HOKKAIDO UNIVERSITY

Institute for Catalysis ICAT

Institute for Catalysis（ICAT）
Hokkaido University

Institute for Catalysis, Hokkaido University

Founded in 1943 by Prof. Juro Horiuchi
as Institute for Catalysis

And

Remodel in 1989 to Catalysis Research Center(CRC)
reorganized in 2015 to Institute for Catalysis (ICAT)

8 Professors. 8 Associate Professors, 8 Assistant Professors

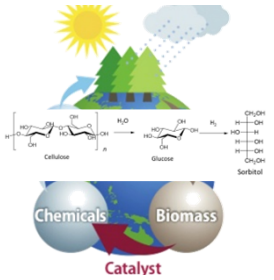
Director :Kiyotaka Asakura
Vice Director :
Junya Hasegawa
Speical Professors.
Prof. E.Negishi
Prof. A.Suzuki

Department of Fundamental Researc
Catalyst Surface Research Division (K.Asakura
Catalysis Theory Research Division(J.Hasegawa
Catalytic Transformation Research Division(A.Fukuoka
Catalyst Material Research Division(K.Shimizu
Photocatalysis Research Division (B.Ohtan
Molecular Catalyst Research Division(T.Takahash
Macromolecular Science Research Division (T.Nakano
Department of Practical Applicatio
Research and Development Division(M.Nishida

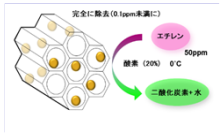
Joint Usage and Research Center in Catalysis Field in Japan

Catalysis is a material to accelerate chemical reactions.
Professors and graphical view of activity

Biomass conversion and mesoporous materials



Biomass

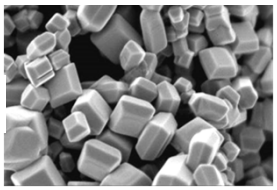


Pt/MCM− 41

Refrigerator catalyst

Fukuoka

Photo catalyst and noble TiO_2 synthesis

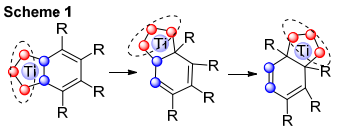


Decahedral-shaped single crystalline

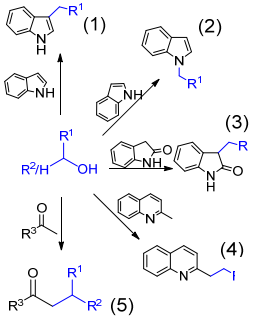
Ohtani

Molecular catalyst and C-C bond formation

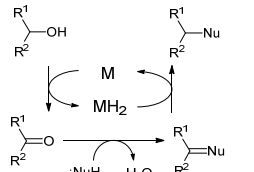
Takahashi

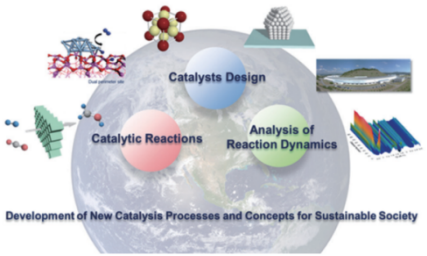


Fine chemistry by heterogeneous catalysts



Shimizu





Catalysis Theory

Hasegawa

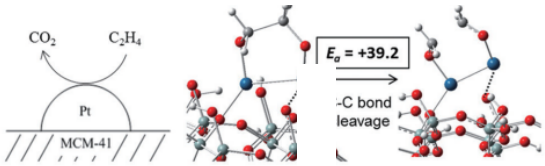
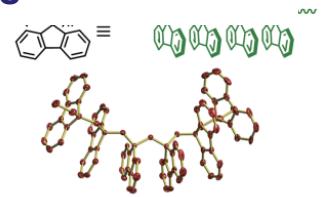


Fig. 1 Complete oxidation of ethylene on the Pt_2/silica surface model.

Advanced Functional polymers

Nakano

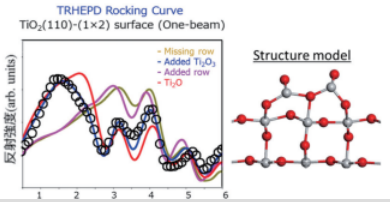


Bridge between Academy and Industry

Nishida

Surface science and catalyst characterization

Asakura



Institute for Catalysis
ICAT

HOKKAIDO UNIVERSITY

1.Purpose of external evaluation

1. Periodical Evaluation
2. We will have the intermediate evaluation about Joint Usage /Research Program by MEXT (Governemt) in 2018.
3. We will submit the proposal to a new program called “International Joint Usage/Research Program” starting in October 2018.

2.1 Missions of ICAT

1. ICAT performs the fundamental researches to reveal the basic concepts about catalysis and to develop the new catalysts.

2. ICAT transfers these new concepts and catalysts to industry and society in order to realize the catalyst-induced innovation and to the sustainable society.

3. ICAT develops next generation researchers and leaders through the above activities.

4. Joint Usage / Research Center

2.3 The ICAT strategy

1. **Three-departments system to promote the fundamental science and to put it into practical application.** ←**diversity of the research**

