



# RCMS NEWS

# 18

2017

NAGOYA UNIVERSITY  
RESEARCH CENTER FOR MATERIALS SCIENCE

Reports and Communications of RCMS Activities  
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May 2017  
Issue #18



## CONTENTS

Integrated Research Consortium on Chemical Sciences .....	2
The 20 <sup>th</sup> Joint Seminar, Core-to-Core Program .....	4
Research Topic .....	6
New Faculty Member .....	8
Integrative Graduate Education and Research Program in Green Natural Sciences .....	10
Report from the Chemical Instrumentation Facility .....	11
Visiting Professor 2016 .....	12
RCMS Seminars .....	14
Chemistry Gallery .....	18
Events 2016 .....	19
Staff List .....	20



# Integrated Research Consortium on Chemical Sciences Established in 2016

In April 2016, the Research Center for Materials Science at Nagoya University established the Integrated Research Consortium on Chemical Sciences with cooperation from the Institute for Catalysis at Hokkaido University, the Science Institute for Chemical Research at Kyoto University, and the Institute for Materials Chemistry and Engineering at Kyushu University.

On June 22 (Wed.) of 2016, an opening ceremony for the Consortium and commemorative lecture was held at the 2nd-Floor Conference Room of the Noyori Materials Science Laboratory. A kick-off symposium was held on the following day. Without delaying the succession of initiatives from the MEXT Project of Integrated Research on Chemical Synthesis which finished in the 2016 academic year, the Consortium will serve as a core international research organization in materials synthesis.

## Opening Ceremony for the Consortium and Commemorative Lecture

(June 22–23, 2016)



Greetings, Director, Prof. Tatsumi



Greetings, President, Prof. Matsuo



Prof. Amano



Prof. Noyori



Congratulate address, MEXT, Mr. Ushio



Prof. Itami



Prof. Erker



Invited, Prof. Takimiya

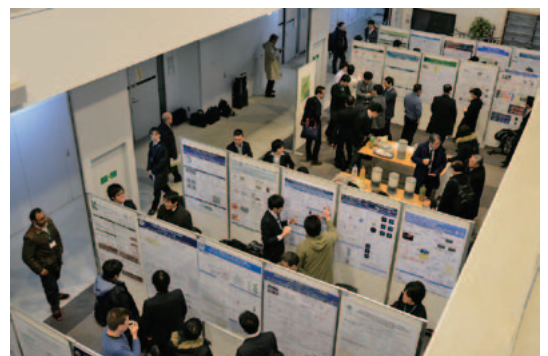
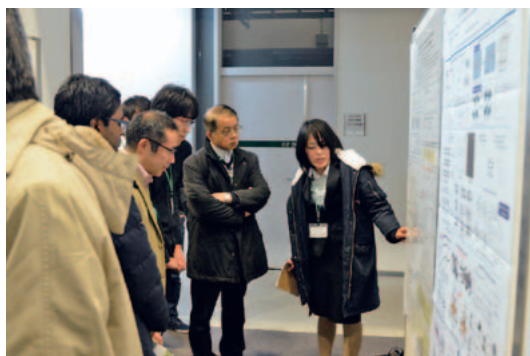


Poster session

IRCCS 2<sup>nd</sup> Symposium, Hokkaido \*\*\*\*\*  
(January 26–27, 2017)



Prof. Kobayashi, The U. of Tokyo



# Core-to-Core Program

## The 20<sup>th</sup> Joint Seminar

As part of the Core-to-Core Program “Strategic Research Networks (Type A)” operated by the Japan Society for the Promotion of Science (JSPS), the program “Elements Function for Transformative Catalysis and Materials” is promoted by the Research Center for Materials Science and the Department of Chemistry, Graduate School of Science at Nagoya University, with Professor Shigehiro Yamaguchi serving as Project Coordinator. This program was selected for the Core-to-Core Program in the 2014 academic year as a successor to the Japanese-German Graduate Externship and The JSPS Strategic Young Researcher Overseas Visits Program for Accelerating Brain Circulation, two programs which were conducted to provide overseas experience at a young age for outstanding young researchers expected to perform internationally. In this program, joint research and dispatch of researchers is actively performed with the participating institutions at the University of Munster (Germany), the Technical University of Berlin (Germany), Queen’s University (Canada), and Kyoto University (Japan).

The 2016 academic year featured the 20<sup>th</sup> Joint Seminar when counting from the Japanese-German Graduate Externship program. The Seminar was held at Queen’s University, marking the first time that the event was held in Canada. “Boron in the Americas – Boram 2016” had been held at Queen’s University immediately prior to the 20<sup>th</sup> Joint Seminar, and many researchers who had attended Boram 2016 also attended the symposium. Researchers participating in joint research for the program were asked many questions by researchers who had come to listen to the symposium. The Joint Seminar was a lively and extremely meaningful event.

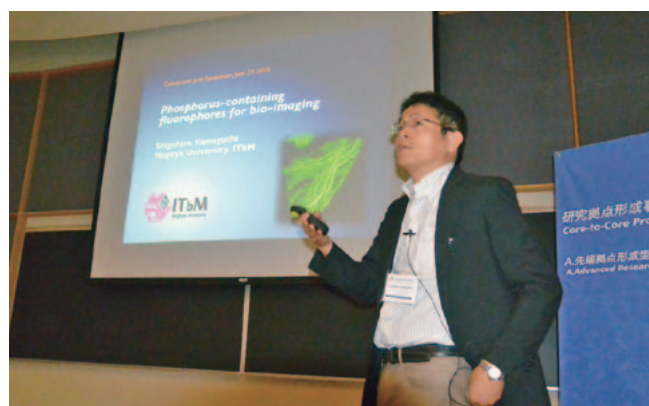
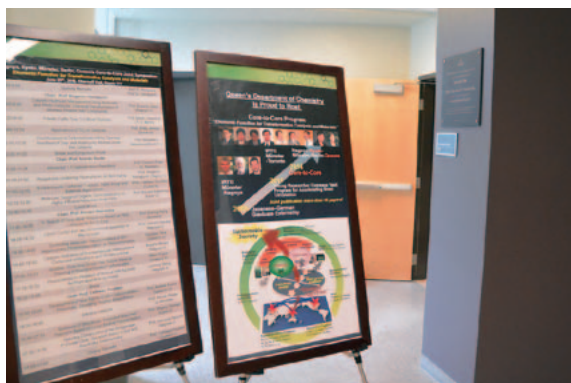
### The 20<sup>th</sup> Joint Seminar

