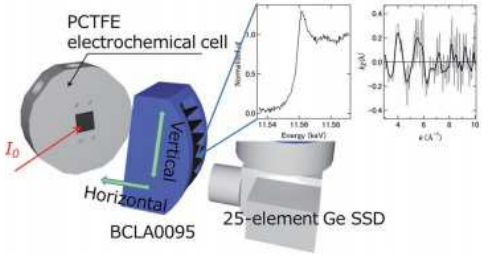
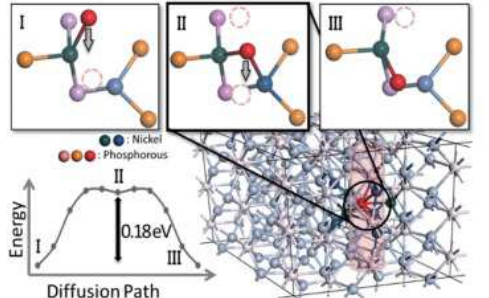


[Table II]

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.

Research Division	Abstract	Contacts
Catalyst Surface	<p>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 Ni₂P, a typical intermetallic catalyst. We have found a P easy diffusion path where beautiful tetrahedral intermediate structure is realized as shown in Fig.2.</p>  <p>Fig. 1 Ultra-high sensitive XAFS measurement system and XAFS spectra of sub monolayer Pt on Highly oriented pyrolytic graphite</p>  <p>Fig. 2 DFT calculation of Ni₂P 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.</p>	<p>Prof.: Kiyotaka ASAKURA e-mail: askr Phone: 9113</p> <p>Assoc. Prof.: Satoru TAKAKUSAGI e-mail: takakusa Phone: 9114</p> <p>Assist. Prof.: Hiroko MIWA e-mail: ariga Phone: 9115</p>

Research Division	Abstract	Contacts
Catalysis Theory	<p>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.</p> <p>Our current research focuses on the following topics:</p> <ol style="list-style-type: none"> 1. Mechanism of hydrolysis by model carbon catalysts. 2. Mechanism of ethylene oxidation with Pt/mesoporous SiO₂ 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. <div style="display: flex; justify-content: space-around; align-items: flex-end;"> <div data-bbox="465 965 1003 1133"> </div> <div data-bbox="1146 837 1467 1141"> </div> </div> <div style="display: flex; justify-content: space-around; align-items: flex-end; margin-top: 10px;"> <div data-bbox="465 1149 1003 1204"> <p>Fig. 1 Complete oxidation of ethylene on the Pt₂/silica surface model.</p> </div> <div data-bbox="1052 1149 1512 1181"> <p>Fig. 2 Catalytic reactions on the CeO₂ surface.</p> </div> </div>	<p>Prof.: Jun-ya HASEGAWA e-mail: hasegawa Phone: 9145</p> <p>Assoc. Prof.: Akira NAKAYAMA e-mail: nakayama Phone: 9145</p> <p>Assist. Prof.: Min GAO e-mail: gaomin Phone: 9145</p>

Research
Division

Abstract

Contacts

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.

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

Catalytic
Transformation

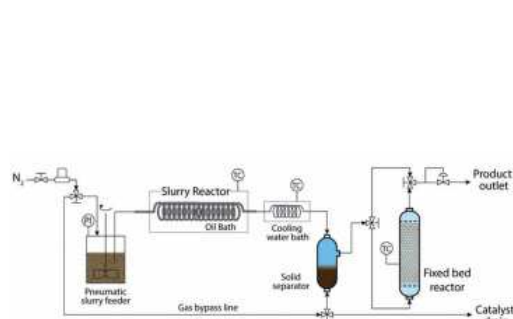


Fig. 1 Continuous flow slurry process for hydrolysis of mix-milled cellulose and *Eucalyptus*.