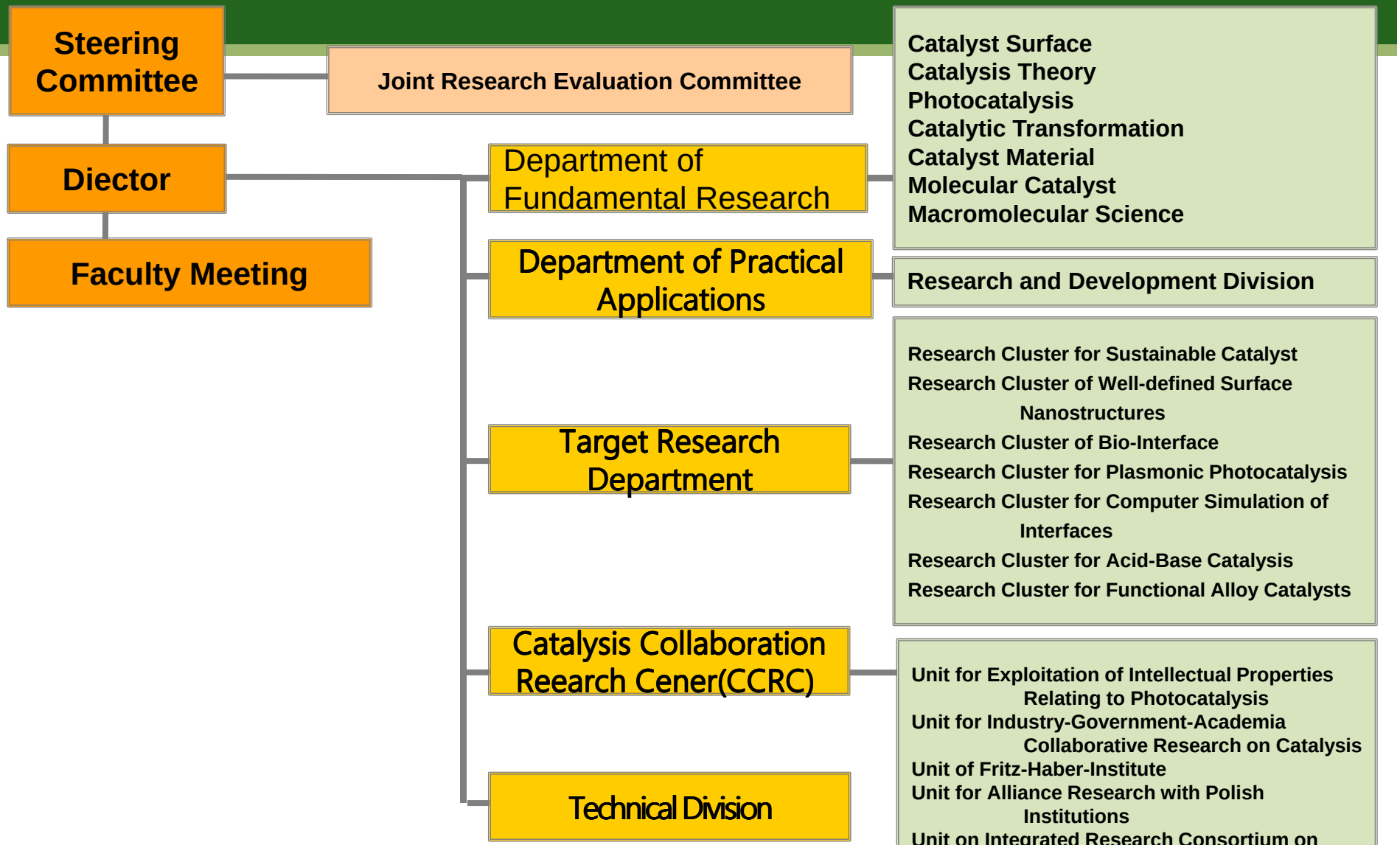
2. **Accumulation and Application of the knowledge about catalysis and catalysts.** ←**Catalyst Informatics**

3. **Expansion of our Activities to Different Science Fields.** ← **diversity of the research**

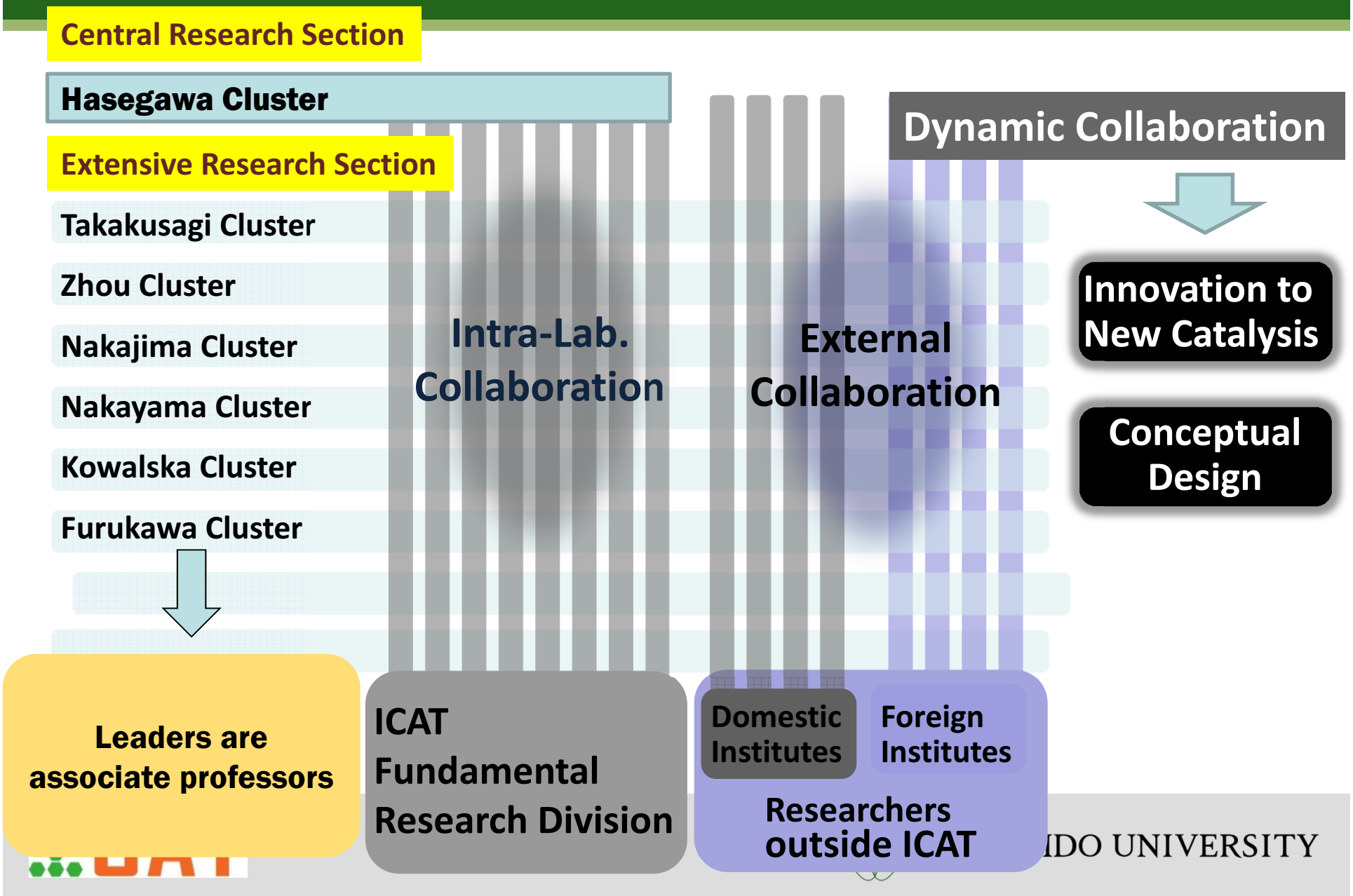
4. **Inter-organizational Cooperation** ← **a member of IRCCS, collaborations with AIST, KEK, RIKEN,and NIMS**

5. **Establishment of Global Catalysis Network** ← **MOU between world-wide research centers and institutes.**

2.4 Institute for Catalysis



Target-Oriented Research Assembly （Poster Presentation） 8



2.6 Principle of human affairs.

(1) All professors are adopted through open recruitment.

(2) Internal promotion is forbidden.

(3) The division is closed after the Full professor retirement.

