



RCMS NEWS

16

2015

NAGOYA UNIVERSITY
RESEARCH CENTER FOR MATERIALS SCIENCE

Reports and Communications of RCMS Activities
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May 2015
Issue #16



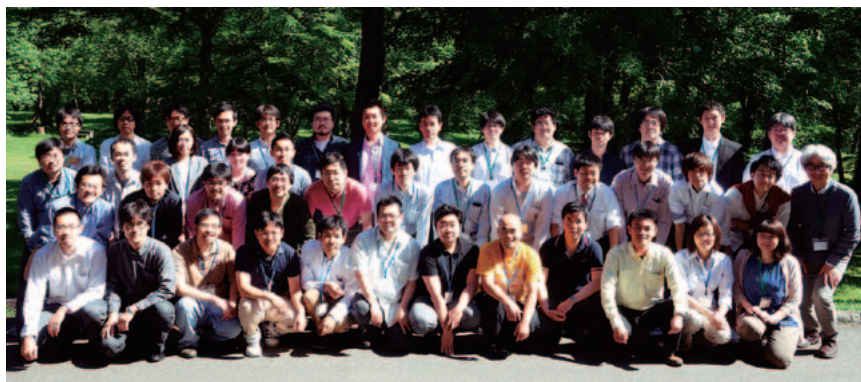
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MEXT Project of Integrated Research on Chemical Synthesis 2014

In 2014, 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 5th Young Researchers Forum (Hokkaido, June 20–21, 2014)



The 4th International Conference on MEXT Project of Integrated Research on Chemical Synthesis (Kyoto University, July 10–11, 2014)



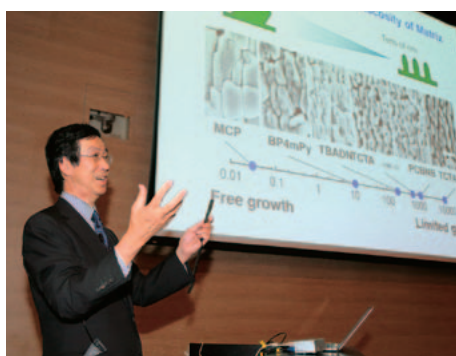
Prof. Holger Braunschweig



Prof. Katsuhiko Tomooka



The 5th Symposium on MEXT Project of Integrated Research on Chemical Synthesis
(Nagoya University, December 19–20, 2014)



Prof. Eiichi Nakamura



Dr. Tahei Tahara



Prof. Kunio Awaga

[Symposium and Forum in 2015]

- The 6th Symposium on MEXT Project of Integrated Research on Chemical Synthesis in Nagoya (April 14, 2015)
- The 6th Young Researchers Forum in Kyusyu (July 3–4, 2015)
- The 5th International Conference on MEXT Project of Integrated Research on Chemical Synthesis in Nagoya (January, 2016)

The 17th & 18th Joint Seminar, Core-to-Core Program

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 17th Core- to-Core Joint Seminar June 12–13, 2014 (Thursday – Friday) at Nagoya University

German Participants:

7 Faculties and 5 Students (Oral Presentations)

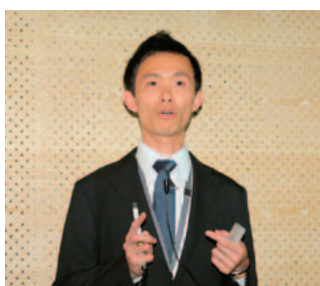
Japanese Participants:

5 Faculties and 4 Students (Oral Presentations),

29 Poster Presentations



Prof. Shigehiro Yamaguchi



Dr. Foo Siong Wan



Ms. Friederike Schröter



The 18th Core-to-Core Joint Seminar

November 27–29, 2014 (Monday – Tuesday) at University of Münster

Japanese Participants: 7 Faculties, 1 Post doc and 4 Students (Oral Presentations)

German Participants: 3 Faculties, 2 Post doc and 6 Students (Oral Presentations), 54 Poster Presentations

Canadian Participants: 1 Faculties



Nozomi Mihara



Prof. Kenichiro Itami



President of U. of Münster,
Prof. Ursula Nelles



Prof. Kazuyuki Tatsumi



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 2014, over 260 graduate students enrolled in this program from graduate school of Science, Engineering and Agricultural Sciences. 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) foreign residency research for 23 students. Furthermore, the program hosted various international symposium / workshop where lots of students could have opportunities to discuss with foreign researchers.

Thirteen 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.

The program had the first 22 alumni at the end of FY 2014. The following are some comments from them.

“The program is one of the best that I have ever participated. Through this program, I got to know many excellent people from diverse fields and talking with them had benefited me a lot from various aspects.”

“I came to realize about the importance of developing good leadership qualities not only for myself, but also for the future of community and society.”

“It had opened up my mindset about what I could achieve in future. Besides, I got to know more about working in a global environment, as in how to deal with people of different cultural background, and how to maximize the outcome from a team comprising of multi-nationality.”

Their future success is greatly anticipated.



A snapshot of foreign residency research



Leadership Program at North Carolina



Alumni from Department of Chemistry

Research Topic

(Organic Synthesis)

Flexible Fluorophores for Materials Imaging Technique

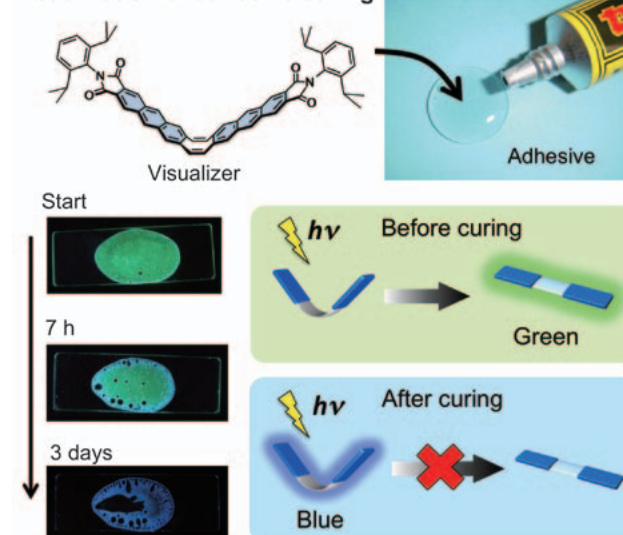
We have proposed hybridization of flexible and rigid π skeletons as a fundamental molecular design for multi-luminescence from a single-component organic system. A series of synthetic hybrid π systems change their conformation, depending on the physical environment in various media. Since the structural transformation is accompanied by the luminescence color change, the visualization of the physical environment can be achieved in the materials. This technique would be called as "materials imaging". Our approach began with the molecular design for the multi-luminescent systems. As for organic systems, π -conjugated skeletons are a fundamental unit for controlling their optoelectronic properties. Since the π skeletons are composed mainly of planar sp^2 carbons and aromatic rings, most of π -conjugated systems are inherently rigid. The rigidity is often favorable for luminescent properties. However, the limitation of conformational diversity confines their properties into static ones. On the other hand, conformational changes of flexible π systems could lead to dynamic properties, although the molecular motion sometimes results in the quenching of emission. Our idea is to combine these advantages of the rigidity and flexibility for the creation of new multi-luminescent molecules.

