[Table II]

Contact Information

* Please input ".hokudai.ac.jp"after "@cat", when you send an E-mail.
Please put “81-11-706-” in front of the phone number.

<table>
<tr><th>Research Division</th><th>Abstract</th><th>Contacts</th></tr>
<tr>
<td>Catalyst Surface</td>
<td>
Our missions are to develop unique surface analysis techniques, to observe the catalytically active solid surfaces on an atomic level, to reveal the reaction mechanisms, to make the catalytically interesting surfaces and to manipulate the surface reactions. We applied the accelerator based beam techniques to the characterization of the surfaces such as synchrotron radiation, positron, muon and X-ray free electron laser. Fig.1 shows the ultra high sensitive XAFS technique to study the Pt on the flat graphite surface in the fuel cell system. We can observe the XAFS of sub monolayer Pt. Also we have successfully observed a new phenomenon called as MARX-RAMAN (Multi Atom Resonance X-ray Raman) sensitive to the local structure of the atom accompanying the specific bond. Intermetallics draw much attention as a new class of catalysts. We are investigating Ni_2P, a typical intermetallic catalyst. We have found a P easy diffusion path where beautiful tetrahedral intermediate structure is realized as shown in Fig.2.

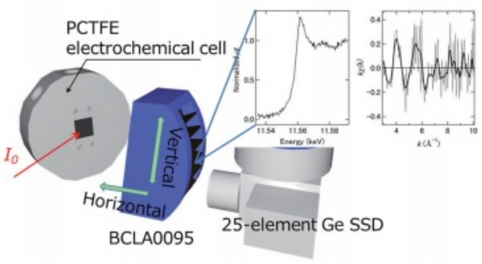


Fig. 1 Ultra-high sensitive XAFS measurement system and XAFS spectra of sub monolayer Pt on Highly oriented pyrolytic graphite

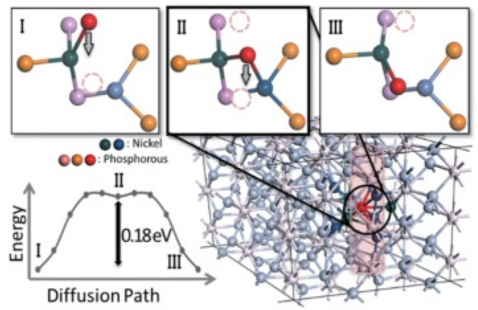
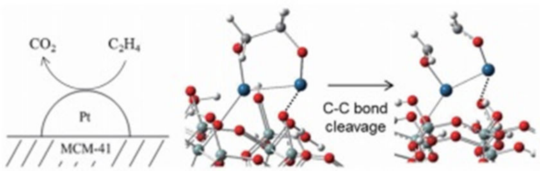
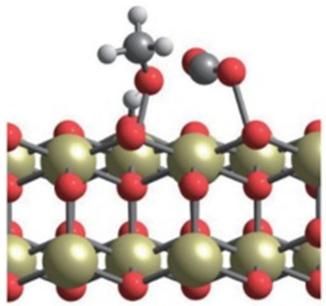


Fig. 2 DFT calculation of Ni_2P during diffusion process. Red one is a diffusing P. In the second stage two Ni atoms have the tetrahedral structures which reduces the activation energy to 0.18 eV.
</td>
<td>
Prof.: Kiyotaka ASAKURA
e-mail: askr
Phone: 9113

Assoc. Prof.: Satoru TAKAKUSAGI
e-mail: takakusa
Phone: 9114
</td>
</tr>
</table>