**June 29 (Wed.), 2016; held at Queen’s University, Canada**

Participants from Japan: 7 professors, 4 students (oral presentation)

Participants from Canada: 20 professors, approx. 70 students

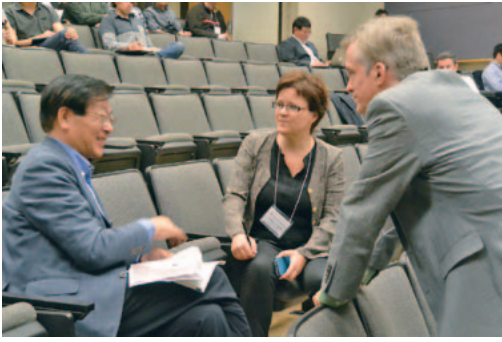
Participants from Germany: 7 professors, 5 students (oral presentation by all participants)



Prof. Yamaguchi



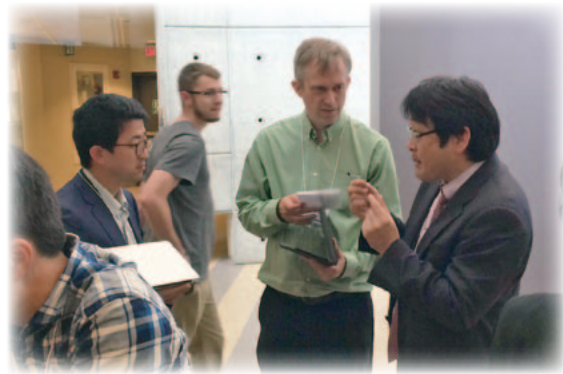
Opening, Prof. Wang



Ms. Mihara, student from Nagoya



Prof. Erker



Prof. Saito



Mr. Wang, student from Nagoya



Closing, Prof. Crudden



Group photo

## Research Topic

(Functional Materials)

# Visualizing photoexcitation in a molecule by laser tunneling ionization imaging

Electron motion governs bond-breaking and bond-making between molecules. Shooting movies of electrons is thus a long-standing goal of physicists and chemists pursuing a deeper understanding of chemical reactions. Laser tunneling ionization is a promising approach towards this goal that requires a high temporal resolution in the femtosecond range or shorter. In fact, the laser tunneling ionization has been successfully applied to static imaging of ground-state molecules. On the other hand, the applicability to excited states is not trivial. This is because of their small ionization potentials, which may introduce significant contributions from multiphoton process (instead of tunneling) to the ionization. Supported by quantitative comparisons with solid theories, the present study on nitric oxide (NO) demonstrates that the laser tunneling imaging can visualize the electron distribution in a short-lived, excited molecules and the change upon photoabsorption. The present study<sup>[1]</sup> demonstrates the visualization of photoexcitation in a molecule – a model reaction involving electron rearrangement – by laser tunneling ionization, thus suggesting a route to shoot ultrafast electron movies during chemical reactions.

We adopted NO as the target, which has a low-lying electronic state ( $A^2\Sigma^+$ ) in the deep UV range (226 nm) from the ground state ( $X^2\Pi$ ) (Fig.1). The ion

image of  $N^+$  fragment ions produced by dissociative tunneling ionization of NO in the ground state,  $NO(X^2\Pi, 2\pi) \rightarrow NO^+ + e^- \rightarrow N^+ + O + e^-$ , exhibits a characteristic momentum distribution peaked at  $45^\circ$  to the laser polarization direction. Since the tunneling ionization rate is determined by the shape of HOMO along the laser electric field, the structure of the  $2\pi$  orbital appears in the ion image. On the other hand, a broad distribution centered at  $\sim 0^\circ$  is seen when the  $A^2\Sigma^+$  excited state (with the  $3s\sigma$  HOMO of a Rydberg character) is prepared as the initial state by deep-UV photoexcitation. The observed angular distributions are in good agreement with the predictions by weak-field asymptotic theory (WFAT) of tunneling ionization, showing that the laser tunneling ionization can probe changes in the highest-occupied molecular orbital by photoexcitation.



### Reference

- [1] T. Endo, A. Matsuda, M. Fushitani, T. Yasuike, O. I. Tolstikhin, T. Morishita and A. Hishikawa, Phys. Rev. Lett. 116 (2016) 163002 (5 pages).

(Akiyoshi HISHIKAWA)

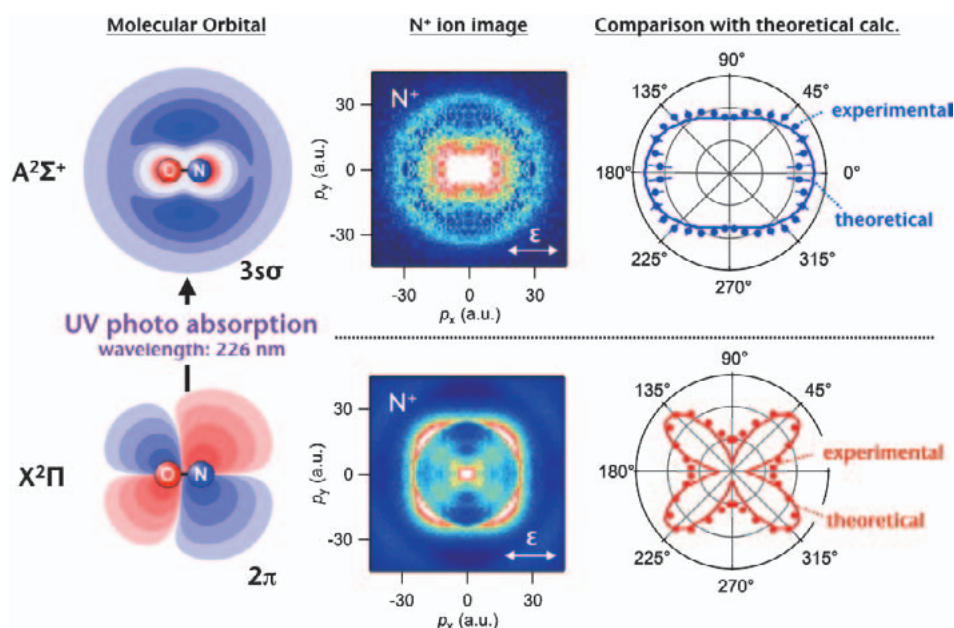


Figure 1. Molecular orbitals before and after UV photoexcitation (226 nm) of NO (left). Experimental results (middle) and comparison with theoretical predictions (right).