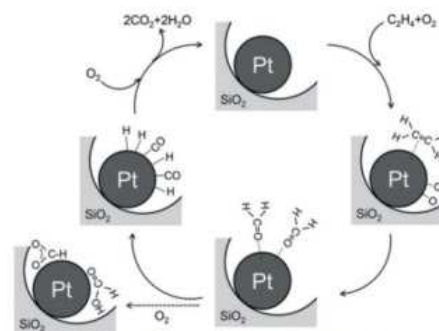
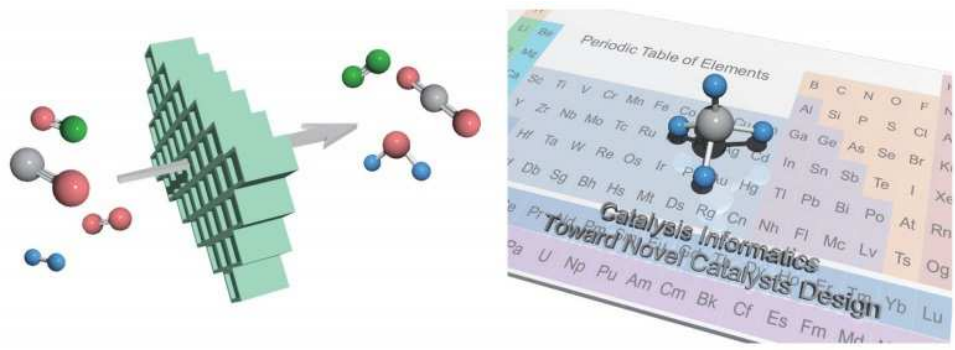
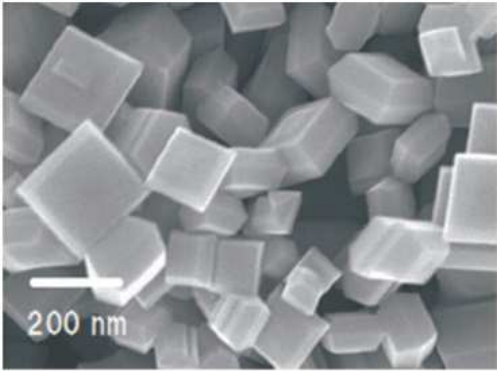
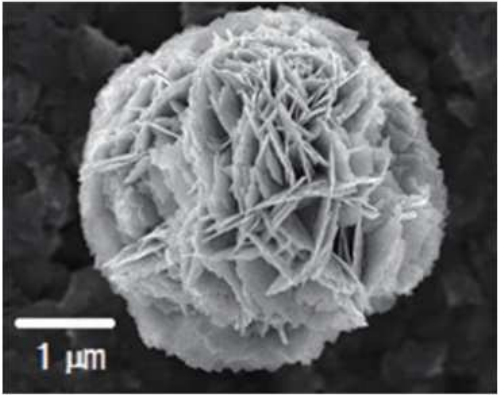


Fig. 2 Proposed mechanism for low-temperature oxidation of ethylene over Pt/mesoporous silica.

Research Division	Abstract	Contacts
Catalyst Material	<p>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.</p> 	<p>Prof.: Ken-ichi SHIMIZU e-mail: kshimizu Phone: 9164</p> <p>Assoc. Prof.: Shinya FURUKAWA e-mail: furukawa Phone: 9162</p> <p>Assist. Prof.: Takashi TOYAO e-mail: toyao Phone: 9165</p>

Research Division	Abstract	Contacts
Photocatalysis	<p>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.</p> <div style="display: flex; justify-content: space-around; align-items: flex-end;"> <div style="text-align: center;">  <p>Fig. 1</p> </div> <div style="text-align: center;">  <p>Fig. 2</p> </div> </div>	<p>Prof.: Bunsho OHTANI e-mail: ohtani Phone: 9132</p> <p>Assoc. Prof.: Ewa KOWALSKA e-mail: kowalska Phone: 9130</p> <p>Assist. Prof.: Mai TAKASHIMA e-mail: takashima.m Phone: 9130</p>

Research
Division

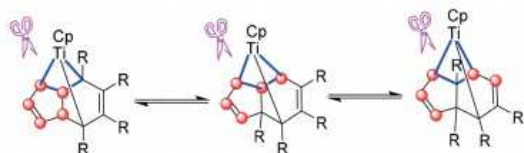
Abstract

Contacts

Molecular
Catalyst

Carbon-carbon bond formation/cleavage remains a tremendous challenge confronting contemporary synthetic organic chemistry. Our group has developed a class of transition metal-mediated reactions that allow for a novel forming/cleaving pattern of C-C bonds. Particularly in the past few years, several novel C-C bond formation and cleavage reactions on titanium have been demonstrated. In this context, as shown in Scheme 1, the five cyclic carbons in dihydroindene moiety were cleaved and transformed to five linearly aligned carbons, which were then further cleaved into one two-carbon and one three-carbon fragments.

In parallel, we also attempted a range of approaches for the synthesis of substituted acenes. Our most recent effort has been focusing on discovering a new route to the synthesis of 2D acenes from acenes (Scheme 2). Toward this end, Mn catalysts were used to promote the dimerization of acenes at the first ring following the introduction of a hydroxyl group. Finally, C-C bonds formed between the remaining carbons one at a time to give 2D acenes.



Scheme 1. Carbon-carbon bond formation and cleavage of Cp ligand on titanium



Scheme 2. Controllable synthesis of 2D acenes from acenes via carbon-carbon bond formations from one side to the other.