A hybrid π system we have first designed displayed environment-dependent RGB luminescence, which is composed of a flexible cyclooctatetraene core and rigid anthraceneimide wings [1,2]. The RGB emissions from a single organic component without changing the excitation energy have not yet been realized, whereas the inorganic quantum dots with different particle sizes and several aromatic systems with different aggregation states show multichromic characteristics. The hybridization of the rigid and flexible substructures plays important roles in the multichromism with the three primary colors. The flexible moiety gives rise to a dynamic conformational change in the excited state from a blue-emissive V-shaped form to a green-emissive planar form. The rigid substructure induces a two-fold π -stacked array of the V-shaped molecules in the crystalline state, which produces a red excimer emission. With the single-component multichromic properties,

a freezing process of organic solvents was monitored by the fluorescence color change. Namely, the green emission from the planar conformer was observed in a solution, while the blue color from the V-shaped form was observed in a frozen part of the solution because the conformational change in the excited state is suppressed. More importantly, this viscochromism was applied to the real-time visualization of a hardening process of solvent-based adhesives, such as Cemedine C[®]. The fluorescence color of the trace additive informed us without any spectrometer when the hardening is completed as well as where is an insufficiently hardened area [3]. The imaging technique will be further developed to visualize the physical environment in various materials by the real-time and contactless method.



Visualization of adhesive curing



References

- [1] S. Saito, S. Irle, S. Yamaguchi, et al. *J. Am. Chem. Soc.* **2013**, *135*, 8842 (Highlighted in *C&EN*).
- [2] S. Saito, S. Irle, S. Yamaguchi, et al. *Chem. Eur. J.* **2014**, *20*, 2193 (Inside Cover).
- [3] Patent Application 2013-257581.

(Shohei SAITO)

Research Topic (Inorganic Synthesis)

Programmable Synthesis of Stacked Assemblies of Porphyrins and Phthalocyanines

Metallo-porphyrins and metallo-phthalocyanines are versatile building blocks for functional molecular assemblies since their redox, spin, spectroscopic, and catalytic properties are tunable by changing the central metal ions. Moreover, it is well-known that these compounds spontaneously stack each other due to their planer structure to form polymeric assemblies with unique chemical and physical properties. We supposed that the precise control of numbers, sequences, and compositions of metallo-porphyrins and/or metallo-phthalocyanines inside their stacked assemblies would lead us to produce the materials with designed functions. Research efforts in our group focus on development of the programmable synthesis of the stacked assemblies of metallo-porphyrins and metallo-phthalocyanines for nanoelectronic devices, supramolecular catalysts, and so on. Until now, we have developed two different strategies for the programmable synthesis of the stacked arrays as mentioned below.

1) Covalently-linked arrays via repetitive stepwise peptide elongation. We developed a novel programmable synthesis of a cofacially-stacked porphyrin array via repetitive construction of a peptide duplex as shown in Figure 1. We designed and synthesized a novel porphyrin having two artificial amino acid moieties at the *trans meso*-positions. Twofold peptide bond formation between two porphyrin units can afford the peptide duplex bridged by porphyrins. By utilizing this method, we synthesized a ladder-type porphyrin array **T1** in which three different square-planar metal ions, namely Cu^{2+} , Ni^{2+} , and Pd^{2+} , were arranged in a programmable fashion. Efficient electronic communication among the arrayed porphyrin units were confirmed by electrochemical

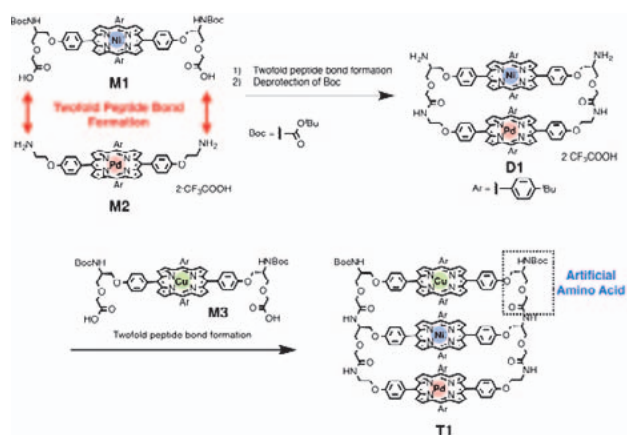


Figure 1. Synthesis of a ladder-type peptide duplex **T1**.

measurements.

2) Mechanically-linked arrays via multiple rotaxane formation.

Rotaxane is a mechanically-interlocked supramolecular structure in which an axle component is threaded through a macrocycle. We reported that the assemblage of a porphyrin having four peripheral alkylammonium sidechains **1** and a phthalocyanine bearing four crown ethers **2**, followed by a stoppering reaction to convert the terminal azide groups of **1** into bulky phosphoramidate stoppers, gave a stacked assembly **3** of a porphyrin and a phthalocyanine connected through fourfold rotaxane (Figure 2). It was also revealed that control of the spin-spin communication between two $S = 1/2$ spins of Cu^{2+} in the dinuclear Cu^{2+} complex **4** was achieved by reversible protonation/deprotonation of the ammonium ions and the phosphoramidate stoppers of the rotaxane structure.

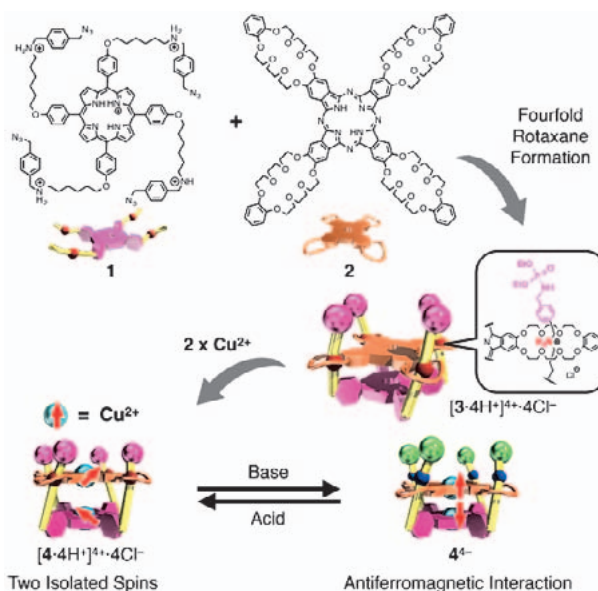


Figure 2. Synthesis of a dinuclear Cu^{2+} complex **4** and the switching of the spin-spin interaction in **4**.

References

- [1] Y. Yamada, T. Kubota, M. Nishio, K. Tanaka, *J. Am. Chem. Soc.*, **2014**, *136*, 6505–6509.
- [2] Y. Yamada, M. Okamoto, K. Furukawa, T. Kato, K. Tanaka, *Angew. Chem. Int. Ed.*, **2012**, *51*, 709–713.