# Research Topic

## (Inorganic Synthesis)

# Development of Imaging XAFS Techniques and Visualization of Heterogeneous Catalysts

Heterogeneous solid catalysts act as key materials for various chemical conversions in industry and their high stability and catalytic performances are often unique for solid catalysts. However, it is still difficult to visualize heterogeneous structures of solid catalysts, which obtain their unique reactivity, and the nature and dynamic behaviors of heterogeneous catalysis are not fully understood yet. X-ray absorption fine structure (XAFS) is a powerful tool to characterize local structures of solid catalysts without crystal structures, which cannot be characterized by X-ray diffraction analysis, and it has been applied for the characterization of various heterogeneous catalysts. Conventional XAFS measurements have been performed using mm-size X-ray beams, and average structural information inside mm-size X-ray beam irradiated to a sample is obtained. Spatial information is reduced to 1 dimensional data by the conventional XAFS and the developments of imaging XAFS techniques with two/three-dimensional spatial information are state-of-the-art.

We have developed several imaging XAFS techniques by use of high-flux synchrotron X-ray source and they have been applied to visualize two/three-dimensional structures of functional solid materials such as heterogeneous catalysts and fuel cell electrode membranes<sup>[1,2]</sup>. Particularly, two-dimensional scanning nano-XAFS has a simple optical setup and X-ray imaging combining XAFS spectroscopy is developed by using 100 nm-size focused X-ray nanobeam<sup>[2]</sup>. Recently, we succeeded in imaging of Ce oxidation states inside a single particle of Ce-Zr solid solution, which is a key material of automobile exhausting process, for oxygen storage and release (OSC) processes. Imaging XAFS clearly showed that the mode of oxygen diffusion in the Ce-Zr solid solution particles for the OSC process<sup>[3]</sup>.

Figure 1 shows two-dimensional mapping of Ce oxidation state inside a single  $\text{Ce}_2\text{Zr}_2\text{O}_x$  ( $x = 7-8$ ) particle at-

tached with a Pt catalyst particle imaged by scanning nano-XAFS using focused X-ray nanobeam of  $409 \times 154$  nm. We determined the positions of Pt particles and  $\text{Ce}_2\text{Zr}_2\text{O}_x$  particles on a substrate by SEM images and selected a  $\text{Ce}_2\text{Zr}_2\text{O}_x$  particle attaching with a Pt particle. After the reduction with  $\text{H}_2$  at 573 K, oxygen storage proceeds into the  $\text{Ce}_2\text{Zr}_2\text{O}_x$  bulk by a reaction with  $\text{O}_2$ , changing the Ce oxidation state from 3+ to 4+. The oxygen storage was not completed at 423 K and the 2D mapping of the Ce valence state showed heterogeneous distribution of the Ce oxidation state inside the  $\text{Ce}_2\text{Zr}_2\text{O}_x$  particle (Fig. 1 (1)). Similar heterogeneous distribution was observed for other  $\text{Ce}_2\text{Zr}_2\text{O}_x$  particles, indicating that heterogeneous reaction modes of the oxygen storage process, independent to the position of the attaching Pt catalyst.

The reverse oxygen release process proceeds by the reduction with  $\text{H}_2$ , changing in the Ce oxidation state from 4+ to 3+. For the reduction process, significant differences in the reactivity of  $\text{Ce}_2\text{Zr}_2\text{O}_x$  particles by the imaging XAFS. The reduction of a  $\text{Ce}_2\text{Zr}_2\text{O}_x$  particle without the attaching Pt particle was slow and did not complete.  $\text{Ce}_2\text{Zr}_2\text{O}_x$  particles with the attaching Pt particle were smoothly reduced and it was visualized that the reaction spread from the interface of the Pt and  $\text{Ce}_2\text{Zr}_2\text{O}_x$  (Fig. 1 (2)). These results suggested that the oxygen release proceeded from the Pt catalyst and oxygen diffusion spread in the  $\text{Ce}_2\text{Zr}_2\text{O}_x$  bulk. The supported Pt catalyst would support the heterogeneous reactivity of the  $\text{Ce}_2\text{Zr}_2\text{O}_x$  particles and improve the overall reactivity.

Imaging XAFS can visualize distribution and chemical states of each elements in solid materials and would provide heterogeneous structures, reactivity, reaction modes, and phenomena of solid heterogeneous materials.

## References

- [1] T. Saida, O. Sekizawa, N. Ishiguro, K. Uesugi, M. Hoshina, T. Uruga, S. Ohkoshi, T. Yokoyama, and M. Tada, *Angew. Chem. Int. Ed.* **51**, 9361-9365 (2012) (Hot paper).
- [2] N. Ishiguro, T. Uruga, O. Sekizawa, T. Tsuji, M. Suzuki, N. Kawamura, M. Mizumaki, K. Nitta, T. Yokoyama, and M. Tada, *ChemPhysChem* **15**, 1563-1568 (2014).
- [3] H. Matsui, N. Ishiguro, K. Enomoto, O. Sekizawa, T. Uruga, and M. Tada, *Angew. Chem. Int. Ed.* **55**, 12022-12025 (2016).

(Mizuki TADA)

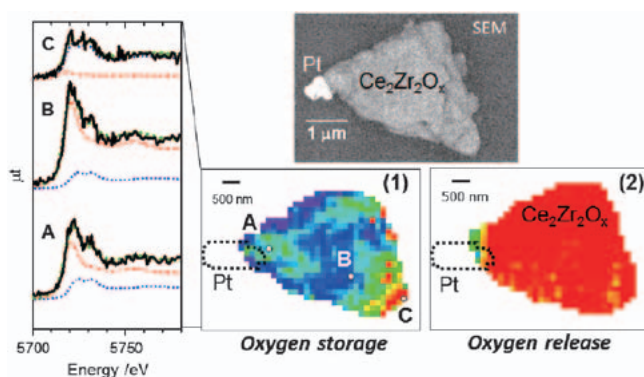


Figure 1.  $\text{Ce L}_{\text{III}}$ -edge scanning nano-XAFS spectra (left), SEM (top), and Ce oxidation-state mappings (1 and 2) of a Pt-attached  $\text{Ce}_2\text{Zr}_2\text{O}_x$  particle. (1) Oxygen storage process, (2) oxygen release process.