To keep the high rate of brain circulations

	2012	2013	2014	2015	2016	Total
Move-in Professors	2	0	1	0	0	3
Associate	2	1	0	2	1	6
Assistant	1	0	0	3	2	6
Move-out Professors	0	1	0	1	0	2
Associate	0	1	1	2	1	5
Assistant	0	0	2	2	1	5

3. Activities

Fiscal Year	2012	2013	2014	2015	2016	Average
Papers (Number of international collaborations)	81 (26)	103 (28)	90 (22)	89 (22)	89 (30)	90.4 (25.6)
Top 10% papers	19	26	15	15	19	18.8
Top 1 % papers	3	2	4	5	6	4
Invited talks	67	84	85	88	94	82

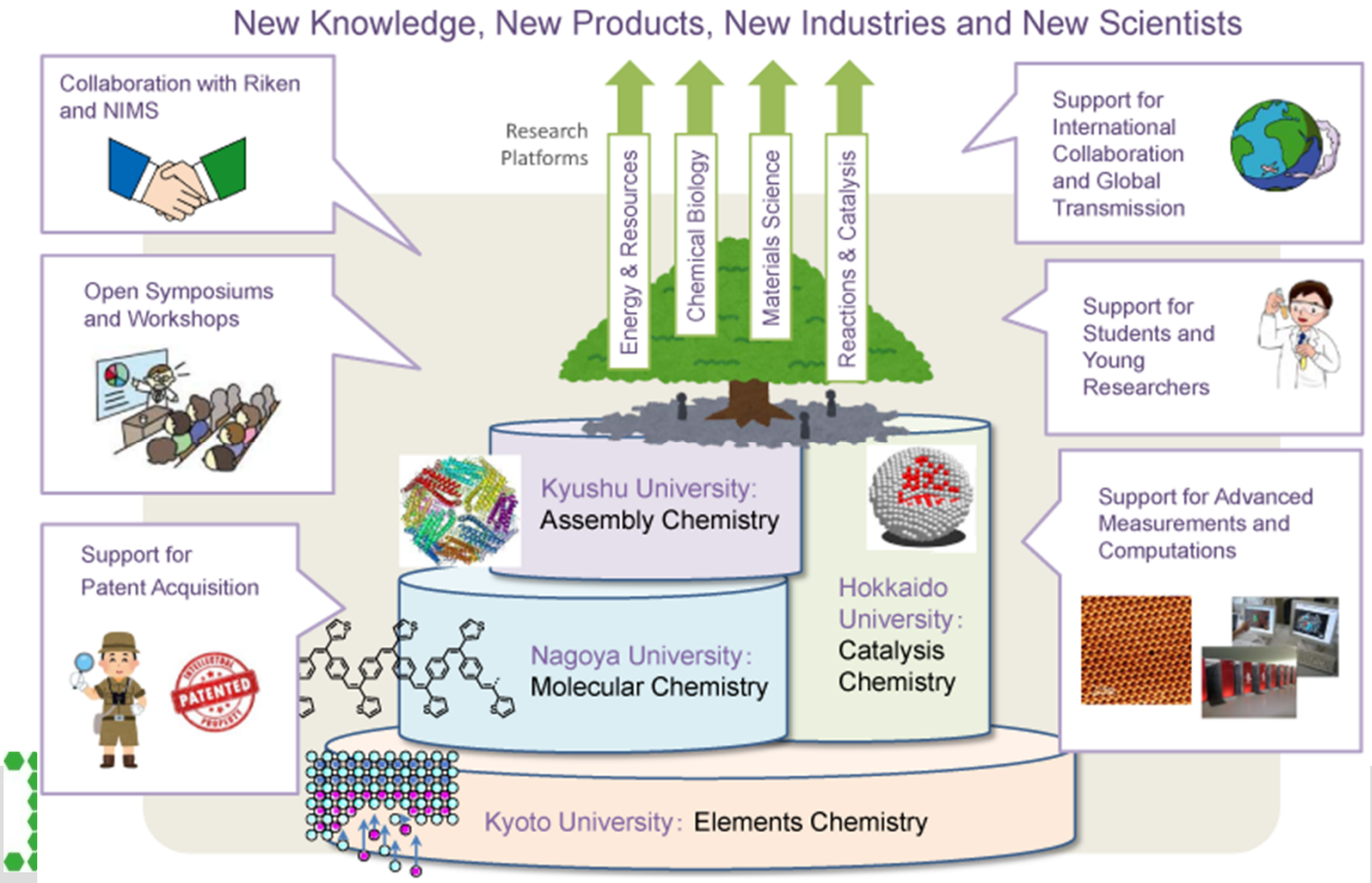
3.Awards(2015-2017)

	Name	Award
2015	M. Osawa	ISE Fellow
2015	A.Fukuoka	Catalysis Society of Japan Award
2015	K.Asakura	Surface Science Society of Japan Award
2015-2017	A.Fukuoka, K.Hara, K.Shimizu, H.Kobayashi,S.Takakusagi,S.Mukai T.Takahashi	Hokkaido U President Award
2016	A.Fukuoka	Green Sustainable Award from MEXT
2016	K.Asakura	Catalysis Society of Japan Award
2017	H.Kobayashi	Chemical SJ, Young Chemist Award
2017	S.Furukawa	Catalyst SJ, Young Scientist Award
2017	S.Furukawa	JIMM, Young Scientist Award

2010–2015,2016–

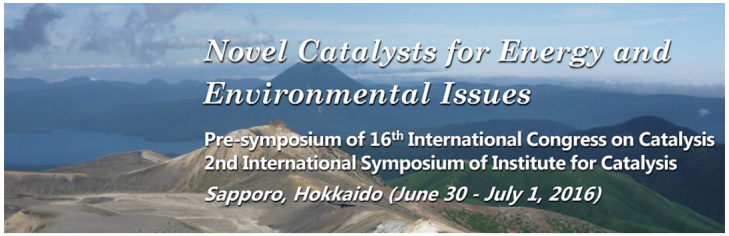
3.2 MEXT Project of Integrated research Consortium on Chemical Sciences

We are working in collaboration with the prestigious research Institutes of Nagoya University, Kyoto University and Kyushu University



UNIVERSITY

3.3 ICAT International Symposium in Japan and Abroad



Program | Presentation guide | Abstract/Paper | Venue/Access | Registration | VISA | Organizer | Picture

Dear all participants,
On behalf of the Organizing Committee of pre-symposium of the 16th ICC-Pre in Sapporo,
we would like to extend our deepest appreciation for your participation in the symposium.
It is our great pleasure to provide this opportunity for all members belonging to international catalysis community.
We believe that you have a lot of fruitful discussion in oral and poster session.

Photos of this symposium have been uploaded. Please check here.

Thanking again all for the highly successful symposium.

Sincerely yours,

Pre-ICC2016

Prof. Atsushi Fukuoka
Chair of the Symposium

Associate Prof. Kiyotaka Nakajima
Secretary of the Symposium

Catalysis Informatics

The 2nd Hokkaido University-Riken-AIST (Catalysis Research) Joint Symposium

October 31(Mon.)