Research Division	Abstract	Contacts
Catalysis Theory	To understand complex mechanisms in catalytic processes, we are developing accurate theories for describing electronic structures in complex molecular systems, the QM/MM methods for large molecular systems, the first principles molecular dynamics simulations for reaction dynamics, and analytical methods based on quantum and statistical mechanics. These methods are applied to various catalytic reactions involving organic, transition-metal, and heterogeneous catalysts. Our current research focuses on the following topics: 1. Mechanism of hydrolysis by model carbon catalysts. 2. Mechanism of ethylene oxidation with Pt/mesoporous SiO_2 catalyst. 3. Organic catalytic reactions on the metal-oxide surface. 4. Computer-aided catalyst design for methane activation. 5. Mechanism of the Pt-catalyzed the reduction of the amide with bifunctional hydrosilane. 6. Reaction mechanism on metal clusters.  Fig. 1 Complete oxidation of ethylene on the Pt_2/silica surface model.  Fig. 2 Catalytic reactions on the CeO_2 surface.	Prof.: Jun-ya HASEGAWA e-mail: hasegawa Phone: 9145 Assoc. Prof.: Kenji IIDA e-mail: k-iida Phone: 9145 Assist. Prof:: Min GAO e-mail: gaomin Phone: 9145

<table>
<tr><th>Research Division</th><th>Abstract</th><th>Contacts</th></tr>
<tr><td>Catalytic Transformation</td><td>

Our strategy is molecular design of heterogeneous catalysts and their application for utilization of renewable energies and environmental protection. One of our topics is conversion of non-food biomass to valuable chemicals by heterogeneous catalysts. We have found that air oxidation of woody biomass provides a weakly acidic carbon that can hydrolyze the woody biomass to glucose and xylose. The solid residue containing the carbon catalyst and lignin after reaction is converted back to a fresh catalyst by the same air oxidation. The carbon catalyst can be utilized in a plug flow slurry reactor for hydrolysis of cellulose to soluble β-1,4 glucans that are further hydrolyzed to glucose in a fixed bed reactor over a conventional solid acid catalyst (Fig. 1). This process is the first example for continuous conversion of cellulose to soluble products in a slurry system.

Our interest also includes catalytic application of mesoporous materials. We reported high activity of Pt/mesoporous silica in low temperature oxidation of ethylene to CO2 (Fig. 2). This catalyst is practically used in the latest models of refrigerators to inhibit aging of vegetables and fruits. We are currently studying the structure-activity relationship in this reaction and also further application for the removal of odorous organic compounds with the Pt catalyst.

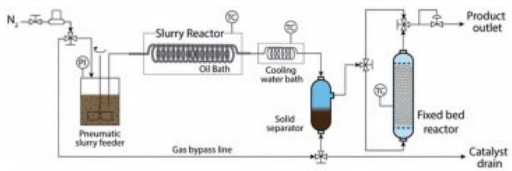


Fig. 1 Continuous flow slurry process for hydrolysis of mix-milled cellulose and *Eucalyptus*.

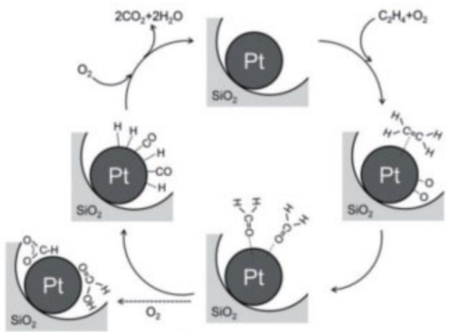


Fig. 2 Proposed mechanism for low-temperature oxidation of ethylene over Pt/mesoporous silica.

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Prof.: Atsushi FUKUOKA
e-mail: fukuoka
Phone: 9140