## New Faculty Member

(Organic Synthesis)

# Material Design based on Living Supramolecular Polymerization

Molecular organization of  $\pi$ -conjugated molecules in a highly ordered manner is an attractive methodology for the development of materials with photo/electronic functions beyond those of molecules. An important class of materials in the field of supramolecular chemistry is supramolecular polymers, which have recently been shown to be synthesized precisely by kinetics, as distinct from thermodynamics. During my postdoctoral career under the guidance of Profs. Masayuki Takeuchi and Kazunori Sugiyasu at National Institute for Materials Science, we have investigated the supramolecular polymerization of porphyrin-based monomers. The assembly phenomenon was found to occur for a delicate interplay of two aggregation pathways based on a kinetic formation of nanoparticles and a formation of thermodynamically stable nanofibres (**Figure 1**). Interestingly, the supramolecular polymerization, which was temporally retarded by the nanoparticle formation, could be initiated by an addition of an aliquot of fragmented nanofibres. Despite the non-covalent polymerization, the kinetics of seed-induced supramolecular polymerization was analogous to those of conventional chain growth polymerization. Thus, we have demonstrated living supramolecular polymerization that enable us to synthesize supramolecular polymers with controlled length and narrow polydispersity.<sup>[1]</sup>

Furthermore, the thermodynamic and kinetic supramolecular polymerizations have been elucidated for an amide-functionalized perylene bisimide (PBI)

organogelator molecule during my postdoctoral career in the Würthner Group at Würzburg University.

This molecule in solvents of low polarity self-assembles by the concerted hydrogen-bonding and  $\pi$ - $\pi$  stacking interactions into highly defined one-dimensional helical nanofibers.<sup>[2]</sup> Spectroscopic studies on the polymerization process revealed that the monomers are kinetically trapped in conformationally restricted state through intramolecular hydrogen bonding between the amide and imide groups. The unique kinetics in the nucleation process was confirmed as a thermal hysteresis in a cycle of assembly and disassembly processes. Under the out-of-equilibrium condition within the hysteresis loop, we have succeeded in demonstrating seeded polymerization by addition of a supramolecular initiator (e.g., pre-assembled short nanofibers) to the kinetically trapped monomer solution.<sup>[3,4]</sup>

The kinetic and mechanistic understanding in the process of molecular organization will open up a new aspect in the design of functional soft matters for applications including the areas of organic electronics and biology. The materials design based on living supramolecular polymerization are currently under investigation in the Yamaguchi Group.

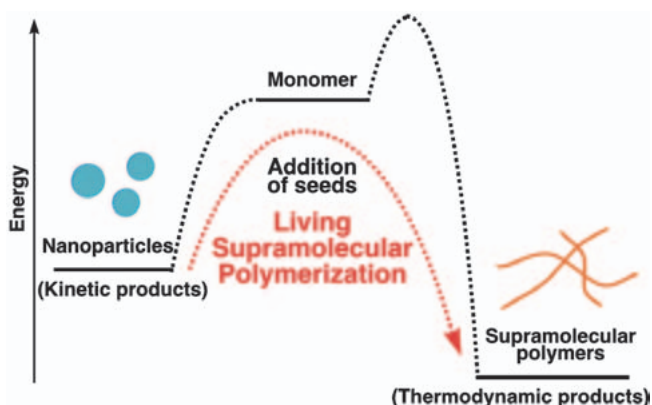


Figure 1. Energy landscape of two competing aggregation pathways of porphyrin-based monomers.

### References

- [1] Ogi, S.; Sugiyasu, K.; Manna, S.; Samitsu, S.; Takeuchi, M. *Nat. Chem.* **2014**, *6*, 188-195.
- [2] Würthner, F.; Saha-Möller, C. R.; Fimmel, B.; Ogi, S.; Leowanawat, P.; Schmidt, D. *Chem. Rev.* **2016**, *116*, 962-1052.
- [3] Ogi, S.; Stepanenko, V.; Sugiyasu, K.; Takeuchi, M.; Würthner, F. *J. Am. Chem. Soc.* **2015**, *137*, 3300-3307.
- [4] Ogi, S.; Stepanenko, V.; Thein, J.; Würthner, F. *J. Am. Chem. Soc.* **2016**, *138*, 670-678.

(Soichiro OGI)



# New Faculty Member

(Organic Synthesis)

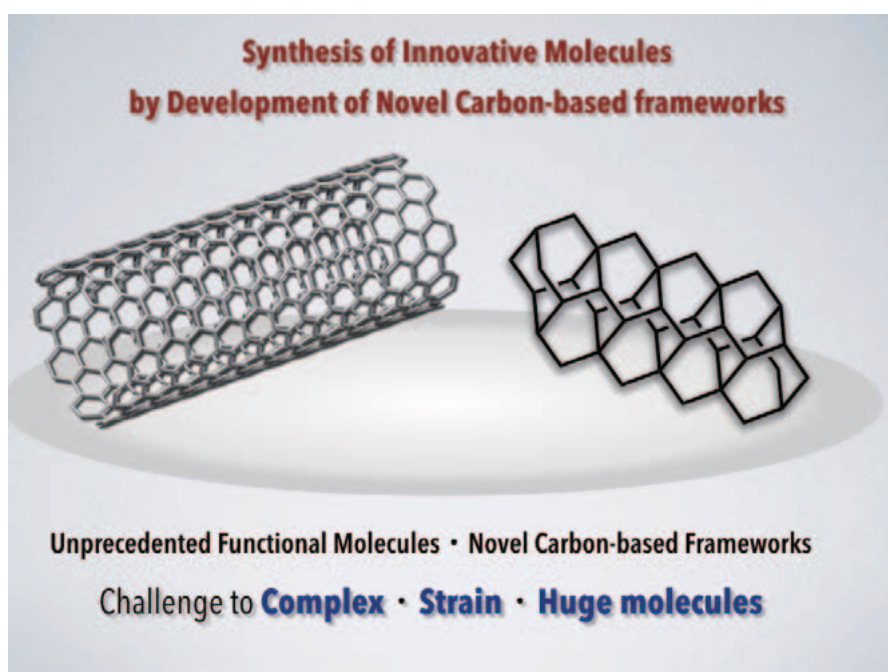
## Synthesis of Innovative Molecules by Development of Novel Carbon-based frameworks

Due to drastic development of organic synthetic chemistry, easy access to various complicated molecules has been enabled. However, current technology still has a significant hurdle to provide some organic molecules. In most cases of such unprecedented molecules, the construction of carbon-based frameworks is difficult because of their strain, large size and so on. Therefore, new synthetic methods to overcome these problematic properties are strongly demanded.

We started to pursue the development of a methodology to construct novel carbon-based frameworks towards synthesis of innovative molecules. Our ultimate goal is making a huge progress in whole science by advancement of organic synthetic chemistry.