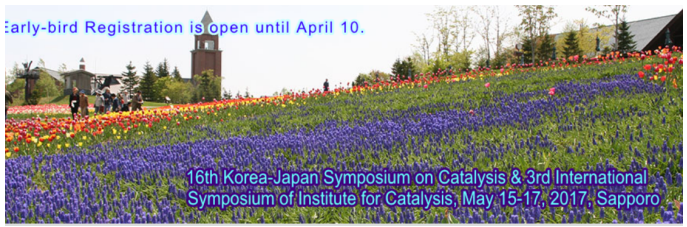
PROGRAM

Chair: *Kiyotaka Asakura (Hokkaido University ICAT)*

13:30	Opening Remarks	**President Advisor Hiroshi Amitsuka** (Hokkaido University)
13:40	Remarks	**Vice President Dr. Yuko Yasunaga** (AIST)
13:50-14:30	Invited Lecture	**Professor Thomas Bligaard** (The SUNCAT Center) 【 】
14:30-15:10	Invited Lecture	**Fellow Dr. Kiyoyuki Terakura** (National Institute for Material Science) 【 】
15:10-15:35		**Professor Kenichi Shimizu** (Hokkaido University ICAT) 【*How to develop a new catalyst? - A classical "scientific" method vs a new approach based on machine learning*】
15:35-15:50	Break	

Chair: *Jun-ya Hasegawa (Hokkaido University ICAT)*

15:50-16:15		**Senior Researcher Dr. Kenji Nagata** (AIST Artificial Intelligence Research Center and Human Informatics Research Institute) 【*AI for catalyst informatics*】
16:15-16:40		**Postdoctoral Researcher Dr. Shigeru Yamaguchi** (RIKEN Center for Sustainable Resource Science) 【*Toward "truly useful" data-driven design of catalytic asymmetric reactions*】
16:40-17:20	Invited Lecture	**Dr. Sergey Levchenko** (Fritz Haber Institute of the Max Planck Society) 【 】
17:20-18:00	Invited Lecture	**Professor Kimito Funatsu** (The University of Tokyo Sch. of Eng. / Dept. of Chemical System Eng.) 【*Paradigm shift to data-driven chemistry*】
18:00	Closing Remarks	**Director Prof. Kiyotaka Asakura** (Hokkaido University ICAT)



Korea-Japan Symposium on Catalysis
May 15-17, 2017

PCOSS-ICAT 2016

北海道大学触媒科学研究所　情報発信型シンポジウム in 厦門

PCOSS-ICAT Joint International Symposium on Catalysis Science for Sustainable Society

Date: December 9-10, 2016
Venue: Xiamen University (China)

3.4 Joint Usage / Research Activity.

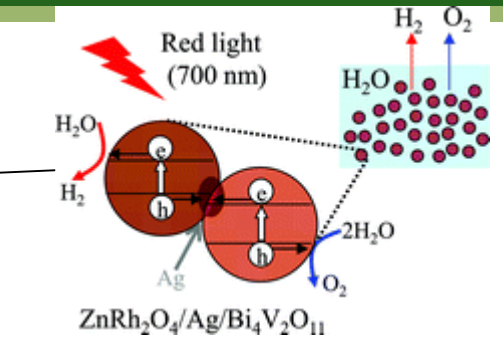
1. Proposal-based Joint Research under the open applications

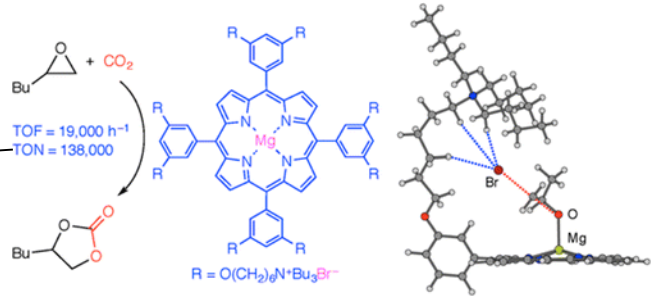
2. APTCC(Advanced Practical Training Course for Catalysis)

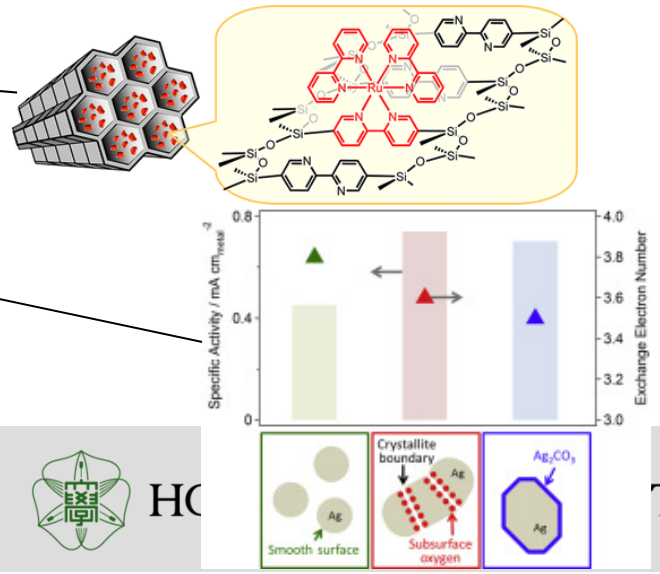
Fiscal year	2012	2013	2014	2015	2016	2012-2016 (ave)
Applications	43	35	30	22	30	32
Accepted	21	25	22	22	30	24
APTCC	11	11	18	19	12	14.2

Selected outcomes of joint research

PI	Collaborator in ICAT	Journal	Title	
Prof. Y.Uemura	K.Asakura	Angewandte Chemi,56 1354(2016)	Dynamics of Photoelectrons and Structural Changes of Tungsten Trioxide Observed by Femtosecond Transient XAFS	Awards from JSSR
Prof. H.Irie	B.Ohtani	J.Material.Chem.A 4,3061(2016)	A Silver-Inserted Zinc Rhodium Oxide and Bismuth Vanadium Oxide Heterojunction Photocatalyst for Overall Pure-Water Splitting under Red Light	Impact factor =8.867
Prof. K.Tanino	A. Nakayama	Nature Commun. 6, 8731(2015)	Total Synthesis of Palau'amine	High Impact factor=12
Prof. H.Ito	K.Asakura	Chem.Sci. 6.2187(2015)	Interconvertible Multiple Photoluminescence Color of a Gold(I) Isocyanide Complex in the Solid State: Solvent-Induced Blue-Shifted and Mechano- Responsive Red-Shifted Photo- luminescence	Top 1% paper
Prof.T.Ema	J. Hasegawa	J.Am.Chem.Soc., 136,15270(2014)	Bifunctional Porphyrin Catalysts for the Synthesis of Cyclic Carbonates from Epoxides and CO2: Structural Optimization and Mechanistic Study	Top 1 % paper
Prof. S.Inagaki	A.Fukuoka	J.Am.Chem.Soc., 136,4003(2014)	A Solid Chelating Ligand: Periodic Mesoporous Organosilica Containing 2,2'-Bipyridine within the Pore Walls	Top 10 % paper
Prof. J.Ohyama	K.Shimizu	J.Power Sources,245,998(2014)	Oxygen Reduction Reaction over Silver Particles with Various Morphologies and Surface Chemical States	Top 10 % paper
Prof. A.Satsuma	K.Shimizu	App.Catal.B 132,511(2013)	Activity Controlling Factors for Low-Temperature Oxidation of CO over Supported Pd Catalysts	Top 10 % paper
Prof. K.Uosaki	A. Nakayama	J.Phys.Chem.C. 117,21359(2013)	Functionalization of Monolayer h-BN by a Metal Support for the Oxygen Reduction Reaction	Top 10 % paper
Pof.A.Onda	A.Fukuoka	J.Cat.296,24(2012)	1-Butanol Synthesis from Ethanol over Strontium Phosphate Hydroxyapatite Catalysts with Various Sr/P Ratios	Top 10 % paper
Prof. H. Kominami	B.Ohtani	Langmuir,28,13105 (2012)	Gold-Titanium(IV) Oxide Plasmonic Photocatalysts Prepared by a Colloid-Photodeposition Method: Correlation Between Physical Properties and Photocatalytic Activities	Top 10 % paper