Prof.: Tamotsu TAKAHASHI

e-mail: tamotsu

Phone: 9149

Assoc. Prof.: Zhiyi SONG

e-mail: songzhiyi


Phone: 9153

Research Division	Abstract	Contacts
Macromolecular Science	<p>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.</p> <p>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).</p> <div style="display: flex; justify-content: space-around; align-items: center;"> <div data-bbox="448 845 985 1181"> </div> <div data-bbox="1030 798 1568 1181"> </div> </div> <div style="display: flex; justify-content: space-around; margin-top: 10px;"> <div data-bbox="448 1189 985 1244"> <p>Fig. 1. Structure of poly(dibenzofulvene), the first π-stacked vinyl polymer.</p> </div> <div data-bbox="1030 1189 1568 1244"> <p>Fig. 2. Chirality switching of helical polymer driven/triggered by circularly polarized light (CPL).</p> </div> </div>	<p>Prof.: Tamaki NAKANO e-mail: tamaki.nakano Phone: 9155</p> <p>Assist. Prof.: Yue WANG e-mail: yue.wang Phone: 9157</p>

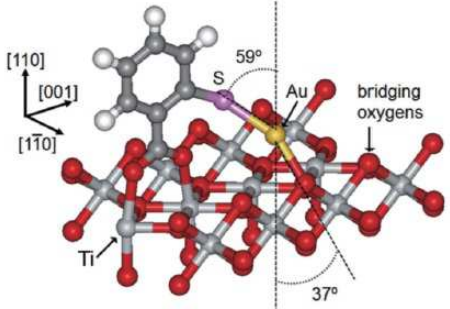
Research Division	Abstract	Contacts
<p>Research and Development</p>	<p>The Research and Development Division was started at the Institute for Catalysis (ICAT) Hokkaido University in 2014 guided by the Ministry of Education, Culture, Sports, Science and Technology (MEXT). At the end of 2014, Hokkaido 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 Artificial 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.</p> <div data-bbox="472 802 1556 1220" data-label="Diagram"> <p style="text-align: center;">Mission of the R&D Division <i>Reinforcing government-industry-academia collaboration</i></p> </div>	<p>Prof.: Mayumi NISHIDA e-mail: m-nishida Phone: 9381</p> <p>Assoc. Prof.: Tomohiro YASUDA e-mail: t-yasuda Phone: 9381</p>

Department of Target Research

Central Research Section

Research Cluster	Abstract	Contacts
Sustainable Catalyst	<p>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.</p>  <p>Fig. 1. Top page of the web site of the catalyst database</p>	Cluster Leader: Jun-ya HASEGAWA e-mail: hasegawa Phone: 9145

Extensive Research Section

Research Cluster	Abstract	Contacts
<p>Well-defined Surface Nanostructures</p>	<p>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.</p> <p>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.</p>  <p>Fig. 1. Atomically dispersed Au on $\text{TiO}_2(110)$ premodified with o-MBA (mercaptobenzoic acid) molecules.</p>	<p>Cluster Leader: Satoru TAKAKUSAGI e-mail takakusa phone: 9114</p>

Research Cluster	Abstract	Contacts
<p style="text-align: center;">Plasmonic Photocatalysis</p>	<p>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.</p> <p>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.</p> <div style="display: flex; justify-content: space-around; align-items: center;"> <div data-bbox="539 774 958 1072" data-label="Image"> <p>The image shows a central diagram of a TiO₂ photocatalyst with Au nanoparticles. Surrounding it are several micrographs: 'healthy bacteriocytes' (top left), '24 h vs 24 h irradiation' (middle left), 'destroyed bacteria' (bottom left), 'mycotoxins' (top right), and 'protoplast' (bottom right).</p> </div> <div data-bbox="1061 724 1368 1072" data-label="Diagram"> <p>The diagram illustrates the photocatalytic mechanism on a TiO₂ surface. It shows the conduction band (CB) and valence band (VB) with energy levels. Light excites electrons from the VB to the CB, creating electron-hole pairs. These pairs react with H₂O and CO₂ to produce reactive species like O₂⁻ and •OH, which then degrade pollutants like CH₃COOH. The surface is modified with Au and Ag nanoparticles.</p> </div> </div> <div style="display: flex; justify-content: space-around; margin-top: 10px;"> <div data-bbox="539 1082 958 1118" data-label="Caption"> <p>Fig. 1. Images of bacteria and fungi: healthy (top) and affected (bottom) by irradiated plasmonic photocatalysts.</p> </div> <div data-bbox="1003 1082 1422 1139" data-label="Caption"> <p>Fig. 2. Scheme of photodegradation of chemical and microbiological pollutants on titania (exposed with {101} facets) modified with NPs of gold and silver.</p> </div> </div>	<p>Cluster Leader: Ewa KOWALSKA e-mail: kowalska phone: 9130</p>

Research Cluster

Abstract

Contacts

Our research focuses on the understanding and theoretical modeling of interfaces (solid/air, solid/liquid, solid/solid interfaces) with the help of computer simulations based on electronic structure theory, reaction dynamics, and statistical mechanics.