(Akiko YAGI)



# 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.

In 2016, the program provided opportunity for 63 students to participate in international conferences held at outside Japan, and also provided opportunity of mid-term (2–3 months) overseas research exchange for 14 students. Furthermore, the program hosted various international symposium / workshop where lots of students could have opportunities to discuss with foreign researchers.

Eleven students participated in the Leadership Program at North Carolina (NC), US. All students not only attended lectures regarding Leadership, Entrepreneurship and Technology Transfer but also visited many laboratories in universities at NC 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. In the last day, Prof. Matsuo, the president of Nagoya University, attended the final presentations of the students and the farewell party.



Poster Prize



Overseas Research Exchange



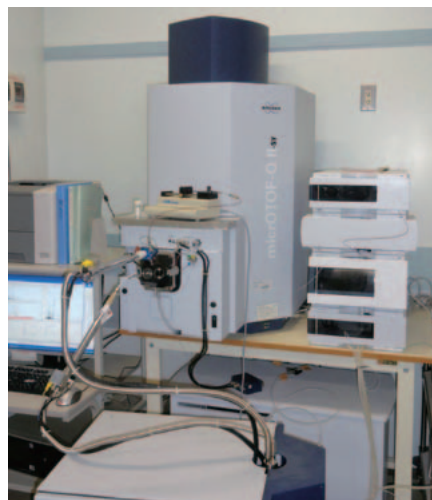
IBM WATSON (NC Program)



Final Presentation (NC Program)

# 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 2016 fiscal year, as shown in "CIF Utilization Status", 71 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 718.



CSI-MS (micrOTOF-QII, Bruker)



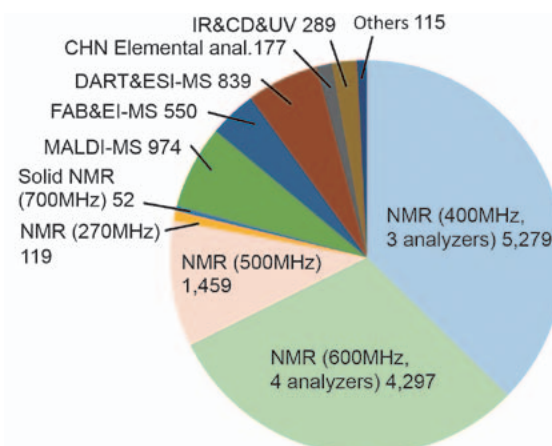
NMR (ECA-600, JEOL)



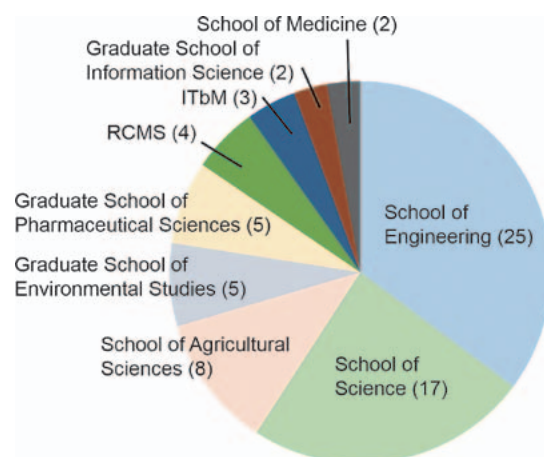
CHN Elemental analyzer, (MT-6, YANACO)

## [CIF Utilization Status]

Utilization Status for the Academic Year 2016  
(April 2016 – April 2017)



Number of Uses/Measurements by Instrument



Utilization Status by Department  
(Total: 71 Groups, 718 People)

## Visiting Professor 2016

### Prof. Eric Rivard

Associate Professor,  
University of Alberta

Period of Stay:

April 25, 2016 – June 26, 2016

Research Theme:

Chemistry of Functional Organo-Main Group Compounds



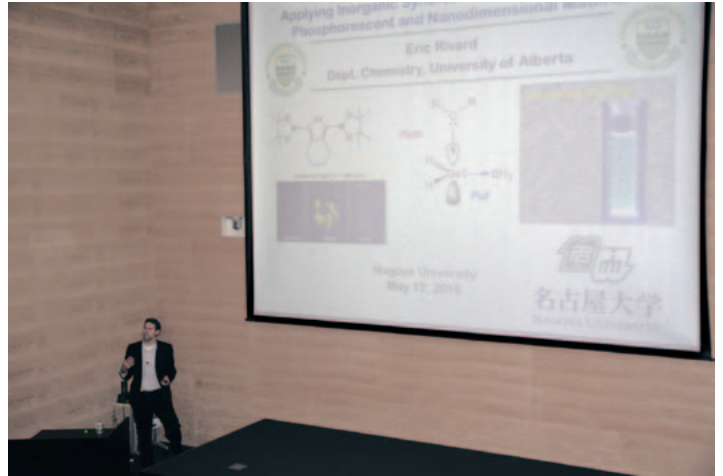
Prof. Eric Rivard from University of Alberta, Canada, stayed as a Visiting Associate Professor in RCMS for two months from April 25th, 2016 to engage in the research about chemistry of functional organo-main group compounds. Prof. Rivard is a highly distinguished young researcher in the field of inorganic chemistry and, particularly, main group chemistry focusing molecular functions.

His chemistry covers broad aspects from the fundamental structural main group chemistry to catalysis as well as electronic functions. For example, his outstanding discovery of room temperature phosphorescence of tellurophene boronic acids gave significant impact on the relevant research community. He has also promoted main group chemistry focusing intriguing structures and reactivity, such as reactive element hydride chemistry and oligogermanium synthesis. To promote these researches in depth, he has visited us and stayed in RCMS.

During his stay, he actively participated in the research in RCMS. He delivered a wonderful lecture on May 12, 2016 with the title of "Applying Inorganic Synthesis to Gain Access to New Phosphorescent and Nanodimensional Materials". Moreover, he also kindly joined group meetings in our research group and gave us many insightful suggestions. He always discussed with our students with great enthusiasm. In addition, he also kindly delivered classes in the graduate course about advanced polymer science. Many students participated were impressed by his elegant lectures with clear explanation. Prof. Eric also enjoyed laboratory parties many times, where he indeed talked with students very frankly and always encouraged them. We all would like to appreciate his significant contributions to the activities in RCMS.