(Yasuyuki YAMADA)

Research Topic

(Functional Materials)

Research on Rechargeable Molecular Batteries

Over the last decade, the evolution of materials has led to numerous innovations in the field. In the recent past, the Li-ion battery (LIB) is the pioneer technology as it provides both high energy density and large output current. Recently, our group focused on the application of molecular clusters, such as “Mn₁₂ acetate” and Keggin-type polyoxometalates as novel cathode active materials due to their large electron uptake numbers. The preliminary results inspired us to develop advanced materials by combining the advantages of organic materials and molecular clusters. The practical strategy was to link the metal clusters with redox active organic bridging ligands to form porous coordination polymers (PCPs), which are also well known as metal-organic frameworks (MOFs).

Herein we selected 2,7-anthraquinonedicarboxylic acid (2,7-H₂AQDC) as a bridging ligand. Anthraquinone (AQ) exhibits two reversible redox steps with one electron uptake for each. The solvothermal reaction between 2,7-H₂AQDC and Cu(ClO₄)₂·6H₂O in DMF led to the formation of a two-dimensional (2-D) metal organic framework with a formula of [Cu(2,7-AQDC)-(DMF)]_∞·xDMF (1·DMF). The framework adopted a Kagome lattice architecture. A single triangular unit of Kagome lattice was composed by the Cu₂(Ac)₄ paddlewheel cluster secondary building units (SBUs) as nodes and anthraquinone groups as bridges (**Figure 1**). Hexagonal pores were formed inside the 2-D layers by surrounding AQ groups and possessed a diameter of 23.4 Å.

CR2032-type coin cell batteries were assembled to characterize the solid state electrochemical behaviors of 1·DMF. To rule out the kinetic effect and investigate the intrinsic behavior, pellets that contained 10% weight of MOF, 70% carbon black as a conductive additive and 20% PVDF (polyvinylidene fluoride) as a binder were used as cathodes, while the anodes were lithium discs, and a 1:1 v/v EC/DEC (ethylene carbonate/diethyl carbonate) solution of LiPF₆ (1M) was used as electrolyte. In the optimization of the measurement conditions, the voltage window and scan current were selected as 4.0–2.0 V and 1 mA, respectively. Two plateaus were clearly observed in the charge-discharge profile within the voltage ranges of 3.4–2.5 V and 2.5–2.0 V, respectively, while the output gravimetric capacity ratio of the two steps was nearly 1:1 (**Figure 2**). In cyclic performance test of the battery, an initial specific capacity of 115 mAh/g was achieved, and there was no decrease within 50 cycles.

Operando Cu K-edge X-ray absorption near edge structure (XANES) analysis. This phenomenon could be assigned to the stepwise two-electron uptake processes in Cu₂(Ac)₄ and AQ subunits. These findings suggest

that MOF materials with good potential for use in industrial batteries could be induced by fine fabrication techniques, such as the introduction of thin films and nanocrystals. By involving other 3d transition metals, such as Mn, Fe, and Co, new MOFs with larger surface areas and higher reduction voltages might be achieved, which could vastly improve the performance of the MOF-based batteries.



Fig. 1 2D sheet structure of [Cu(2,7-AQDC)(DMF)]_∞.

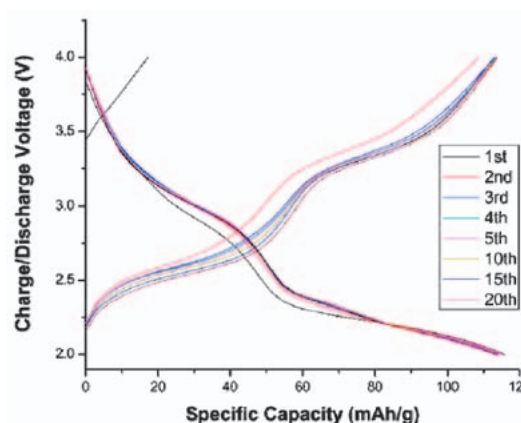


Fig. 2 Charge/discharge curves of 1·DM.

References

- [1] H. Wang, S. Hamanaka, Y. Nishimoto, S. Irle, T. Yokoyama, H. Yoshikawa, K. Awaga, *J. Am. Chem. Soc.*, **134**, 4918 (2012).
- [2] Z. Zhang, H. Yoshikawa, K. Awaga, *J. Am. Chem. Soc.*, **136**, 16112 (2014).

(Kunio AWAGA)

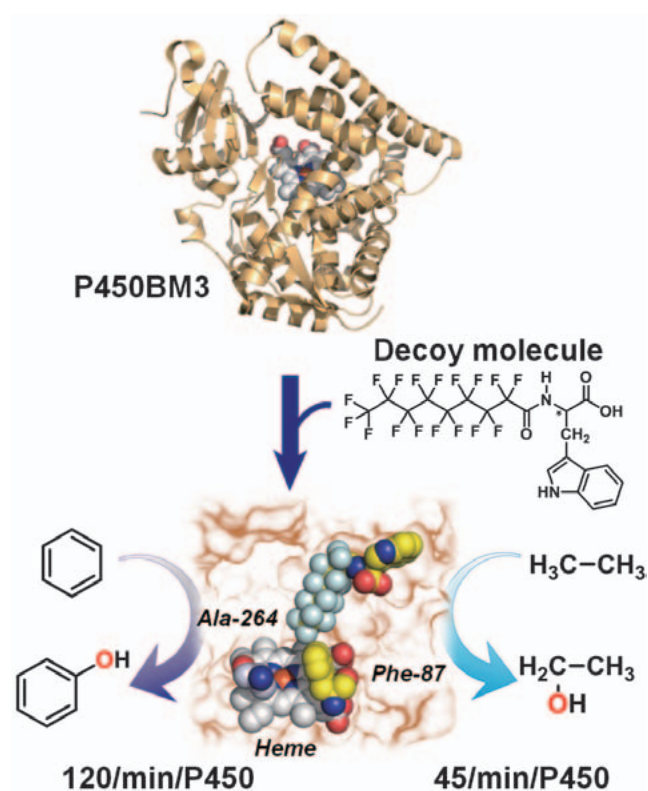
Research Topic (Biomaterials Research)

Molecular Design of Monooxygenases for Hydroxylation of Small Alkanes

Gaseous alkanes such as methane and ethane are important fuels and potential chemical feedstock, but the selective hydroxylation of gaseous alkanes is a long-standing challenge and a current topic of interest considering increasing industrial and economic requirements. Cytochrome P450s (P450s) are a superfamily of heme-containing monooxygenases that are capable of breaking strong C–H bonds of hydrocarbons. Because recombinant forms of P450s are prepared by using common expression systems such as *Escherichia coli*, P450s have great potential for further engineering and subsequent application in synthetic chemistry. Unfortunately, the substrate specificity of cytochrome P450s makes them unsuitable for the hydroxylation of gaseous small alkanes, because P450s, especially those isolated from bacteria, recognize their specific substrates by intermolecular interactions to ensure their specificity and efficiency. Thus, first challenge for us is to provide general methodologies to control its substrate specificity of P450s.