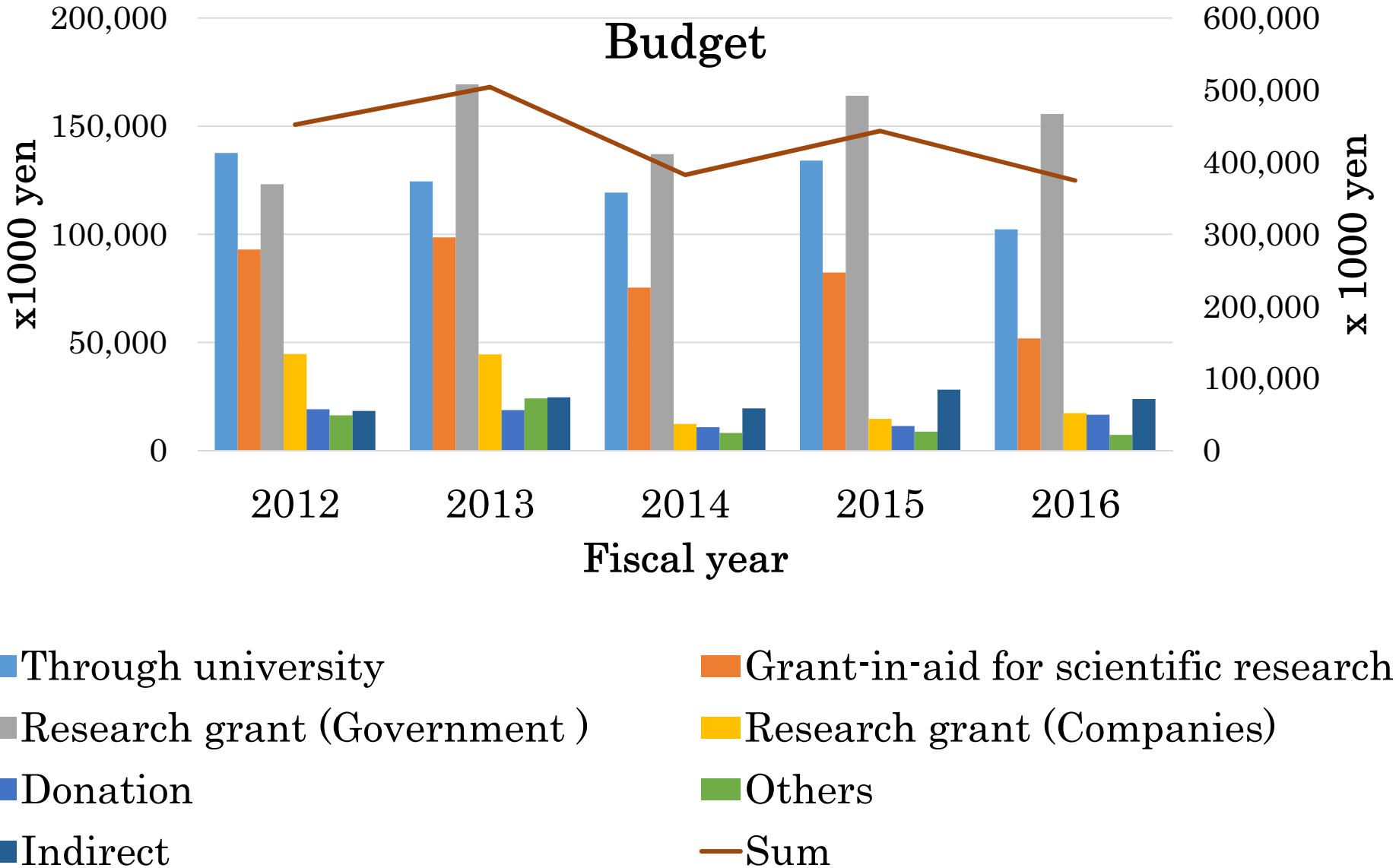
4.1 Education = Each professor has classes in each department.

Fiscal Year	2012	2013	2014	2015	2016	Sum
Temporal Researchers	38(12)	58(21)	42(23)	42(23)	17(8)	197(87)
Graduate Students	69(19)	68(24)	59(19)	57(19)	51(20)	304(101)
Undergraduate	8	11	11	8	7	45
Research Student	4(4)	1(1)	0(0)	2(2)	6(6)	13(13)
Oversea training	2	1	2	0	1	6
PhD	3(2)	4(3)	9(3)	7(2)	9(4)	32(14)

(From abroad)

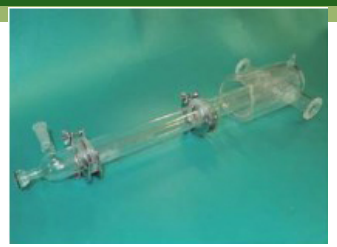
5 professors belong to Graduate School of Chemical Science and Engineering. Each of 3 others belong to Graduate Schools of Life Science, Environmental Science and Engineering.

5 Logistics and administration
5.2 Budget



5.3 Technical Division

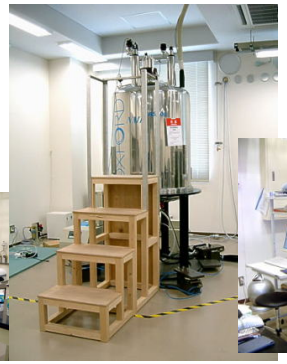
Glassblowing



Machine shop

Catalyst Instrument

NMR, XPS,TEM,SEM, BET



Ishikawa Yamagishi Hasegawa Mukai Shimoda Kawamura

Director Junya Hasegawa

Mission

To promote catalyst science for sustainable society.

To construct International catalysis network.

To reinforce collaborations with the other institutes.

To accelerate practical applications.

To promote the database and catalysis informatics.