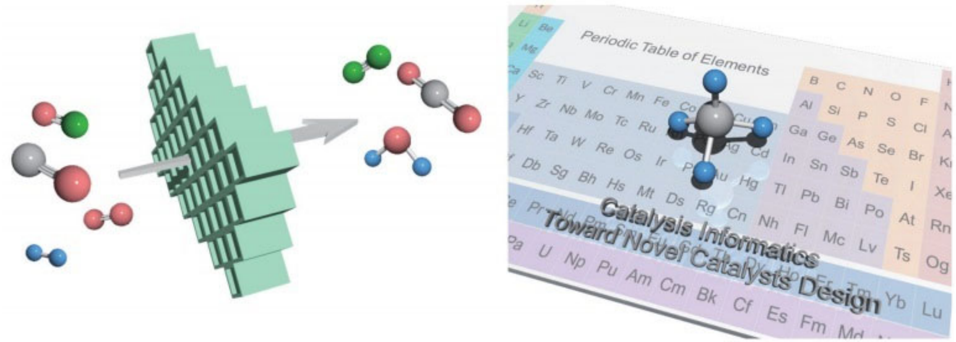
Assoc. Prof.: Kiyotaka NAKAJIMA
e-mail: nakajima
Phone: 9136

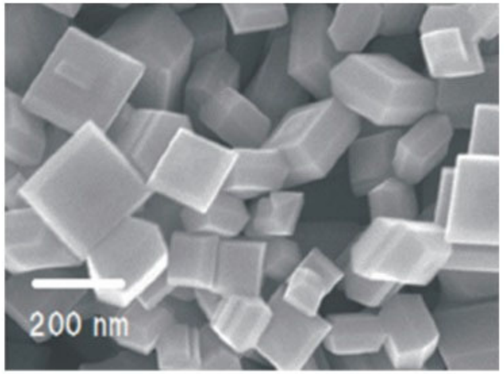
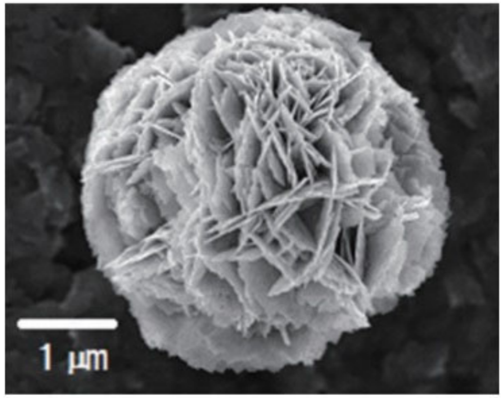
Assist. Prof.: Hirokazu KOBAYASHI
e-mail: kobayashi.hi
Phone: 9137

Assist. Prof.: Abhijit SHROTRI
e-mail: ashrotri
Phone: 9137

</td></tr>
</table>

Research Division	Abstract	Contacts

Catalyst Material	Our aim is to design new heterogeneous catalysts for green organic reactions and automotive pollution control with minimum use of precious metal resources. Mechanistic and structural studies by various in situ spectroscopic methods establish the structure-activity relationship, which provides fundamental aspects for catalyst design. We have found that creation of multifunctional active sites at metal-metal or metal-support interfaces is a key factor for design of novel catalysts. Interplay of experiments, computational chemistry and data science is our new methodology to develop heterogeneous catalysts for energy and environmental issues.  	Prof.: Ken-ichi SHIMIZU e-mail: kshimizu Phone: 9164 Assoc. Prof.: Shinya FURUKAWA e-mail: furukawa Phone: 9162 Assist. Prof:: Takashi TOYAO e-mail: toyao Phone: 9165

Research Division	Abstract	Contacts
Photocatalysis	We are aiming to design, fabricate and characterize photocatalyst particles and to clarify the mechanism of their photocatalysis. (1) reversed double-beam photoacoustic spectroscopy (RDB-PAS) for evaluation of energy-resolved density of electron traps in photocatalyst particles to be compared with their photocatalytic activity; (2) examination of light-intensity dependence of photocatalytic reactions using an ultrahigh-intensity continuous monochromatic light source to find electron-transfer mechanism depending on the density of electrons or holes in a particle; (3) preparation of highly active titanium(IV) oxide (titania) photocatalyst particles (Fig. 1) using a newly developed gas-phase reactor; (4) development of metal oxide particles with micro-macro hierarchical structure (Fig. 2) through hydrothermal reaction, and clarification of the mechanism of those particle formation and photocatalysis on them.  Fig. 1  Fig. 2	Prof.: Bunsho OHTANI e-mail: ohtani Phone: 9132 Assoc. Prof.: Ewa KOWALSKA e-mail: kowalska Phone: 9130 Assist. Prof:: Mai TAKASHIMA e-mail: takashima.m Phone: 9130