Welcome party



Seminar



With assist. Prof. Ogi



With Prof. Yamaguchi



Farewell party



Farewell party

# RCMS Seminars

**April 19, 2016** Prof. Michael Haley  
 (Department of Chemistry and Biochemistry, University of Oregon, USA)  
 "Indenofluorenes and Quinoidal Analogues  
 – A New Class of Electron-Accepting Materials"



ITAMI  
ERATO-ITbM-IGER-RCMS  
**Seminar**

**Prof. Michael Haley**  
 Department of Chemistry and Biochemistry  
 University of Oregon  
 USA

*Indenofluorenes and Quinoidal Analogues –  
 A New Class of Electron-Accepting Materials*

Date: Apr 19, 2016  
 Time: 16:00~17:30  
 Lecture Room  
 Noyori Materials Science Laboratory 2F  
 Language: English

Contact:  
 Kenichiro Itami  
 Email: itami@chem.nagoya-u.ac.jp  
 Yasutomo Segawa  
 ysegawa@nagoya-u.jp  
 Aki (Matsuoka) Miura  
 matsuoka.aki@f.mbox.nagoya-u.ac.jp



**RCMS-IGER-ITbM Seminar**

**Prof. Eric Rivard**  
 University of Alberta, Canada

*"Applying Inorganic Synthesis to Gain Access to  
 New Phosphorescent and Nanodimensional Materials"*

May 12, 2016 (Thur) 16:00~17:30  
 Noyori Materials Science Laboratory 2F,  
 Lecture Hall  
 Host: Shigehiro Yamaguchi (789-2291)

IGER  
 NAGAYA UNIVERSITY

プラットフォーム・グリーン物質変換コース

**May 12, 2016** Prof. Eric Rivard  
 (University of Alberta, Canada)  
 "Applying Inorganic Synthesis to Gain Access to New  
 Phosphorescent and Nanodimensional Materials"

**July 19, 2016** Dr. Michael J. Shevlin  
 (Senior Scientist, Chemistry MSD, USA)  
 "High-Throughput Experimentation-Enabled Reaction  
 Discovery, Development, and Mechanistic Elucidation:  
 Cobalt- and Nickel- Catalyzed Asymmetric Hydrogenation  
 of Olefins"



**PS-IGER-RCMS SEMINAR**

**Dr. Michael J. Shevlin**  
 Senior Scientist, Chemistry  
 MSD, USA

*"High-Throughput Experimentation-Enabled Reaction Discovery,  
 Development, and Mechanistic Elucidation: Cobalt- and Nickel-  
 Catalyzed Asymmetric Hydrogenation of Olefins"*

July 19, 2016 (Tue) 16:30-  
 Noyori Materials Science Laboratory 2F, Lecture Room

Host: Masato Kitamura  
 Graduate School of Pharmaceutical Sciences

IGER



**CtC • RCMS • IGER Seminar**

**"Synthesis and Structure of  
 Group 16 systems"**

**Lecturer : Prof. J Derek Woollins**  
 (University of St Andrews)  
 Date : Wed. 31st Aug. 15:30 – 17:00  
 Place : Chemistry Gallery

This talk will describe the synthesis, structural studies and applications of sulfur, selenium and tellurium compounds. Small molecule S-N chemistry, metal-S-N chemistry, P-S, P-Se and P-Te heterocycles as well as imidylphosphate complexes will be described. Recent work on developing automated chemical crystallography (joint with A.M.Z. Slawin) will also be described.

Contact: Kunio Awaga (ext. 2487)

**August 31, 2016** Prof. J Derek Woollins  
 (University of St Andrews)  
 "Synthesis and Structure of Group 16 systems"

RCMS Nagoya University

Platform: Theoretical Chemistry Colloquium  
Nano-Energy

**October 14, 2016 (Fri), 16:00-17:00**  
RCMS, 2<sup>nd</sup> floor, Chemistry Gallery

**Low dimensional nanomaterials. Theoretical predictions and experimental support**

**Dr. Dmitry G. Kvashnin**  
Emanuel Institute of Biochemical Physics Russian Academy of Sciences, Moscow, Russia & National University of Science and Technology "MISIS", Moscow, Russia

**Abstract:** Successful synthesis of graphene opens a new field in material sciences - the field of low dimensional materials. Nowadays a high number of scientific groups over the world take many attempts to fabricate and investigate novel two dimensional materials with unexpected physical and chemical properties. This presentation is devoted to the theoretical investigation of low dimensional materials with various compounds. Using classical molecular dynamic calculations the unusual effect of hardening of graphene with the low concentration of vacancy defects was described from atomistic point of view (J. Phys. Chem. Lett., 6, 2384 (2015)). By means of ab initio calculations the physical properties of novel two-dimensional materials based on bilayered graphene and copper oxide were studied in details. All obtained results were confirmed by experimental data (Nano Research 8 (4)-1250 (2015), NanoScale (2016), submitted).

Contact: Stephan Irie  
siri@itbm.nagoya-u.ac.jp Tel.: 6397

**October 14, 2016** Dr. Dmitry G. Kvashnin  
(Emanuel Institute of Biochemical Physics Russian Academy of Sciences, Moscow, Russia & National University of Science and Technology "MISIS", Moscow, Russia)  
"Low dimensional nanomaterials. Theoretical predictions and experimental support"

**IGER-ITbM-RCMS Seminar**

**Prof. Evamarie Hey-Hawkins**  
University Leipzig, Germany

*"Carborane Meets Phosphorus"*

**October 18, 2016 (Tue) 13:00-14:30**  
Institute of Transformative Bio-Molecules (ITbM) 1F, Lecture Room

Host: Shigehiro Yamaguchi (789-2291)

IGER  
NAGOYA UNIVERSITY

プラットフォーム: グリーン物質変換コース

**October 18, 2016** Prof. Evamarie Hey-Hawkins  
(University Leipzig, Germany)  
"Carborane Meets Phosphorus"

**IGER and RCMS Seminar**

**"Structural Diversity in Copper(II) Complexes Influenced by External Factors - Structural and Magnetic Studies."**

**Assist. Prof. Sailaja S. Sunkari**  
Department of Chemistry,  
Mahila Mahavidyalay of Banaras Hindu University, India

**Nov. 1<sup>st</sup>, 2016 (Tue) 16:00-17:00**  
Noyori Materials Science Laboratory  
Chemistry Gallery

Contact: Satoshi Muratsugu (6093)  
E-mail: smuratsugu@chem.nagoya-u.ac.jp

IGER

**November 1, 2016** Assist. Prof. Sailaja S. Sunkari  
(Department of Chemistry, Mahila Mahavidyalay of Banaras Hindu University, India)  
"Structural Diversity in Copper(II) Complexes Influenced by External Factors - Structural and Magnetic Studies"