CCRC news

CCRC News #1

May 1, 2016

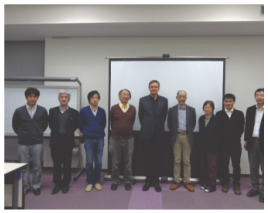
Catalysis Collaborative Research Center (CCRC)

平成２７年１０月の改組において、触媒科学研究所内に附属触媒連携研究センター(Catalysis Collaborative Research Center, CCRC)が発足しました。これまでコーポレートユニットして培われた学外連携を更に発展させることを目的としています。第三期中期目標中期計画期間の開始に伴う組織改編を経て、新たに５つのユニットで構成される附属センターとして再出発しました。

連携センターでは、ユニットなどにおける学外連携をサポートすべく、実験室や居室などの提供を行い、研究所内で実施する連携研究や、学外からの滞在型研究を促進します。

４月２５日には、フリッツ・ハーバー研究所のシェフラー所長が来日されました。研究所間の連携活動についての議論、マテリアルインフォマティクスについての講演など忙しい一日でした。ユニット研究室での写真を下に紹介します。

（記　長谷川淳也）



シェフラー所長の講演会にて
After the lecture by Prof. Scheffler

CCRC News #11

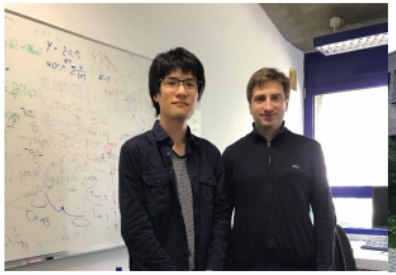
October 9, 2017

北海道大学総合化学院ではAdvanced Graduate School of Chemistry and Materials Science(AGS)と呼ばれる国際教育プログラムが提供されています。総合化学院博士課程に在籍する学生に、海外の研究期間に短期滞在して研究を実施する機会を提供しています。連携センター・Fritz-Haber-Institute(FHI)ユニットの協力を得て、触媒理論研究部門Ｄ１の宮崎玲君が、FHIの理論部門に二か月間滞在し、固体表面における分子吸着に関する理論的研究に関して、FHIのScheffler所長、Levchenkoグループリーダーと共同研究を行いました。FHI理論部門は、ab initio熱力学と呼ばれる計算手法やNOMADと呼ばれる固体物理計算データベースの構築と情報学的活用などにおいて先進的な役割を果たす世界拠点です。世界の俊英の中に揉まれて、宮崎君は一回りたくましくなって帰国したように思えます。FHIユニットのご協力に心から感謝申し上げます。

（記　長谷川淳也）

Graduate School of Chemical Sciences and Engineering, Hokkaido University, provides a global educational program, “Advanced Graduate School of Chemistry and Materials Science (AGS)”. In this program, highly motivated Ph. D. Students have an opportunity to stay and do collaboration work at prominent research institutes in overseas countries. Owing to the cooperation by Theory Department at Fritz-Haber-Institute (FHI), Ray Miyazaki (D1) enjoyed a collaborative research work with Prof. Schaeffler (Director) and Dr. Levchenko (Group leader). The theory department at FHI is a world-wide prominent institute where advanced theory, catalytic concept, and computational techniques have been developed. Ray acquired precious experience by working together with the top scientists. We sincerely thank Theory department, FHI for the cooperation on collaborations, education, and warm hospitality.

(Jun-ya Hasegawa)



（左）研究室にて　（右）FHI の理論部門

CCRC News #4

August 26, 2016

連携センターでは、ロシア・ボレスコウ触媒研
士が特任教授として滞在
）。BIC は 400 人の研究
雇する世界最大の触媒研
触媒開発の基礎研究から
lberberg 博士は理論化学
量子化学研究室を率いて
創成棟にて BIC-ICAT
部門間の共同研究を越
を促進できれば喜ばし
らは Zilberberg 博士、
元 BIC）が参加され、触
に関する講演をされま
所長が XFEL を用いた
クスについての pump-
が系間交差反応の遷移
講演を行い、学術交流

（記　長谷川淳也）

Since July, Prof. Zilberberg from Boreskov Institute of Catalysis (BIC), Russia, is visiting ICAT. BIC is the world largest institute in the field of catalytic science. The scope of the BIC spans from basic development of catalysis to industrialization of promising catalysts. About 400 academic researchers and 1300 staffs are involved! Prof. Zilberberg is leading the quantum chemistry laboratory. On August 25, we organized BIC-ICAT Workshop. I wish that this event promotes to expand the collaborative network at institution level. From the BIC side, Prof. Zilberberg and Prof. Zhanpeisov (Tohoku Univ., a former member of BIC) gave talks on the electronic mechanism of catalytic reactions. From ICAT, Prof. Asakura (director) presented the excited-state dynamics of WO_3 studied with the pump-probe XFEL measurement. Hasegawa showed transition state and reaction pathway of the intersystem crossing reactions.

(Jun-ya Hasegawa)

p (from the left, Nakayama, Hasegawa, Asakura, Zilberberg, Zhanpeisov, Sarode)