Research Division	Abstract	Contacts
Molecular Catalyst	Based on manipulating and understanding chemical reactions, we cultivate a novel molecular catalysis for contributing sustainable production of organic fine chemicals and materials. Particularly, we are focusing on the control of fundamental active species (anions, radicals, and cations) involved in chemical reactions by creating unprecedented molecules and eliciting the catalytic power inherent in their structure. Our original catalysts enable various selective transformations and thus, precise construction of complex organic frameworks. In addition, we aim to develop new chemical reactions through the experimental and theoretical understanding the behavior of molecules.	Prof.: Daisuke URAGUCHI e-mail: uraguchi Phone: 9149

<table>
<tr><th>Research Division</th><th>Abstract</th><th>Contacts</th></tr>
<tr>
<td>Macromolecular Science</td>
<td>
Our research activities focus on the synthesis of polymers having controlled structures including helices, π-stacked conformations, and hyperbranches and supramolecules including ordered liquid crystalline phases aiming at creating advanced materials showing catalytic activities, photo emission, photo-electronic functions, non-linear optical properties, separation functions, and pharmaceutical activities.
We have succeeded in the synthesis and
structural elucidation of π-stacked vinyl polymer, poly(dibenzofulvene), for the first time (Fig. 1). Based on the π-stacked structure, this polymer shows valuable photo electronic properties that have been thought to be unique to main-chain conjugated polymers. Another goal is to create a polymer helix using light: we have, for the first time, prepared a preferred-handed helix on the basis of chirality of light (circularly polarized light) in a reversible manner and further extended this work to a helical-sense switching driven/triggered by light (Fig. 2).

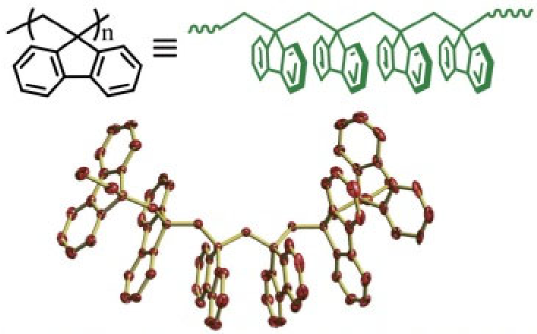


Fig. 1. Structure of poly(dibenzofulvene), the first π-stacked vinyl polymer.