**November 4, 2016** Prof. Roald Hoffmann  
(Novel Laureate (1981, Chemistry), Cornell University, USA)  
"Two new games for carbon, we hope"

**ITbM-RCMS Seminar**

**Prof. Roald Hoffmann**  
Novel laureate (1981, Chemistry)  
Cornell University, USA

*"Two new games for carbon, we hope"*

Date: 4 November, 2016  
Time: 13:30-15:30  
Lecture Room  
Noyori Materials Science Laboratory 2F  
Language: English

Contact:  
Kenichiro Itami  
E-mail: itami@chem.nagoya-u.ac.jp

**IGER & RCMS Seminar**  
**Engineered metalloenzymes for selective carbene and nitrene transfer reactions**



**Prof. Rudi Fasan**  
 University of Rochester  
 Nov. 8, 2016 16:00 ~ 17:00  
 Noyori Materials Science Laboratory  
 Chemistry Gallery



up to 99% conversion  
 up to 11,300 turnovers  
 $k_{cat}/K_M = 4.8 \times 10^5 \text{ M}^{-1} \text{ s}^{-1}$  (benzyl azide)

Contact: Osami Shoji  
 E-mail: shoji.osami@a.mbox.nagoya-u.ac.jp

**November 8, 2016** Prof. Rudi Fasan  
 (University of Rochester)  
 "Engineered metalloenzymes for selective carbene and nitrene transfer reactions"

**November 9, 2016** Professor Mark Gandelman  
 (Technion – Israel Institute of Technology, Israel)  
 "New Bonding and Reactivity: Chemistry of N-Cations and N-Radicals"

**IGER & RCMS Seminar**



**Professor Mark Gandelman**  
 Technion – Israel Institute of Technology  
 Israel


**"New Bonding and Reactivity: Chemistry of N-Cations and N-Radicals"**

**November 9<sup>th</sup> (Wed) 2016, 15:30–17:00**  
 Noyori Materials Science Laboratory 2F  
 Conference Room

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

**RCMS • IGER Seminar**

**"LANTHANIDES-TTF COMPLEXES DISPLAYING SINGLE MOLECULE MAGNET BEHAVIOUR AND LUMINESCENCE"**



**Lecturer : Prof. Lahcène OUAHAB**  
 (Université de Rennes)  
**Date : Wed. 9th Nov. 15:30 – 17:00**  
**Place: Noyori Materials Science Laboratory Chemistry Gallery**


Lanthanide-based complexes have greatly contributed to the development of molecular magnets in the last decade and more particularly in the branch of single molecule magnets (SMMs). The main reasons are their large magnetic moments associated to their intrinsic large magnetic anisotropy. The splitting of the multiple ground state of a singlet in a given environment is responsible of the trapping of the magnetic moment in one direction in SMMs. However, the analysis of the crystal field effects on the magnetic anisotropy are not so common. A better understanding of the magneto-structural correlation in lanthanide-based complexes should provide tools to improve their potentialities. In this presentation we will focus on the specific magnetic properties of TTF-based lanthanide mononuclear and polynuclear complexes. We will show how optimize the SMM behavior playing on i) the modulation of the supramolecular effects via chemical modification of the TTF ligand, ii) single molecular engineering modifying the structure, distribution and symmetry of the coordination polyhedron, iii) magnetic dilution (inclusion and doping) and iv) entropic enrichment of the dysprosium.

Contact: Kunio Awaga (ext. 2487)

**November 9, 2016** Prof. Lahcène OUAHAB  
 (Université de Rennes)  
 "LANTHANIDES-TTF COMPLEXES DISPLAYING SINGLE MOLECULE MAGNET BEHAVIOUR AND LUMINESCENCE"

**November 16, 2016** Prof. Amir H. Hoveyda  
 (Department of Chemistry, Boston College, USA)  
 "New Concepts, Catalysts and Methods in Catalytic Olefin Metathesis"

**PS-IGER-RCMS SEMINAR**



**Prof. Amir H. Hoveyda**  
 Department of Chemistry  
 Boston College, USA

**"New Concepts, Catalysts and Methods in Catalytic Olefin Metathesis"**

November 16, 2016 (Wed) 14:00-  
 Noyori Materials Science Laboratory 2F, Lecture Room

Host: Masato Kitamura  
 Graduate School of Pharmaceutical Sciences



**IGER & RCMS Seminar**

光または電気化学的活性化を用いた  
バイオインスパイアード触媒の創製と機能開拓



九州大学大学院工学研究院  
**久枝良雄 先生**

2016年11月16日 16:30 ~ 18:00  
野依記念物質科学研究館講演室



Vitamin B<sub>12</sub>  
C21H38CoN6O14P



IGER  
NAGOYA UNIVERSITY


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

**November 16, 2016** Prof. Yoshio Hisaeda  
(Graduate School of Engineering, Kyushu University)

**January 23, 2017** Prof. Jonathan Nitschke  
(University of Cambridge)  
“How Does Self-Assembly Work in Groups?  
Towards an Understanding of Molecular Sociology”

**IGER & RCMS Seminar** RCMS

“How Does Self-Assembly Work in Groups?  
Towards an Understanding of Molecular Sociology”



**Prof. Jonathan Nitschke**  
University of Cambridge

**Jan. 23, 2017 16:30-17:30**  
Noyori Materials Science Laboratory 2F, Lecture Room

Contact: Kentaro Tanaka (2940)  
E-mail: kentaro@chem.nagoya-u.ac.jp

**CiC-RCMS-IGER Seminar** IGER

“Tales from the Supramolecular Photochemistry Crypt”



**Lecturer : Dr. Eli Zysman-Colman**  
(University of St Andrews)  
**Date : Tue. 24th Jan. 15:30 – 17:00**  
**Place: Lecture Room No3 (C-219)**

In this talk, I will outline strategies for the supramolecular assembly and pre-organization of photoactive materials, discuss and contrast their optoelectronic properties with those of reference small molecule compounds. The motivation for this work is to (1) improve the performance of electrochromic devices, (2) to develop selective sensors and photoredox catalysts, and (3) on a more fundamental level, to understand how the photophysical properties of the assembly can be modulated as a function of the structure of its constituent components.