Institute for Catalysi
ICAT

HOKKAIDO UNIVERSITY

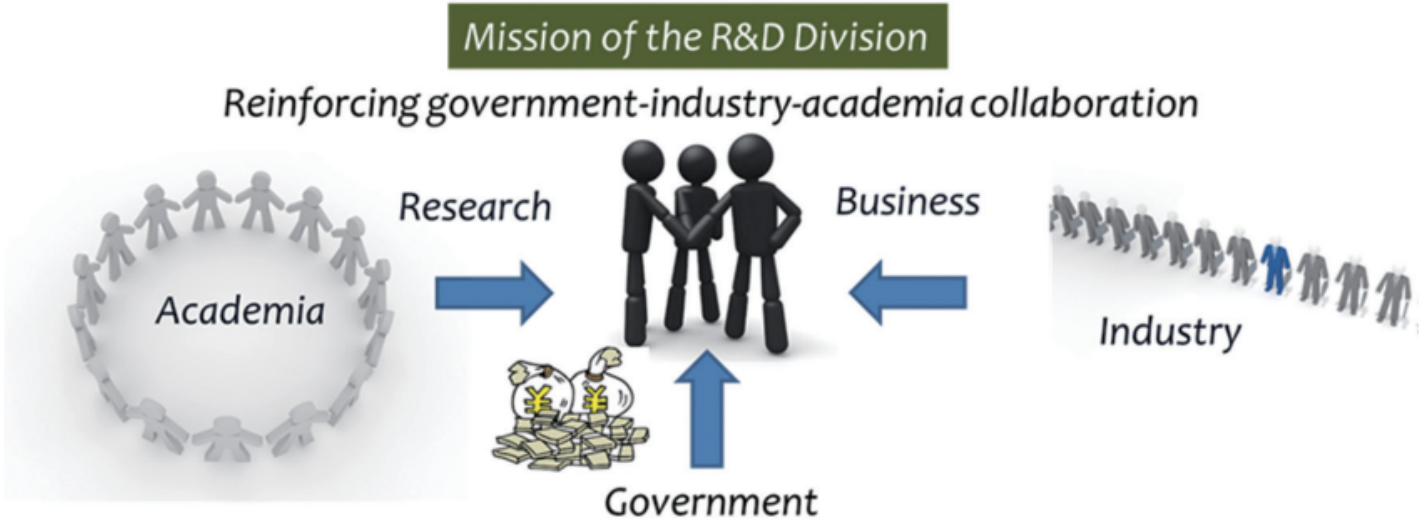
6.1.2 Research and Development Division

Prof. Mayumi Nishida

Industrialize the University's Technology

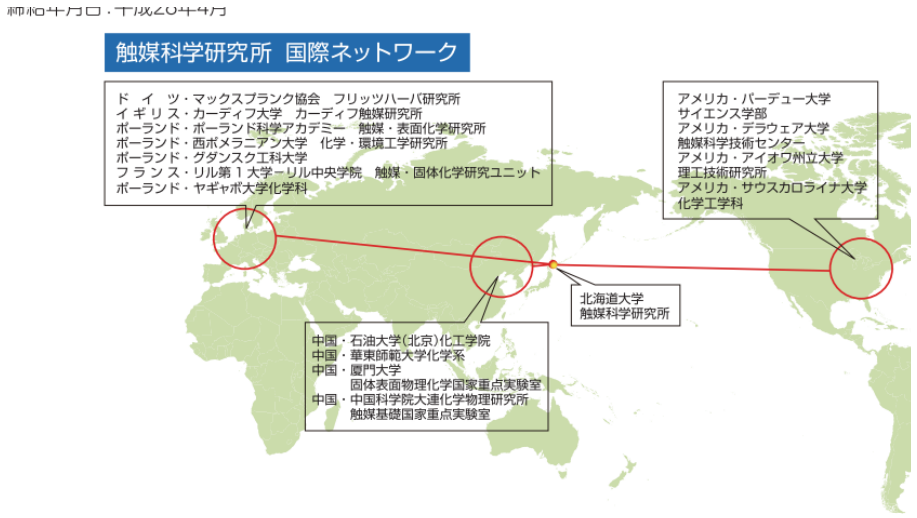
Induce Problem-Solution Research

Cross Appointment Professor with AIST



6.1.4 International Collaborations.

To promote international exchange, the ICAT has concluded agreements with its counterparts in many other countries.



laborations

の国際交流の一環として部局間協定

1) 中国・石油大学 (北京) 化工学院 (平成13年12月7日)
2) 中国・華東師範大学化学系 (平成17年3月18日)
3) ドイツ・マックスプランク協会 フリッツハーバ研究所 (平成17年12月26日)
4) アメリカ・デラウェア大学 触媒科学技術センター (平成19年7月9日)
5) 中国・厦門大学 固体表面物理化学国家重点実験室 (平成19年10月9日)
6) 中国・中国科学院大連化学物理研究所 触媒基礎国家重点実験室 (平成19年10月10日)
7) アメリカ・アイオワ州立大学 理工技術研究所 (平成21年3月10日)
8) イギリス・カーディフ大学 カーディフ触媒研究所 (平成22年1月26日)
9) ポーランド・ポーランド科学アカデミー 触媒・表面化学研究所 (平成22年3月15日)
10) ポーランド・西ポメラニアン大学 化学・環境工学研究所 (平成22年3月17日)
11) ポーランド・グダンスク工科大学 (平成22年3月18日)
12) フランス・リル第1大学―リル中央学院 触媒・固体化学研究ユニット (平成23年1月17日)
13) アメリカ・パーデュー大学サイエンス学部 (平成26年4月26日)
14) アメリカ・サウスカロライナ大学 化学工学科 (平成28年3月24日)
15) ポーランド・ヤギャボ大学化学科 (平成28年5月11日)
16) ロシア・ボレスコフ触媒研究所 (平成28年10月11日)
17) アメリカ・サンキャットセンター (平成28年11月2日)
18) 中国・中国人民大学化学系 (平成28年11月18日)

To promote international exchange, we have concluded agreements with its counterparts in many other countries.

1) School of Chemical Engineering, China University of Petroleum, China (December 7, 2001)
2) Department of Chemistry, East China Normal University, China (March 18, 2005)
3) Fritz Haber Institute of the Max Planck Society, Germany (December 26, 2005)
4) Center for Catalytic Science and Technology, Delaware University, USA (July 9, 2007)
5) State Key Laboratory of Physical Chemistry of Solid Surfaces, Xiamen University, China (October 9, 2007)
6) State Key Laboratory of Catalysis, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, China (October 10, 2007)
7) Institute for Physical Research and Technology, Iowa State University, USA (March 10, 2009)
8) Cardiff Catalysis Institute, Cardiff University, UK (January 26, 2010)
9) Institute of Catalysis and Surface Chemistry, Polish Academy of Sciences, Poland (March 15, 2010)
10) Institute of Chemical and Environment Engineering, West Pomeranian University of Technology in Szczecin, Poland (March 17, 2010)
11) Gdansk University of Technology, Poland (March 18, 2010)
12) Unité de Catalyse et de Chimie du Solide Université Lille 1 et Ecole Centrale de Lille, France (January 17, 2011)
13) College of Science, Purdue University, USA (April 26, 2014)
14) Department of Chemical Engineering, University of South Carolina, USA (March 24, 2016)
15) Faculty of Chemistry, Jagiellonian University, Poland (May 11, 2016)
16) Boreskov Institute of Catalysis, Russia (October 11, 2016)
17) SUNCAT Center for Interface Science and Catalysis, USA (November 2, 2016)
18) Department of Chemistry, Renmin University of China, China (November 18, 2016)

6.1.4 Invited Guest Professors

Stay with us for more than 1 month.

To carry out collaboration researches and education.

2017 Prof. Janczarek Marcin

Prof. Jochen Lauterbach

Prof. A.Bedilo

2016 Prof. P.R.Sarode(from Goa University)

Prof. I. Zilberberg(from Boreskov Institute of Catalysis)

Prof. Zhiping Li (Renmin University of China)

Prof. E. J.M. Hensen(TU Eindohoven)

2015 Prof. H.J.Freund(FHI, Germany)

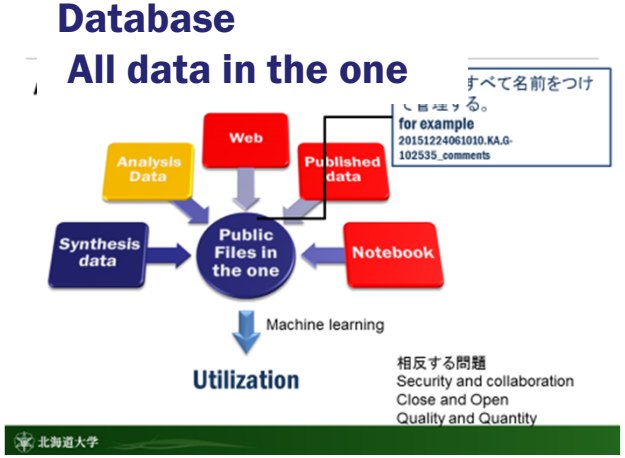
Prof. Chang Wei(China, University Soochow)