P450BM3 isolated from *Bacillus megaterium* catalyzes the hydroxylation of long-alkyl-chain fatty acids. Because the substrate binding is crucial to initiate the catalytic cycle of P450BM3, substrates whose structures are largely different from those of fatty acids cannot be hydroxylated by P450BM3. P450BM3 thus does not catalyze the hydroxylation of small hydrocarbons. However, we have demonstrated that even wild-type P450BM3 can catalyze the hydroxylation of gaseous alkanes such as ethane and propane as well as benzene by using perfluorinated carboxylic acids (PFCs) as decoy molecules.^{1–3} Recently, we have demonstrated that *N*-perfluoroacyl amino acids strongly activate wild-type P450BM3 for the hydroxylation of inert alkanes.⁴ The turnover rate for hydroxylation of ethane and propane catalyzed by P450BM3 with *N*-perfluorononanoyl *L*-leucine (PFC9-L-Leu) as the decoy molecule reached 45/min and 256/min, respectively. More importantly, we have succeeded in the crystal structure analysis of P450BM3/*N*-perfluorononanoyl *L*-tryptophan (PFC9-L-Trp) complex.⁴ The binding of PFC9-L-Trp reforms the active site pocket to allow the accommodation of small substrates and simultaneously influences the formation of active

species of P450BM3.



References

- [1] N. Kawakami, O. Shoji, Y. Watanabe, *Angew. Chem. Int. Ed.* **2011**, *50*, 5315–5318.
- [2] N. Kawakami, O. Shoji, Y. Watanabe, *Chem. Sci.* **2013**, *4*, 2344–2348.
- [3] O. Shoji, T. Kunimatsu, N. Kawakami, Y. Watanabe, *Angew. Chem. Int. Ed.* **2013**, *52*, 6606–6610.
- [4] Z. Cong, O. Shoji, C. Kasai, N. Kawakami, H. Sugimoto, Y. Shiro, Y. Watanabe, *ACS Catalysis* **2015**, *5*, 150–156.

(Yoshihito WATANABE)

Research Topic

(Molecular Catalysis)

New Trends in Molecular Catalysis

The major mission of the Division of Molecular Catalysis at RCMS is to establish new trends and high-standard academic basis in chemical synthesis by exploring new science in molecular catalysis. This article focuses on our recent representative research in the Division of Molecular Catalysis. Each project is initiated by identifying and discussing "What is the scientific basis requested for academia and industry in the next generation?". A part of the results has been published as academic papers^[1-4] and patents.^[5]

Chemical Synthesis by Catalytic Hydration^[2,3]

Catalytic hydration of organic compounds is a fundamental reaction both in the academic chemistry and industrial chemical production. We have recently disclosed that water-soluble cobalt(III) porphyrin complexes promote the hydration of terminal alkynes to give methyl ketones (Figure 1).

Organic Synthesis with Light Energy: the Noyori Forum Joint Project^[4,5]

Chemical synthesis using sunlight energy is a dream of the whole human beings. Photochemical transformation of biomass-derived or renewable substances is an important challenge for promoting green and sustainable chemistry. During the course of our joint research program with the Noyori Forum, aiming at the development of new technology for the industry in the next generation, we have succeeded in developing a organic reaction that catalytically utilize light energy.

The photocatalytic transfer hydrogenolysis of allyl alcohol gives potentially sustainable propylene with high chemo- and redox-selectivity, promoted by powdered Pd/TiO₂ in CH₃OH under near-ultraviolet-visible light irradiation at ambient temperature. Noteworthy in this transformation is the unusual selectivity for C–O bond cleavage over C=C bond reduction. With the similar strategy, we have also developed the photocatalytic dehydrogenation of alcohols and the photocatalytic N-methylation of amines with methanol.



References

- [1] *Chem. Asian J.* **10**, 112–115 (2015).
- [2] *J. Am. Chem. Soc.* **135**, 50–53 (2013).
- [3] (a) *RSC Adv.* **5**, 12152–12160 (2015). (b) *Chem. Asian J.* **6**, 1740–1743 (2011).
- [4] (a) *Chem. Eur. J.* **19**, 9452–9456 (2013); *Synfacts* **9**, 1138 (2013). (b) *Catal. Sci. Technol.* **4**, 4093–4098 (2014). (c) *Org. Lett. in press* (2015). (d) *Chem. Lett.* **42**, 146–147 (2013).
- [5] (a) JP2013-213167. (b) JP2013-193470. (c) JP2013-65083. (d) JP2012-181888. (e) JP2012-70113. (f) JP2012-28845. (g) JP2010-208526. (h) JP2010-203712. (i) JP2010-49823. (j) JP2010-49735. (k) JP2010-1557. (l) JP2009-299231. (m) JP2009-233817.

(Hiroshi NAKA)

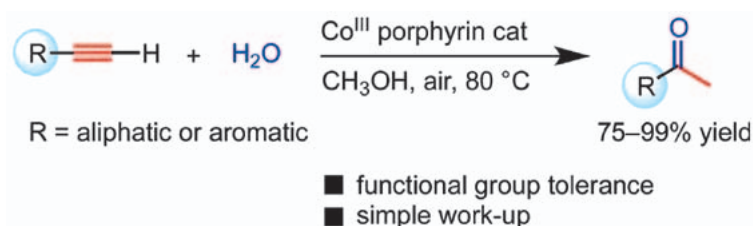


Figure 1. Catalytic Hydration of Alkynes by a Cobalt Catalyst

Visiting Professor 2014

Prof. Refat Moustafa Hassan Abzied

Professor, Assiut University



metal complexes. The joint research includes (1) oxidation reactions of polysaccharides and carrageenans by aqueous cerium(IV), permanganate, chromic acid, hexachloroiridate, and by alkaline hexacyanoferrate. He also studied (2) the behavior of biopolymeric metal-alginate ionotropic hydrogels, and (3) non-isothermal decomposition of cross-linked thorium (IV)-alginate complex in relation to the coordination geometry and thermal stability. He is very active and his recent publication is related to (4) the corrosion inhibition of aluminum using water-soluble polyvinylalcohol. All these results have been published as more than 10 articles since 2011. Professor Hassan also shared his precious time with the students, and enjoyed English conversation with them a couple of hours a week.

