case studies illustrating the strengths and challenges of computational catalysis. For these topics, I will highlight the importance of solvent effects in catalysis and present recent tools for including solvation effects in computational studies.

Contact: Stephan Irie  
E-MAIL: irie@chem.nagoya-u.ac.jp Tel.: 8297

**May 12, 2015** Prof. Dr. Andreas Heyden  
(Associate Professor of Chemical Engineering,  
University of South Carolina, Columbia, SC, USA)  
"Understanding and Designing Heterogeneous Catalysts  
from First Principles"

**May 14, 2015** Dr. J. B. Brown  
(Assistant Professor, Department of Clinical System Onco-Informatics  
Graduate School of Medicine, Kyoto University)  
"Computational studies of photosensitive flavoproteins : from  
spectroscopy to understanding functional mechanisms"

**ITbM-RCMS Seminar**

**Dr. J. B. Brown**  
Assistant Professor, Department of Clinical System Onco-Informatics  
Graduate School of Medicine,  
Kyoto University

**Computational studies of photosensitive  
flavoproteins: from spectroscopy to  
understanding functional mechanisms**

**May 14th, 2015, 15:00-16:00**  
Chemistry Gallery  
Noyori Materials Science Laboratory 2F  
Language: English

Contact: Stephan Irie  
E-mail: irie@chem.nagoya-u.ac.jp

**RCMS & IGER Seminar**

“New Materials for Hybrid Photovoltaics”

**Lecturer : Dr. Neil Robertson**  
(University of Edinburgh)  
**Date : Sat. 6th June 13:30 – 15:30**  
**Place : SA321**

Sulfonate dye-sensitized solar cells (DSSCs) have shown promise as a light-weight, flexible and easily-fabricated photovoltaic technology. Efficiencies however, remain lower than that of liquid electrolyte DSSCs and new dyes and new hole-transport materials (HTM) are required to optimize these devices. Recently, perovskite solar cells, derived from inorganic absorbers and materials, have emerged as a new high-efficiency thin-film solar cell technology and these also require new HTMs with enhanced stability, charge stability and lower cost. The talk will introduce the above hybrid solar cells and will describe the design, synthesis, characterization and application of new dyes and HTMs.

Contact: Kunio Awaga (ext. 2487)

**June 6, 2015** Dr. Neil Robertson  
(University of Edinburgh)  
“New Materials for Hybrid Photovoltaics”

**IGER & RCMS Seminar**

**Professor Philip JESSOP**  
Queen's University, Canada

“Switchable Solvents”

**July 3<sup>rd</sup> (Fri) 2015, 16:30-18:00**  
Noyori Materials Science Laboratory 2F  
Conference Room

Contact: Susumu SAITO, ext. 5945  
: saito.susumu@f.mbox.nagoya-u.ac.jp

IGER  
プラットフォーム:  
グリーン物質実証コース

**July 3, 2015** Professor Philip JESSOP  
(Queen's University, Canada)  
“Switchable Solvents”

**RCMS & IGER Seminar**

“Magnetic Molecules and Hybrid Materials for Molecular Spintronics”

**Lecturer : Prof. EUGENIO CORONADO**  
(University of Valencia)  
**Date : Tue. 18th Aug. 13:30 – 15:00**  
**Place : SA321**

Spin-based electronics is one of the emerging frontiers in today's nanotechnology and the most active area within nanotechnology. In the meantime has been based on conventional materials like magnetic oxides and semiconductors. In 1, molecular electronics emerged several decades ago as a promising possibility to manufacture or even to replace conventional magnetic electronics when it goes into. In this system, a novel extension of molecular electronics is that of using magnetic molecules, as well as molecular-based materials, as components of new spintronic systems.

In the talk we explore into the laboratory one play in molecular electronics is highlighted. In the first part I will show that magnetic molecules based on lanthanide complexes are possible candidates of spin qubits which can be used as quantum computing. In the second part the manipulation of the spin through the temperature or through an electric field will be illustrated in molecules formed by spin-conjugated compounds. In the third part molecular materials will be designed in spintronic transistors in order to fabricate molecule-based spintronic devices. In particular, I will report the fabrication of spin-LED devices in which the light can be turned through a magnetic field.

Contact: Kunio Awaga (ext. 2487)

**August 18, 2015** Prof. EUGENIO CORONADO  
(University of Valencia)  
“Magnetic Molecules and Hybrid Materials for Molecular Spintronics”

**RCMS & IGER Seminar**

**新谷 亮 先生**  
東京大学大学院工学研究科化学生命工学専攻

「有機ケイ素化合物の選択的合成における新展開」

2015年9月7日 (月) 10:00-11:30  
野依記念研究館2F ケミストリーギャラリー

IGER  
プラットフォーム: グリーン物質実証コース

Host: 山口茂弘 (789-2291)

**September 7, 2015** Dr. Ryo Shintani  
(Department of Chemistry and Biotechnology,  
Graduate School of Engineering,  
The University of Tokyo)