2014 Prof. W. MACYK; M. Kotora; T. Cuenca

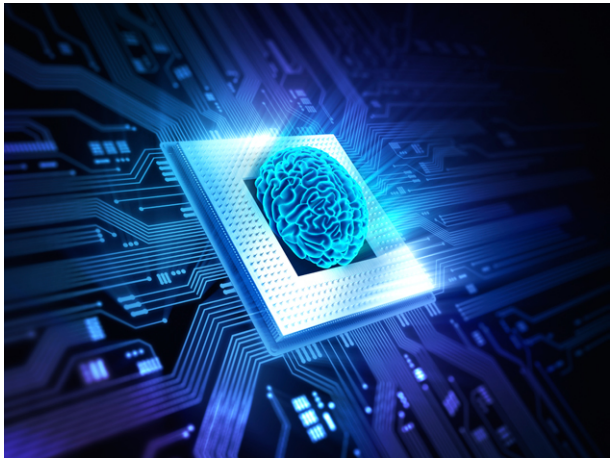
2013 Prof. B.C.Gates; Mauriello Francesco; Chen Zhan; Sanchez Cortes Santiago; Adriana Pietropaolo

6.2 Catalyst Informatics

Collect all data and extract new catalysts or new concept by machine learning



Joint Symposium on Catalyst Informatics (2015～) with AIST, RIKEN, and NIMS。



Machine learning helps researchers tackle challenging tasks, such as designing pollution filter catalysts at industrial scale

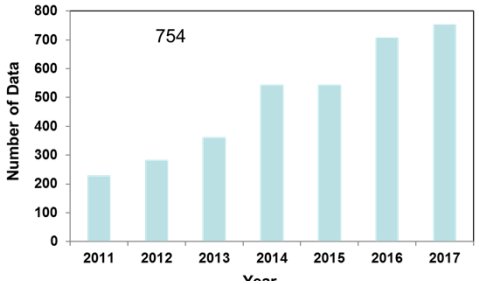
Chemistry World

http://www.rsc.org/chemistryworld/2016/06/machine-learning-catalyst-metal-trends

Takigawa, I., Shimizu, K.-i., Tsuda, K. & Takakusagi, S.
Machine-learning prediction of the d-band center for metals and bimetals.
RSC Advances **6**, 52587-52595, doi:10.1039/c6ra04345c (2016).

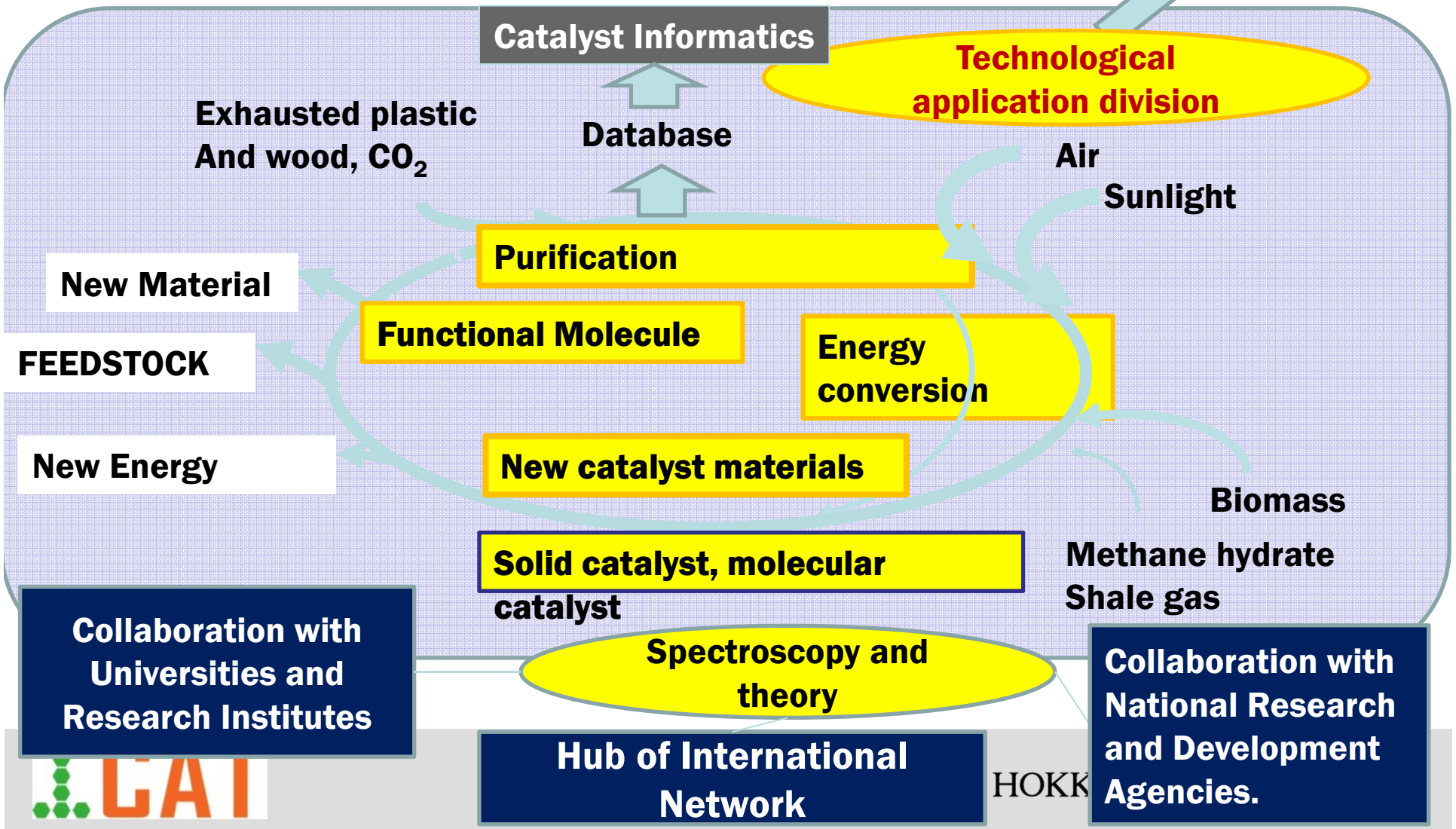
6.2Database

Database	Content	Registered No
Catal. Mat. (J)	Abstract of Paper and Patent about Catalyst Materials and their reactions	900
XAFS (En)	XAFS Spectra database	218
Photo Catalysis(J)	Full page database for Photocatalyst news letter(J)	413 +1528



Database

http://www.cat.hokudai.ac.jp/catdb/

6.3 Future vision of ICAT

Catalyst driven Innovations
Catalysts for Sustainable Society