Period of Stay:

May 19 – August 29, 2014

Research Theme:

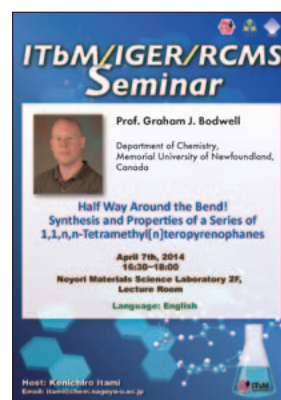
Syntheses of macro ligands as products of natural and synthetic polymers with hydroxy groups and removal of heavy and / or radioactive metals from the environment

This is the second visit to the RCMS for Professor Hassan from Assiut University, Egypt. He started joint research with a member of RCMS in 2010, and keeps producing high-quality research papers concerning the oxidation reactions of various natural and artificial polymers such as alginate and its derivatives by various



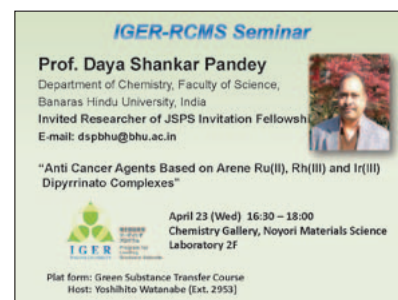
RCMS Seminars

April 7, 2014 Prof. Graham J. Bodwell
(Department of Chemistry, Memorial University of Newfoundland, Canada)
"Half Way Around the Bend! Synthesis and Properties of a Series of 1,1,n,n-Tetramethyl[n]teropyrenophanes"



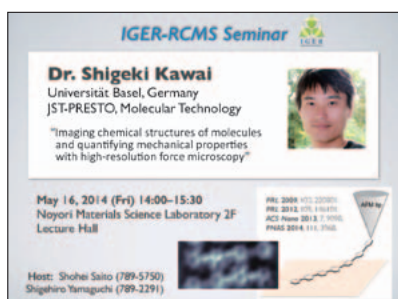
April 10, 2014 Prof. Rik R. Tykwinski
(Universität Erlangen-Nürnberg, Germany)
"Synthesis and structure-property relationships of 1-D carbon chains"

April 23, 2014 Prof. Daya Shankar Pandey
(Department of Chemistry, Faculty of Science, Banaras Hindu University, India)
"Anti Cancer Agents Based on Arene Ru(II), Rh(III) and Ir(III) Dipyrrinato Complexes"



April 30, 2014 Prof. Mats Larsson
(Stockholm University, Department of Physics, Sweden)
"Charged chiral molecules at ev and keV energies"

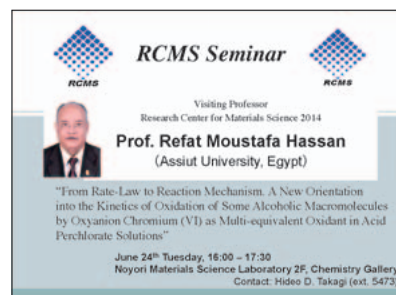
May 1, 2014 Asst. Prof. Dr. Pornpan Pungpo
(Department of Chemistry, Faculty of Science Ubonratchathani University Ubonratchathani, THAILAND)
"Rational design of InhA inhibitors as highly potential anti-tubercular agents, based on computer aided molecular design"



May 16, 2014 Dr. Shigeki Kawai
(Universität Basel, Germany JST-PRESTO, Molecular Technology)
"Imaging chemical structures of molecules and quantifying mechanical properties with high-resolution force microscopy"

June 24, 2014 Prof. Refat Moustafa Hassan
(Assiut University, Egypt)

“From Rate-Law to Reaction Mechanism. A New Orientation into the Kinetics of Oxidation of Some Alcoholic Macromolecules by Oxyanion Chromium(VI) as Multi-equivalent Oxidant in Acid Perchlorate Solutions”



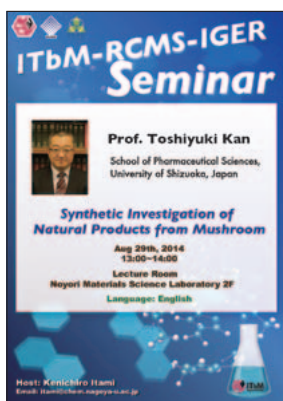
June 24, 2014 Prof. Donna G. Blackmond
(Department of Chemistry, The Scripps Research Institute, USA)
“Chemical and Physical Models for the Origin of Biological Homochirality”

July 9, 2014 Prof. David Spring
(Department of Chemistry University of Cambridge, UK)
“Enriching Chemical Space to Drug Undruggable Targets”



July 16, 2014 Dr. Heide Ibrahim
(INRS – EMT, Canada)
“Analysis and control of hydrogen and electron movement using Coulomb explosion imaging”

July 25, 2014 Prof. Yasumichi Matsumoto
(Graduate School of Science and
Technology, Kumamoto University)



August 29, 2014 Prof. Toshiyuki Kan
(School of Pharmaceutical Sciences, University of Shizuoka, Japan)
“Synthetic Investigation of Natural Products from Mushroom”

August 29, 2014 Prof. Hirokazu Kawagishi
(Research Institute of Green Science and Technology / Graduate School of Science and Technology / Graduate School of Agriculture, Shizuoka University, Japan)

“Chemical explanations for mysteries related to mushrooms – ‘Sughiratake-acute encephalopathy’ and ‘fairy ring’ –”



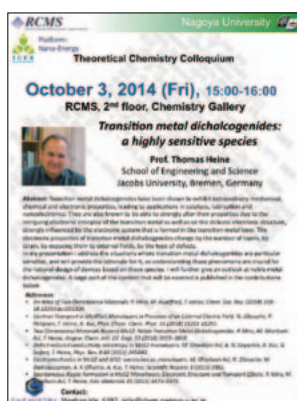
September 16, 2014 Prof. Chao Chen
(Tsinghua University, Beijing, China)
“Efficient Ring Synthesis with Diaryliodonium Salts through Electrophilic Activation of Small molecules”

October 3, 2014 Dr. Jérôme Canivet
(The Institute of Researches on Catalysis and Environment in Lyon (IRCELYON), France)
“Metal-Organic Frameworks: A new tale of the Emperors’s new clothes”



October 3, 2014 Prof. Emad Flear Aziz
(Department of Physics, Free University of Berlin, Germany)
“Charge Transfer to Solvent Dynamics in Aqueous Solution”

October 3, 2014 Dr. Matthew A. Addicoat
(School of Engineering and Science, Jacobs University, Bremen, Germany)
“AuToGraFS: Automatic Topological Generator for Framework Structures”



October 3, 2014 Prof. Thomas Heine
(School of Engineering and Science, Jacobs University, Bremen, Germany)
“Transition metal dichalcogenides: a highly sensitive species”

October 10, 2014 Dr. Christian Doonan
(University of Adelaide, Australia)
"Robust porous organic cage molecules"



ITAMI ERATO-ITbM-RCMS Seminar

Dr. Christian Doonan
Associate Professor,
University of Adelaide, Australia

Robust porous organic cage molecules

Oct 10th, 2014
16:30-18:00
Lecture Room
Noyori Materials Science Laboratory 2F
Language: English

Contact:
Kentichiro Hamada
Email: khamada@nagoya-u.ac.jp
Hirotoshi Sakamoto
Email: sakamoto@nagoya-u.jp



IGER-ITbM-RCMS Seminar

Prof. Amos B. Smith, III
University of Pennsylvania, USA

"Evolution and Exploitation of Anion Relay Chemistry (ARC)"

October 16, 2014 (Thu) 16:30-18:00
Noyori Materials Science Laboratory 2F,
Lecture Hall

Host: Shigehiro Yamaguchi (789-2291)

October 16, 2014 Dr. Amos B. Smith, III
(University of Pennsylvania, USA)
"Evolution and Exploitation of Anion Relay Chemistry (ARC)"

October 22, 2014 Prof. Lawrence T. Scott
(Boston College, USA)
"Geodesic Polyarenes: Precursors to Single-index Carbon Nanotubes"