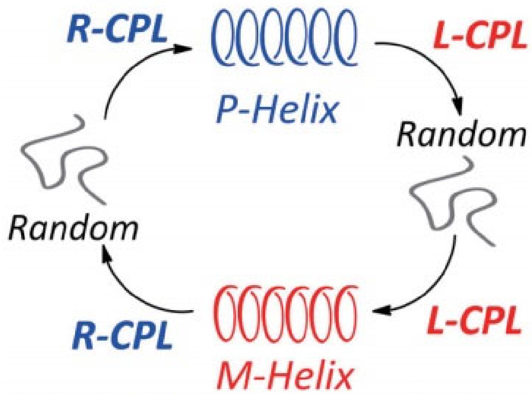


Fig. 2. Chirality switching of helical polymer driven/ triggered by circularly polarized light (CPL).
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<td>
Prof.: Tamaki NAKANO
e-mail: tamaki.nakano
Phone: 9155
Assoc. Prof.: Zhiyi SONG
e-mail: songzhiyi
Phone: 9157
Assist. Prof:: Masayoshi Bando
e-mail: masayoshi.bando
Phone: 9157
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<table>
<tr><th>Research Division</th><th>Abstract</th><th>Contacts</th></tr>
<tr><td>Research and Development</td><td>The Research and Development Division was started at the Institute for Catalysis (ICAT) Hokkaido University in 2014 guided by the Ministry of Education, Culture, Sports, Science and Technology (MEXT). At the end of 2014, Hokkaido University and the National Institute of Advanced Industrial Science and Technology (AIST) drew up a contract to realize the cross-appointment system to reinforce the government-industry-academia network. In 2015, I was appointed the leader of the Hokkaido University Cross-appointment Team, that was set up in the Interdisciplinary Research Center for Catalytic Chemistry AIST. Then, with the cooperation of ICAT, AIST and Riken (the Institute of Physical and Chemical Research), we launched the project named “Catalyst Informatics.” The Arti cial Intelligence Research Center AIST helped facilitate and drove the project. In 2017, the National Institute for Materials Science (NIMS) joined the project and “Catalyst Informatics Symposium” was held in the collaboration with ICAT-Riken-AIST- NIMS.

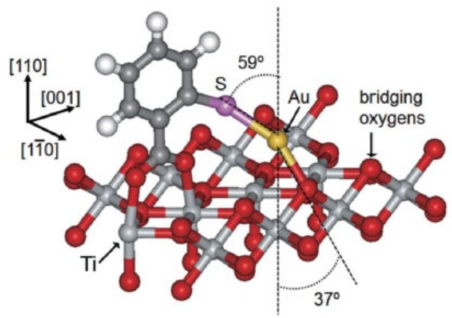
</td><td>Prof.: Mayumi NISHIDA
e-mail: m-nishida
Phone: 9381</td></tr>
</table>

Department of Target Research

Central Research Section

Research Cluster	Abstract	Contacts
Sustainable Catalyst	This cluster is aiming at promoting advanced catalysis research. Our projects are to develop and maintain both hard and soft infrastructures in the institute, to promote and enhance the collaborations and cooperation in the community of catalysis science and engineering, and to develop the forefront of the interdisciplinary area related to catalysis. (1) Sustainable catalysis research project is to promote and support advanced catalysis researches as well as to introduce transcendental approaches in catalysis. (2) Training and education program is to contribute in developing human resources and in outreach activities to the society. (3) Database project is to accumulate experimental and XAFS information of catalytic systems and to develop catalysis informatics.  Fig. 1. Top page of the web site of the catalyst database	Cluster Leader: Jun-ya HASEGAWA e-mail: hasegawa Phone: 9145

Extensive Research Section

Research Cluster	Abstract	Contacts
Well-defined Surface Nanostructures	The objective of our research group is to create well-defined active nanostructures by modifying oxide single crystal surfaces with various functional molecules and metals. The origin of the catalytic activity is elucidated by using advanced surface science techniques such as STM and PTRF-XAFS. Machine-learning technique is also applied to predict nanostructures with higher activity. We are now focusing on metal clusters on oxide surfaces because they are technologically important as oxide-supported metal catalysts and electronic devices. It is not easy to prepare homogeneous subnanometersized clusters on oxides because they are easily aggregated to form large clusters. We succeeded in preparing an atomically dispersed metal species by premodifying an oxide surface with functional molecules before metal deposition (Fig. 1), which may enable precise size control of subnanometer-sized clusters with unique catalytic properties.  Fig. 1. Atomically dispersed Au on TiO_2(110) premodified with o-MBA (mercaptobenzoic acid) molecules.	Cluster Leader: Satoru TAKAKUSAGI e-mail takakusa phone: 9114