**IGER & RCMS Seminar**

The Amazing Nonheme High-Valent Iron-Oxo Reaction Landscape

**Prof. Lawrence Que, Jr.**  
University of Minnesota

Sep. 30, 2015 13:00 ~ 14:30

Noyori Materials Science Laboratory 2F,  
Chemistry Gallery

Contact: Yoshitomo Watanabe  
E-mail: yoshi@nucc.nagoya-u.ac.jp

**September 30, 2015** Prof. Lawrence Que, Jr.  
(University of Minnesota)  
“The Amazing Nonheme High-Valent Iron-Oxo Reaction Landscape”

**IGER & RCMS Seminar**

**中村 慎吾 博士 (Shingo NAKAMURA)**  
(株) 産業革新機構 戦略投資グループ  
健康・医療チームディレクター

特定の mRNA を狙った低分子医薬品創出のこころみ:  
siRNA 様の効果を低分子で実現する

Sep 30<sup>th</sup> (Wed) 2015, 16:30-18:00  
Noyori Materials Science Laboratory 2F  
Nobel Prize Exhibition Room

Contact: Susumu SAITO, ext. 5945  
: saito.susumu@f.mbox.nagoya-u.ac.jp

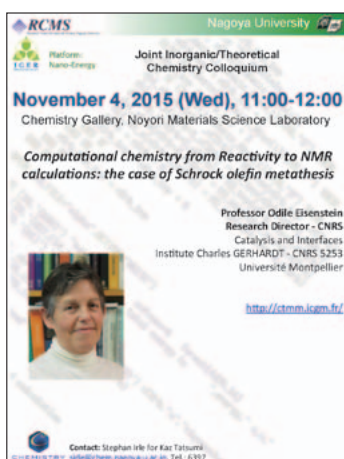
IGER  
プラットフォーム:  
システムバイオ

**September 30, 2015** Dr. Shingo Nakamura  
(Innovation Network Corporation of Japan: INCJ)



**October 20, 2015** Prof. Daniel B. Werz  
(Technical University of Braunschweig Germany)  
"Domino Reactions with Three-Membered Rings and Triple Bonds"

**November 2, 2015** Prof. Masahiro Yamashita  
(Department of Chemistry, Graduate School of Science,  
Tohoku University)



**November 4, 2015** Professor Odile Eisenstein, Research Director - CNRS  
(Catalysis and Interfaces Institute Charles GERHARDT - CNRS 5253  
Université Montpellier)  
"Computational chemistry from Reactivity to NMR calculations:  
the case of Schrock olefin metathesis"

**November 4, 2015** Prof. Légaré François  
(Institut national de la recherche scientifique-Centre Énergie,  
Matériaux, Télécommunications (INRS-ENT), Canada)  
"Ultrafast and biomedical imaging at the Advanced Laser Light Source"  
Part 1: Ultrafast, Part 2: Biomedical "

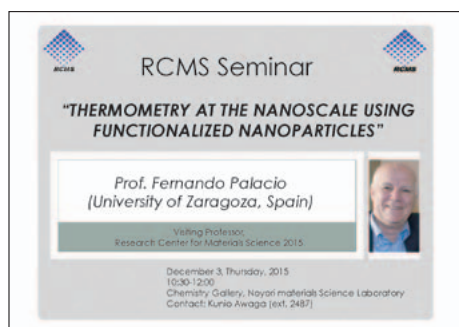


**November 4, 2015** Prof. Jin-Quan Yu  
(The Scripps Research Institute USA)  
"Developing diverse catalytic cycles for C-H activation reactions"



**November 30, 2015** Prof. Jeremiah A. Johnson  
(Department of chemistry, Massachusetts Institute of Technology, USA)  
"Closing the loop: towards control of structure and topology in polymers"

**November 30, 2015** Prof. Hiroki Oshio  
(Graduate School of Pure and Applied Sciences,  
University of Tsukuba)



**December 3, 2015** Prof. Fernando Palaco  
(University of Zaragoza, Spain)  
"THERMOMETRY AT THE NANOSCALE USING  
FUNCTIONALIZED NANOPARTICLES"

**January 15, 2016** Prof. Kazunari Domen  
(Graduate School of Engineering,  
The University of Tokyo)



**January 20, 2016** Prof. Tae-Lim Choi  
(Seoul National University, Korea)  
"Applying New Synthetic Methodologies to Versatile Polymerizations"



**RCMS, IGER, & ITbM Seminar**

**入江 正浩 先生**  
立教大学未来分子研究センター・教授  
名古屋大学物質科学国際研究センター・客員教授

**「光機能を創る」**



平成28年2月5日 (金) 16:00-17:30  
野依記念研究館2F 講演室  
連絡先：山口茂弘 (789-2291)

RCMS IGER ITbM

プラットフォーム：グリーン物質実演コース

February 5, 2016 Prof. Masahiro Irie  
(Research Center for Smart Molecules,  
Rikkyo University)