ITAMI ERATO-ITbM-RCMS Seminar

Prof. Lawrence T. Scott
Professor of Chemistry
Boston College, USA

Geodesic Polyarenes: Precursors to Single-index Carbon Nanotubes

Oct 22th, 2014
16:00-17:30
Lecture Room
Noyori Materials Science Laboratory 2F
Language: English

Contact:
Kentichiro Hamada
Email: khamada@nagoya-u.ac.jp
Yasutomo Sogawa
Email: ysogawa@nagoya-u.jp



IGER & RCMS Seminar

Professor Martin OESTREICH
Technische Universität Berlin, Germany

"Catalytic Si-H Bond Activation"

October 23rd (Thu) 2014, 16:30-18:00
Noyori Materials Science Laboratory 2F
Conference Room

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

October 23, 2014 Prof. Martin Oestreich
(Technische Universität Berlin, Germany)
"Catalytic Si-H Bond Activation"

October 30, 2014 Prof. Matthew S. Sigman
(Department of Chemistry, The University of Utah, USA)
"Analyzing and Predicting Selectivity in Asymmetric Catalysis"



ITbM/IGER/RCMS Seminar

Prof. Matthew S. Sigman
Peter J. Christine S. Stang Presidential
Endowed Chair of Chemistry
Department of Chemistry,
The University of Utah, USA

Analyzing and Predicting Selectivity in Asymmetric Catalysis

October 30th, 2014
16:30-18:00
Noyori Materials Science Laboratory 2F,
Lecture Room
Language: English

Host:
Takashi Ooi
Email: tooi@nagoya-u.ac.jp



IGER-ITbM-RCMS Seminar

Prof. Ming-Chang Yeh
National Taiwan Normal Univ., Taiwan

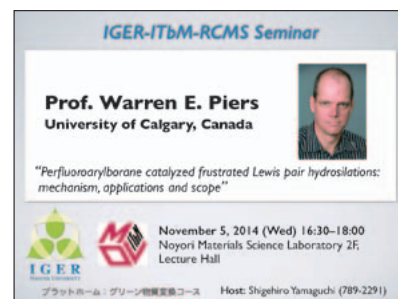
"Facile Synthesis of Heterocycles via Iron- and Indium-Promoted Cyclization Reactions"

October 31, 2014 (Fri) 16:00-17:30
Noyori Materials Science Laboratory 2F,
Chemistry Gallery

Host: Shigehiro Yamaguchi (789-2291)

October 31, 2014 Prof. Ming-Chang Yeh
(National Taiwan Normal Univ., Taiwan)
"Facile Synthesis of Heterocycles via Iron- and Indium-Promoted Cyclization Reactions"

November 5, 2014 Prof. Warren E. Piers
(University of Calgary, Canada)
"Perfluoroarylborane catalyzed frustrated Lewis pair hydrosilations:
mechanism, applications and scope"



IGER-ITbM-RCMS Seminar

Prof. Warren E. Piers
University of Calgary, Canada

"Perfluoroarylborane catalyzed frustrated Lewis pair hydrosilations:
mechanism, applications and scope"

November 5, 2014 (Wed) 16:30-18:00
Noyori Materials Science Laboratory 2F,
Lecture Hall

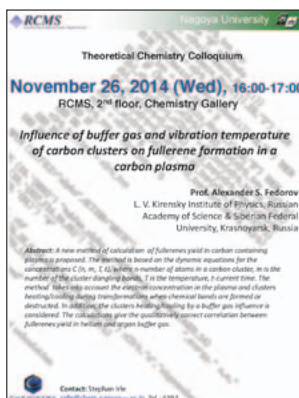
Host: Shigehiro Yamaguchi (789-2291)



November 11, 2014 Prof. Thomas Baumgartner
(University of Calgary, Canada)
"Organophosphorus Avenues Toward Powerful Electron Acceptors and Self-Assembled Nanomaterials"



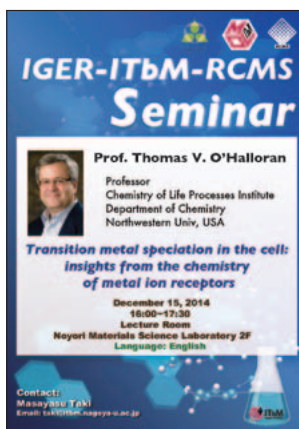
November 12, 2014 Dr. Shigeyuki Masaoka
(Associate Professor, Institute for Molecular Science, National Institutes of Natural Sciences)



November 26, 2014 Prof. Alexander S. Fedorov
(L.V. Kirensky Institute of Physics, Russian Academy of Science & Siberian Federal University, Krasnoyarsk, Russia)
"Influence of buffer gas and vibration temperature of carbon clusters on fullerene formation in a carbon plasma"



December 8, 2014 Prof. Dr. Thomas Niehaus
(Faculty of Physics, University of Regensburg, Germany)
"Range separated functionals in the density functional based tight-binding method: Formalism, implementation and first results"



December 15, 2014 Prof. Thomas V. O'Halloran
(Chemistry of Life Processes Institute, Department of Chemistry, Northwestern Univ, USA)
"Transition metal speciation in the cell: insights from the chemistry of metal ion receptors"



December 16, 2014 Prof. Simon Blakey
(Associate Professor, Department of Chemistry, Emory University, USA)
"C-H Functionalization: An Enabling Technology for Pharmaceutical, Natural Products and Materials Chemistry"



RCMS-ITbM Seminar

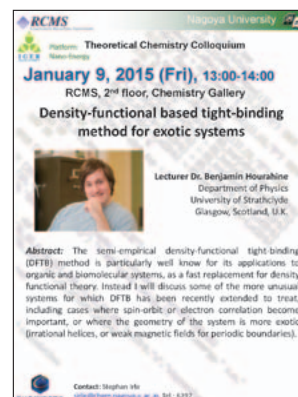
入江 正浩 先生
立教大学理学部未来分子研究センター・教授
名古屋大学物質科学国際研究センター・客員教授

「光機能を創る」

平成26年12月22日(月) 16:00-17:30
野依記念研究館2F 講演室
連絡先：山口茂弘 (789-2291)

December 22, 2014 Prof. Masahiro Irie
(Research Center for Smart Molecules, Department of Chemistry,
Rikkyo University)

January 9, 2015 Dr. Benjamin Hourahine
(Department of Physics, University of Strathclyde, Glasgow, Scotland, U.K.)
“Density-functional based tight-binding method for exotic systems”

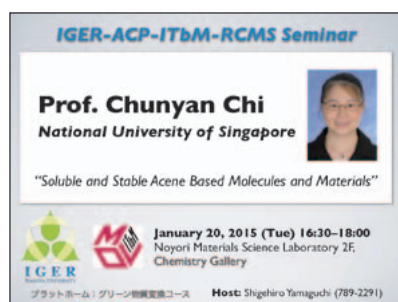


Theoretical Chemistry Colloquium
January 9, 2015 (Fri), 13:00-14:00
RCMS, 2nd floor, Chemistry Gallery
Density-functional based tight-binding method for exotic systems

Lecturer Dr. Benjamin Hourahine
Department of Physics
University of Strathclyde
Glasgow, Scotland, U.K.