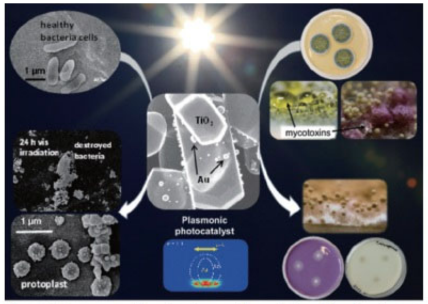
<table>
<tr><th>Research Cluster</th><th>Abstract</th><th>Contacts</th></tr>
<tr><td>Plasmonic Photocatalysis</td><td>
Our research focuses on development of plasmonic photocatalysis with ability of working at visible range of solar spectrum, i.e. mono and bimetallic photocatalysts composed of gold, silver, copper, platinum and wideband semiconductor. The influence of structural properties on the photocatalytic activity and the mechanism of chemical and microbiological (bacteria and fungi) pollutants degradation is investigated.
The mechanism of photocatalytic action under visible light irradiation will be studied by a few methods, e.g., photoacoustic spectroscopy (PAS), reversed double beam photoacoustic spectroscopy (RDB-PAS), time-resolved microwave conductivity (TRMC), electron paramagnetic resonance (EPR) spectroscopy, fluorescence spectroscopy, quasi-Fermi level determination, action spectrum analysis. The influence of titania facets (101 and 001) on properties of metal deposits, and thus on resultant photo- and antimicrobial properties will be also examined.


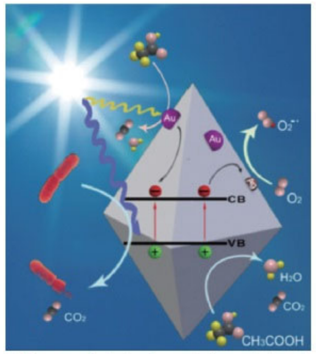
Fig. 1. Images of bacteria and fungi: healthy (top) and affected (bottom) by irradiated plasmonic photocatalysts.


Fig. 2. Scheme of photodegradation of chemical and microbiological pollutants on titania (exposed with (101) facets) modified with NPs of gold and silver.
</td><td>Cluster Leader:
Ewa KOWALSKA
e-mail: kowalska
phone: 9130</td></tr>
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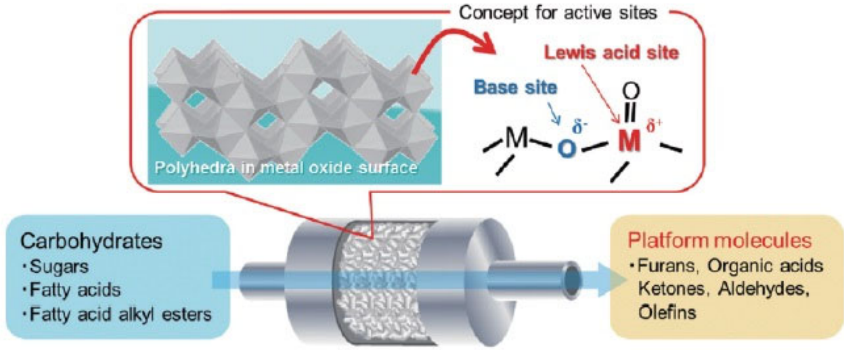
<table>
<tr><th>Research Cluster</th><th>Abstract</th><th>Contacts</th></tr>
<tr><td>Acid-Base Catalysis</td><td>

Chemical production from renewable and easily accessible carbohydrates in nature is increasingly important in recent years for the development of sustainable society. Plant-derived carbohydrates, which show higher reactivity than fossil fuel-derived hydrocarbons, can be converted to attractive platform molecules (furans, organic acids, ketones, aldehydes, olefin, etc.) by acid-base catalysis in the presence of water. In this project, acid and base functionality of electron-deficient metal species and electron-rich lattice oxygen sites, respectively, on metal oxides has been studied for the carbohydrates conversion in the presence of water. Precise control of basicity for oxide catalysts would enable selective production of various small (C2-C4) and large (> C12) hydrocarbons though fragmentation and condensation reactions. The resulting molecules can be used as sustainable resources for the production of a variety of industrially important chemicals.