March 14, 2016 Dr. Carla Bittencourt  
(Department of Chemistry, Université de Mons, Belgium)  
"Scanning Photoelectron Microscopy as a tool to analyze  
plasma fluorinated graphene"

**RCMS** **Nagoya University**

Theoretical Chemistry Colloquium

**March 14, 2016 (Mon), 14:00-15:00**  
RCMS, 2<sup>nd</sup> floor, Chemistry Gallery

**Scanning Photoelectron Microscopy as a tool to  
analyze plasma fluorinated graphene**



Dr. Carla Bittencourt  
Department of Chemistry  
Université de Mons  
Mons, Belgium

**Abstract:** X-ray photoelectron spectroscopy (XPS) has been extremely used for probing the composition and electronic structure of solid surfaces and interfaces. The instruments using X-ray photon optics for demagnifying the photon beam to submicrometer dimensions are called scanning photoelectron microscopes (SPEM).

In the first part of the seminar we will discuss the recent developments in Scanning Photoelectron Microscopy (SPEM) and their use for analyzing functionalized graphene.

In the second part of the seminar we use the SPEM to compare the plasma fluorination of graphene using two different gases CF<sub>4</sub> and SF<sub>6</sub>. These results pave the way towards optimization of fluorination mechanism and selectivity in covalent modification of graphene chemistry.

Contact: Stephan Irie  
sirie@chem.nagoya-u.ac.jp, Tel: 6397

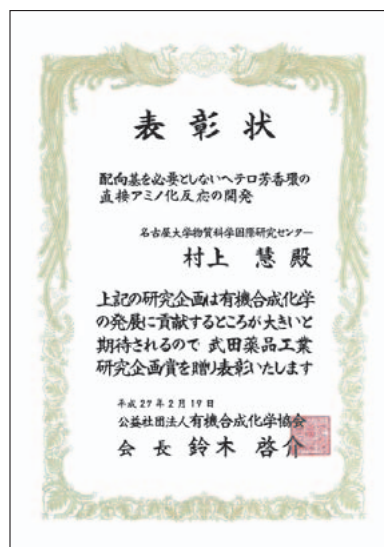
## Awards List 2015

Assistant Prof. Kei Murakami

**ITbM Research Award**



**Takeda Pharmaceutical Company Award  
in Synthetic Organic Chemistry, Japan**



# Chemistry Gallery

The Chemistry Gallery (2<sup>nd</sup> Floor of the Noyori Materials Science Laboratory) continued to host a large number of visitors in 2015.

This includes many high school students and their parents visiting Nagoya University to tour the Chemistry Gallery and follow University Professor Ryoji Noyori's steps in his path to receiving the Nobel Prize, as well as people who came to see special exhibitions held at the Gallery. In addition, the Gallery held many events such as seminars and lectures by overseas guest researchers. And also many people visited during Open Campus in August (641 people) and Nagoya University Home Coming Day in October. (1,200 people)



Guests from University of Strasbourg, France



Guest from Aichi prefecture office



Looking at the shine nobel medal



Kindergarten pupil



Visiting Prof. Palacio (right)

# This Year's Event



New waiting space in front of the guest professor's office



Setting of the wireless LAN system in the public space



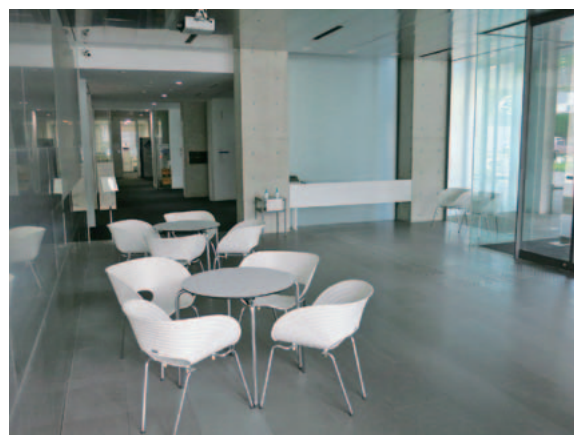
Repairing of the building model in the lobby



Renewed building model (Chemistry Gallery)



New Entrance Lobby



New Entrance Lobby

# Staff List

Director	Professor	Kunio Awaga	(2487)	awaga@mbx.chem.nagoya-u.ac.jp
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	Guest Professor	Palacio Fernand (Professor, Zaragoza University)		
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		Roald Hoffman (Professor Emeritus, Cornell University – Laureate, Nobel Prize in Chemistry)		
		Henri Boris Kagan (Professor Emeritus, Paris-Sud 11 University)		
		Atsuko Tsuji (Editorial Writer, Asahi Shimbun)		
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	Administrative Staff	Chiaki Yamamoto	(5902)	yamamoto@os.rcms.nagoya-u.ac.jp
	Administrative Staff	Sonoe Tankiku	(5908)	tankiku@os.rcms.nagoya-u.ac.jp