Abstract: The semi-empirical density-functional tight-binding (DFTB) method is particularly well known for its applications to organic and biomolecular systems, as a fast replacement for density functional theory. Instead I will discuss some of the more unusual systems for which DFTB has been recently extended to treat, including cases where spin-orbit or electron correlation become important, or where the geometry of the system is more exotic (irrational helices, or weak magnetic fields for periodic boundaries).

Contact: Stephen Irie
siri@chem.nagoya-u.ac.jp, Tel. 6397



IGER-ACP-ITbM-RCMS Seminar

Prof. Chunyan Chi
National University of Singapore

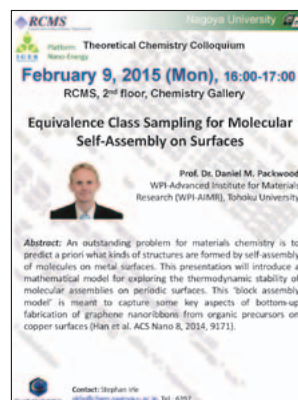
“Soluble and Stable Acene Based Molecules and Materials”

January 20, 2015 (Tue) 16:30-18:00
Noyori Materials Science Laboratory 2F,
Chemistry Gallery

Host: Shigehiro Yamaguchi (789-2291)

January 20, 2015 Prof. Chunyan Chi
(National University of Singapore)
“Soluble and Stable Acene Based Molecules and Materials”

February 9, 2015 Prof. Dr. Daniel M. Packwood
(WPI-Advanced Institute for Materials Research (WPI-AIMR), Tohoku University)
“Equivalence Class Sampling for Molecular Self-Assembly on Surfaces”



Theoretical Chemistry Colloquium
February 9, 2015 (Mon), 16:00-17:00
RCMS, 2nd floor, Chemistry Gallery
Equivalence Class Sampling for Molecular Self-Assembly on Surfaces

Prof. Dr. Daniel M. Packwood
WPI-Advanced Institute for Materials
Research (WPI-AIMR), Tohoku University

Abstract: An outstanding problem for materials chemistry is to predict a priori what kinds of structures are formed by self-assembly of molecules on metal surfaces. This presentation will introduce a mathematical model for exploring the thermodynamic stability of molecular assemblies on periodic surfaces. This “block assembly model” is meant to capture some key aspects of bottom-up fabrication of graphene nanoribbons from organic precursors on copper surfaces (Han et al. ACS Nano 8, 2014, 9171).

Contact: Stephen Irie
siri@chem.nagoya-u.ac.jp, Tel. 6397



ITbM-IGER-RCMS Seminar

Dr. Tatiana Domratheva
Group Leader
Computational Photobiology
Department of Biomolecular Mechanisms
Max-Planck Institute for Medical Research
Germany

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

Feb. 17th, 2015, 16:00-17:30
Chemistry Gallery
Noyori Materials Science Laboratory 2F
Language: English

Contact: Stephen Irie
siri@chem.nagoya-u.ac.jp

February 17, 2015 Dr. Tatiana Domratheva
(Department of Biomolecular Mechanisms, Max-Planck Institute for Medical Research, Germany)
“Computational studies of photosensitive flavoproteins: from spectroscopy to understanding functional mechanisms”

February 20, 2015 Prof. Dr. Hanmin Huang
(Lanzhou Institute of Chemical Physics)
“Exploring metal-complexes for catalytic transformation of C-H and C-N bonds”



PS-RCMS-IGER SEMINAR

Dr. Hanmin Huang
Professor
Lanzhou Institute of Chemical Physics

“Exploring metal-complexes for catalytic transformation of C-H and C-N bonds”

February 20, 2015 (Fri) 16:30-18:00
Noyori Materials Science Laboratory 2F, Lecture Room

Host: Masato Kitamura
Graduate School of Pharmaceutical Sciences

German Students from University of Münster



Artur Kokornaczyk

Period of Stay:

April – September, 2014

Research Theme:

Regioselective Arylation of Thiazole Derivatives as New Potential Sigma 1 Antagonists



Thomas Özgün

Period of Stay:

April – September, 2014

Research Theme:

Frustrated Lewis Pairs; Ambiphilic Ligands in Transition Metal Catalyzed Reactions



Till Böckermann

Period of Stay:

April – September, 2014

Research Theme:

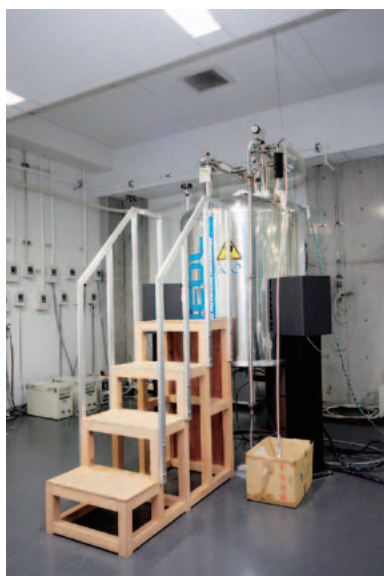
Controlling Liquid Crystalline Phases by Host Guest Chemistry of Functionalized Cyclodextrin



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 2014 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. Since the Institute of Transformative Bio-Molecules began and large-scale projects such as ERATO started at the university, the number of users is increasing.

During the 2014 fiscal year, a "Lecture for Promoting Shared Usage of High Magnetic Field Solid-State NMR spectrometer" was held on November 7th with the support of the University Collaboration Research Equipment Network. In recent years, measurement technology related to solid-state NMR spectrometry has seen remarkable advances, and it is expected that it will be applied to various research fields. Therefore, in order to cultivate potential users of the solid-state NMR spectrometer, lectures were held on solid-state NMR measurement methods, sample preparations, data analysis methods, data interpretation, and application examples for using the 700MHz solid state NMR spectrometer.



High Magnetic Field Solid-State NMR
(JNM-ECA700, JEOL)

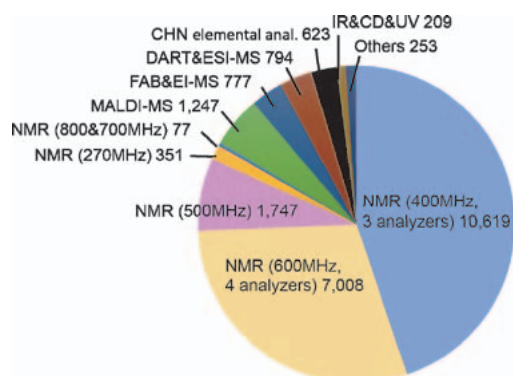
In addition, on September 25th and 26th, the FY2014 Nagoya University Technical Staff Training (Analysis and Material Course) was held at the Research Center for Material Science. A special lecture was held at the Chemistry Gallery of the Noyori Materials Science Laboratory on basics related to the NMR spectrometer and mass spectrometer as well as their applications, and measurement training for the NMR spectrometer and mass spectrometer was held at the Chemical Instrumentation Facility.