Contact: Kunio Awaga (ext. 2487)

**January 24, 2017** Dr. Eli Zysman-Colman  
(University of St Andrews)  
“Tales from the Supramolecular Photochemistry Crypt”

**February 22, 2017** Prof. Hiroshi Kitagawa  
(Graduate School of Science,  
Kyoto University)

**RCMS & IGER Seminar** IGER

**元素間融合を基軸とする  
物質開発と応用展開**

京都大学大学院理学研究科 教授  
物質科学国際研究センター 客員教授



**北川 宏 先生**

日時：2017年2月22日（水） 16:00-17:30  
場所：野依記念物質科学研究館2階講演室

連絡先：唯 美津木（内線6200）

# Chemistry Gallery

The Chemistry Gallery (2<sup>nd</sup> Floor of the Noyori Materials Science Laboratory) welcomed many visitors again in the 2016 academic year. Thanks to a Japanese scientist being selected for the Nobel Prize in Physiology or Medicine (Satoshi Omura, Professor Emeritus at Kitasato University), the gallery attracted more than 20,000 visitors throughout the year.

The Chemistry Gallery also features a replica exhibition of the venue for the Nobel Prize Awards Ceremony. In a year in which a Japanese scientist won the Nobel Prize, many visitors took commemorative photographs at this exhibition. 23,206 people visited the gallery as of March 31, 2017 (according to an automatic counter for entry/exit to the gallery).

A particularly large number of visitors were welcomed during the following periods when Nagoya University was open to the public.

Number of visitors during Open Campus (August 8 to 10): 845

Number of visitors on Homecoming Day (October 5): 2,010



Exhibition of Nobel Ceremony venue



Exhibition of RCMS Members



Record of RCMS Directors

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# Events 2016

## **[Establishment of the Integrated Research Consortium on Chemical Sciences]**

The Research Center for Materials Science at Nagoya University led the establishment of the Integrated Research Consortium on Chemical Sciences

Through the Joint Project of Chemical Synthesis Core Research Institutions (Nagoya University, Kyoto University, Kyushu University) which was held from 2005 to 2009 and the MEXT Project of Integrated Research on Chemical Synthesis (Nagoya University, Kyoto University, Kyushu University, Hokkaido University) which was held from 2010 to 2015, Nagoya University has implemented projects aimed at achieving world-class research standards for fulfilling the role of a core international research institute in materials synthesis. The Consortium will inherit and build upon these projects while working to further strengthen the ability of practical implementation.



## Integrated Research Consortium on Chemical Sciences

## **[Professor Shigehiro Yamaguchi selected as next Director of the Research Center for Materials Science]**

Professor Shigehiro Yamaguchi (Institute of Transformative Bio-Molecules, current Director of the Chemical Instrumentation Facility) has been selected to serve as Director of the Research Center for Materials Science from the 2017 academic year.



## **[Appointment of two new Assistant Professors]**

Two new Assistant Professors have been appointed in the field of organic materials synthesis research.

Assistant Professor Soichiro Ogi (appointed on May 1, 2016)

Assistant Professor Akiko Yagi (appointed on March 1, 2017)

# Staff List

Director	Professor	Kunio Awaga	(2487)	awaga@mbx.chem.nagoya-u.ac.jp
Special Advisor	University Professor	Ryoji Noyori		
Organic Synthesis	Professor	Shigehiro Yamaguchi	(2291)	yamaguchi@mbx.chem.nagoya-u.ac.jp
	Assistant Professor	Soichiro Ogi	(5750)	ogi.soichiro@chem.nagoya-u.ac.jp
	Assistant Professor	Akiko Yagi	(5873)	yagi.akiko@d.mbx.nagoya-u.ac.jp
Inorganic Synthesis	Professor	Mizuki Tada	(6200)	mtada@chem.nagoya-u.ac.jp
	Associate Professor	Hideo Takagi	(5473)	htakagi@chem.nagoya-u.ac.jp
	Associate Professor	Yasuyuki Yamada	(2471)	yy@chem.nagoya-u.ac.jp
	Designated Professor	Kazuyuki Tatsumi	(2474)	i45100a@nucc.cc.nagoya-u.ac.jp
Functional Materials	Professor	Akiyoshi Hishikawa	(2494)	hishi@chem.nagoya-u.ac.jp
	Assistant Professor	Zhang Zhongyue	(5106)	zhangzhongyue@i.mbx.nagoya-u.ac.jp
	Assistant Professor	Haruka Omachi	(3660)	omachi.haruka@a.mbx.nagoya-u.ac.jp
Biomaterials Research	Professor	Yoshihito Watanabe	(3049)	p47297a@nucc.cc.nagoya-u.ac.jp
	Assistant Professor	Fumiaki Tomoike	(2950)	tomoike@chem.nagoya-u.ac.jp
Molecular Catalysis	University Professor	Ryoji Noyori	(2956)	noyori@chem3.chem.nagoya-u.ac.jp
	Assistant Professor	Hiroshi Naka	(5411)	h_naka@nagoya-u.jp
	Assistant Professor	Shinji Tanaka	(2960)	tanaka@os.rcms.nagoya-u.ac.jp
Collaborative Studies	Guest Professor	Hiroshi Kitagawa (Professor, Kyoto University)		
	Guest Associate Professor	Eric Rivard (Associate Professor, University of Alberta)		
Chemical Instrumentation Facility	Manager / Professor	Shigehiro Yamaguchi	(2291)	yamaguchi@mbx.chem.nagoya-u.ac.jp
	Assistant Professor	Chunguang Han	(3072)	hanc@ic.nagoya-u.ac.jp
	Technical official	Yutaka Maeda	(3069)	maeda@ic.nagoya-u.ac.jp
	Technical official	Kin-ichi Oyama	(3069)	oyama@ic.nagoya-u.ac.jp
International Advisory Board		Michael Grunze (Professor Emeritus, Heidelberg University)		
		Roald Hoffman (Professor Emeritus, Cornell University – Laureate, Nobel Prize in Chemistry)		
		Henri Boris Kagan (Professor Emeritus, Paris-Sud 11 University)		
		Atsuko Tsuji (Designated Professor, Nagoya University)		
Cooperating Faculty	Professor	Hisanori Shinohara (Graduate School of Science)	(2482)	noris@nagoya-u.jp
	Professor	Kenichiro Itami (Institute of Transformative Bio-Molecules)	(6098)	itami.kenichiro@a.mbx.nagoya-u.ac.jp
	Professor	Masato Kitamura (Graduate School of Pharmaceutical Sciences)	(2957)	kitamura@os.rcms.nagoya-u.ac.jp
	Professor	Susumu Saito (Graduate School of Science)	(5945)	saito.susumu@f.mbx.nagoya-u.ac.jp
	Distinguished Invited University Professor	Sumio Iijima	(6460)	ijimas@nagoya-u.jp
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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