Conceptual illustration of acid-base pair on metal oxide surface available for carbohydrates conversion in water

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Cluster Leader:
Kiyotaka NAKAJIMA
e-mail: nakajima
phone: 9136

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<table>
<tr><th>Research Cluster</th><th>Abstract</th><th>Contacts</th></tr>
<tr><td>Functional Alloy Catalysts</td><td>

Alloys have been recognized as effective catalyst materials. However, the general methodology and theory for catalyst design remain under debate and construction. To develop efficient alloy catalysts and establish the corresponding chemistry, it is important to understand the surface structures and electronic states of the alloys in an atomic level. For this purpose, we study the following themes from the viewpoints of catalytic chemistry, metallurgy, surface science, and theoretical chemistry:

(1) Achieving stereo and regioselective molecular transformations using specific atomic arrangementsof ordered alloys.

(2) Development of surface-modified intermetallics for efficient molecular conversion.

(3) Synthesis and application of “intermetallic-sloid solution hybrid alloys” for well-controllable catalyst design.

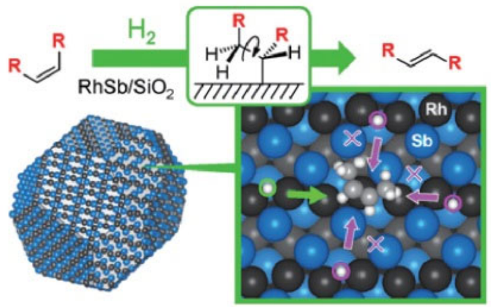

Fig. 1. Hydrogen-mediated stereoselective alkene isomerization using specific surface atomic arrangement of RhSb ordered alloys.

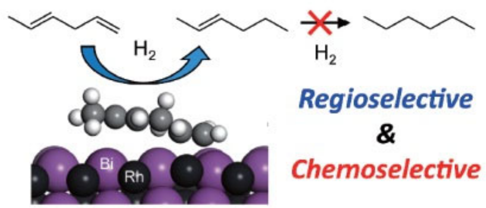

Fig. 2. Regio- and chemoselective hydrogenation of diene to monoene governed by RhBi ordered alloy. Combination of one-dimensional Rh arrays and steric hindrance of Bi inhibits adsorption of inner C=C moiety.

</td><td>

Cluster Leader:
Shinya FURUKAWA
e-mail: furukawa
phone: 9162

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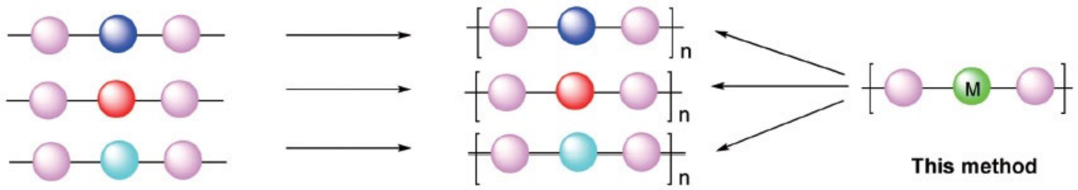
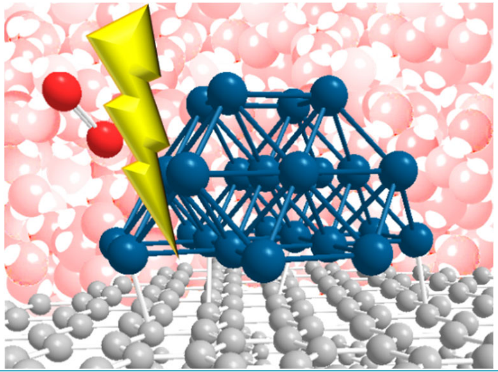
Research Cluster	Abstract	Contacts
Transition-metals-induced Synthesis and Transformation of Polymer	Carbon-carbon bond formation/cleavage on transition metals has been almost exclusively investigated due to the numerous contributions to organic synthesis. In this cluster, carbon-carbon bond formation/cleavage on transition metals were applied to develop new synthetic methodologies for polymers or oligomers. Processes for producing co-oligomers with high regioregularity are important objects in many researches. Herein, metallacycle-including polymer or oligomer were synthesized. Through the carbon-carbon bond formation/cleavage on transition metals, the metallacycle moiety was converted to a variety of aromatic rings. Subsequently, a variety of highly regioregular co-oligomers were synthesized from the same metallacycle-including oligomer.  	Cluster Leader: Zhiyi SONG e-mail: songzhiyi phone: 9153