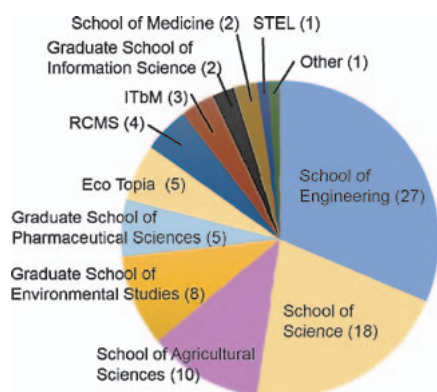
Training by technical staff

[CIF Utilization Status]

Utilization Status for the Academic Year 2014
(April 2014 – February 2015)



Number of Uses/Measurements by Instrument



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

Chemistry Gallery

The Chemistry Gallery (2nd Floor of the Noyori Materials Science Laboratory) continued to host a large number of visitors in 2014. In particular there may be a Japanese Nobel laureates has also been selected from Nagoya University, annual visitors has exceeded 20,000 people for the first time (From April 2014 to March 2015, 23,908 people).

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 (1,904 people) and Nagoya University Home Coming Day in October. (2,173 people)

Exhibition of Nobel Ceremony venue



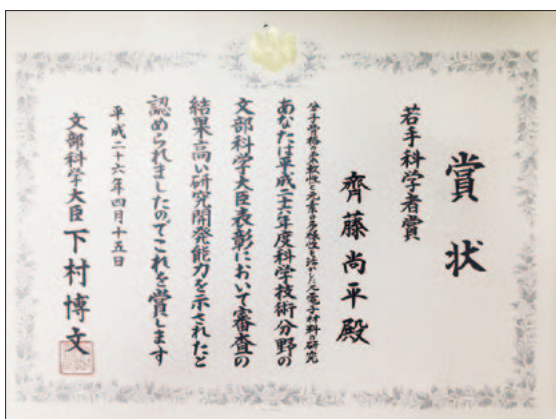
Director, Prof. Awaga with the guests from Ministry of Education, Culture, Sports, Science and Technology



Prizes Awarded 2014

Assistant Prof. Shohei Saito

The Commendation for Science and Technology by the Minister of Education, Culture, Sports, Science and Technology 2014



The 64th the Chemical Society of Japan Award 2014

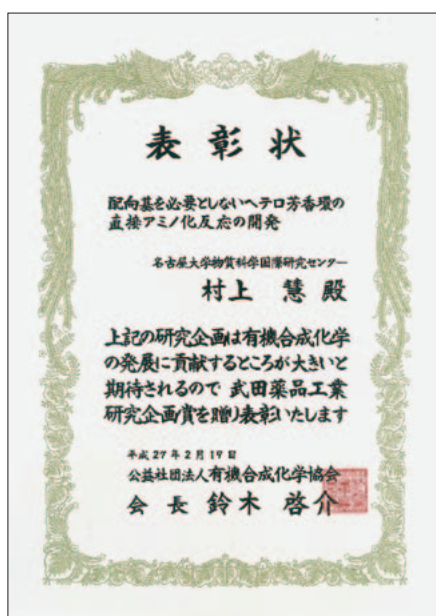
(category of under 37 years old)



Assistant Prof. Kei Murakami

Takeda Award in Synthetic Organic Chemistry, Japan

January 6, 2015



Assistant Prof. Haruka Omachi

Reaxys PhD Prize 2014 Finalist

September 21, 2014



Events in 2014

September, 2014

Designated Professor Kazuyuki Tatsumi elected as a member of new executive board of International Council for Science.

- Former Director of RCMS
- President of IUPAC (2013–2014)



October, 2014

New organization "Institute for Integrated Chemical Sciences" establishment preparation committee set up

<http://www.rcms.nagoya-u.ac.jp/english/news/141001.html>

October, 2014

New Internal rules for use have come into effect for the use of the Noyori Lecture Room, the Chemistry Gallery and the Chemistry Lounge in the Noyori Materials Science Laboratory.

<http://www.rcms.nagoya-u.ac.jp/english/news/141031.html>

November, 2014

Special lecture of Ambassador of the Republic of South Africa was held at Noyori Lecture Hall.

Ambassador Mohau Pheko



December, 2014

Designated Professor Kazuyuki Tatsumi selected as a new member of the Japan Academy.

<http://www.rcms.nagoya-u.ac.jp/news/141215.html>

Staff List

Director	Professor	Kunio Awaga	(2487)	awaga@mbbox.chem.nagoya-u.ac.jp
Special Advisor	University Professor	Ryoji Noyori		
Organic Synthesis	Professor	Shigehiro Yamaguchi	(2291)	yamaguchi@mbbox.chem.nagoya-u.ac.jp
	Assistant Professor	Shohei Saito	(5750)	s_saito@mail.chem.nagoya-u.ac.jp
	Assistant Professor	Kei Murakami	(4525)	murakami@chem.nagoya-u.ac.jp
	Research Fellow	Gore Sangram	(2960)	gore@os.rcms.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
	Assistant 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	Kunio Awaga	(2487)	awaga@mbbox.chem.nagoya-u.ac.jp
	Assistant Professor	Akitaka Matsuda	(2945)	amatsuda@chem.nagoya-u.ac.jp
	Assistant Professor	Haruka Omachi	(3660)	omachi.haruka@a.mbox.nagoya-u.ac.jp
Biomaterials Research	Professor	Yoshihito Watanabe	(3049)	p47297a@nucc.cc.nagoya-u.ac.jp
	Associate Professor	Yasushi Tamura	(2950)	tamura@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	Masahiro Irie (Designated Professor, Rikkyo University)		
	Guest Professor	Hassan Refat Moustafa (Professor, Assiut University)		
Chemical Instrumentation Facility	Manager / Professor	Shigehiro Yamaguchi	(2291)	yamaguchi@mbbox.chem.nagoya-u.ac.jp
	Assistant Professor	Chunguang Han	(3072)	hanc@cic.nagoya-u.ac.jp
	Technical Personnel	Yutaka Maeda	(3069)	maeda@cic.nagoya-u.ac.jp
	Technical Personnel	Kin-ichi Oyama	(3069)	oyama@cic.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 (Editorial Writer, Asahi Shimbun)		
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.mbox.nagoya-u.ac.jp
	Professor	Akiyoshi Hishikawa (Graduate School of Science)	(2494)	hishi@chem.nagoya-u.ac.jp
	Professor	Masato Kitamura (Graduate School of Pharmaceutical Sciences)	(2957)	kitamura@os.nagoya-u.ac.jp
	Associate Professor	Susumu Saito (Institute for Advanced Research)	(5945)	saito.susumu@f.mbox.nagoya-u.ac.jp
	Distinguished Invited University Professor	Sumio Iijima	(6460)	ijimas@nagoya-u.jp
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	Administrative Staff	Sakiko Komura	(5902)	komura@os.rcms.nagoya-u.ac.jp
	Administrative Staff	Sonoe Tankiku	(5908)	tankiku@os.rcms.nagoya-u.ac.jp