Research Cluster	Abstract	Contacts
Nano-Interface Reaction Field	Our research purpose is understanding and designing catalytic reactions near solid/liquid and substrate/nanoparticle interfaces under external fields. By combining theoretical frameworks of quantum and statistical mechanics, we develop a theoretical method which can be applied to interface systems under light or electrode bias. The method is used to formulate theoretical guidelines for controlling catalytic activity by both microscopic chemical bonds and macroscopic interface shapes. Our present study focuses on the following topics: (a) Controlling optoelectronic properties of plasmonic nanoalloys for photocatalysts. (b) Mechanism of photoreactions catalyzed by organic metal complexes and metal nanoparticles supported on a metal-oxide. (c) Role of light and electrode bias in chemical reactions. (d) Development of a theoretical method for electrode catalytic reactions. 	Cluster Leader: Kenji IIDA e-mail: k-iida phone: 9145

Catalysis Collaboration Research Center

Unit	Abstract	Host researcher	
		e-mail	phone
HU Catalysis Alliance	Precise synthesis of ligand-protected subnanometer metal clusters, Interface of inorganic nanoentities and organic-based molecules, Supramolecular aassembly of Clusters ("Cluster of clusters"), Supramolecular/macromolecular chemistry of multimetallic compounds.	Katsuaki KONISHI (Faculty of Environmental Earth Science)	
		konishi@ees.	4538
	Development of "predictive" chemical theory for reaction, electron, and spectroscopy and programs, as well as advanced computational chemistry applications. First-principle excited-state reaction dynamics, Theory-guiding catalysis design with elementary strategy, Development of a large-scale electronic structure theory, Near-field molecular theory, Reaction informatics.	Tetsuya TAKETSUGU (Faculty of Science)	
		take@sci.	3535
	Synthetic organic chemistry, Asymmetric catalysis, Bimetallic cooperative catalysis, Natural product synthesis, Oligosaccharide synthesis based on new glycosidation method.	Shigeki MATSUNAGA (Faculty of Pharmaceutical Sciences)	
		smatsuna@pharm.	3236
	Bio-engineering of carbohydrates and related compounds, including α-glucans, β-mannosides, and others, for production of functional foods and biomaterials. Exploring novel enzymatic activities and engineering of the enzymes. Carbohydrate metabolic pathways and relevant enzymes in living organisms.	Haruhide MORI (Research Faculty of Agriculture)	
		hmori@chem.agr.	2497
	Fabrication of oxide nanofilms, Nanoporous films and functional surfaces using electrochemical processes, Tailoring of novel materials for batteries and fuel cells for next generation.	Hiroki HABAZAKI (Faculty of Engineering)	
		habazaki@eng.	6575
	Development of nano materials and evaluation of properties by quantum beam analysis method, Multi quantum beam high voltage electron microscope (MQB-HVEM), Nonequilibrium materials science, Materials involving quantum beams, Development of nanomaterials, Nuclear reactor materials, Fusion reactor materials, Fine structure analysis using transmission electron microscopy.	Tamaki SHIBAYAMA (Faculty of Engineering)	
		shiba@qe.eng.	6774
	Material design and engineering, Adsorption engineering, Separation engineering, Precise structural controlling of porous materials, Development of new production systems of nanomaterials, Development of devices for reaction and separation using nanomaterials, Material recycling.	Shin MUKAI (Faculty of Engineering)	
		smukai@eng.	6592
	Solid catalyst for purification of water, Solid catalyst with heteropoly compounds, Solid material for recovery of resources.	Yuichi KAMIYA (Faculty of Environmental Earth Science)	
		kamiya@ees.	2217