In particular, we focus on the following topics.

- (a) Role of the acid-base and redox sites in catalytic reactions on the metal-oxide surface.
- (b) First-principles thermodynamics and molecular dynamics simulations in heterogeneous catalysis.
- (c) Catalyst design for direct conversion of methane and lower alkanes
- (d) Heterogeneous catalysis of carbon dioxide conversion to value-added chemical compounds.
- (e) Development of the enhanced sampling scheme based on the first-principle molecular dynamics simulations.

Cluster Leader:
Akira NAKAYAMA
e-mail: nakayama
phone: 9145

Computer Simulation of Interfaces

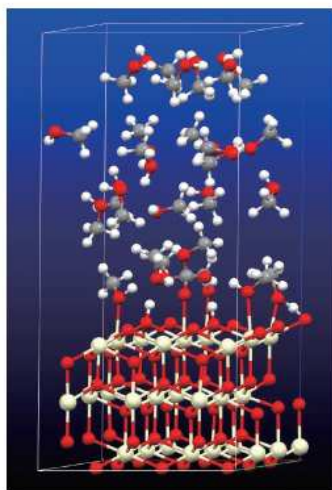


Fig. 1 First-principles simulations of catalytic reactions at the solid/liquid interface

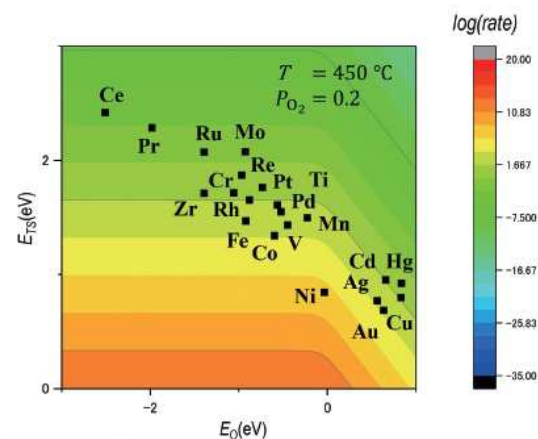
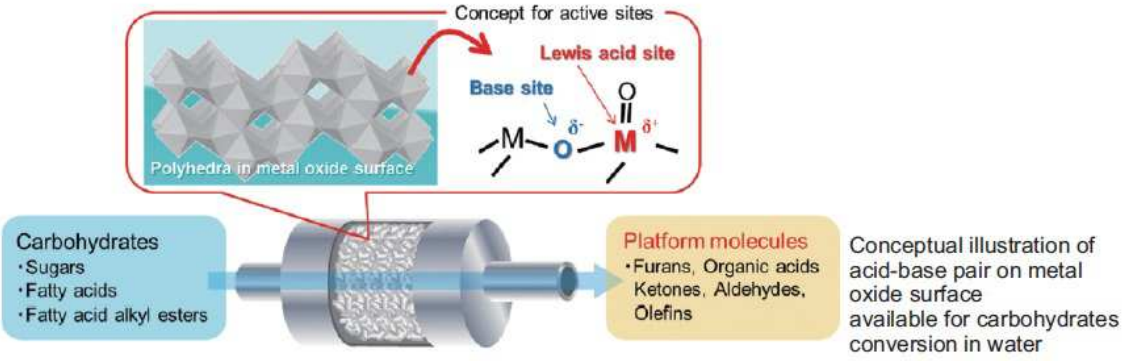
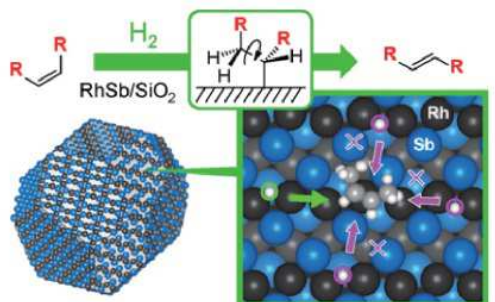
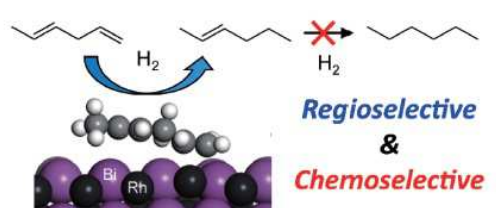
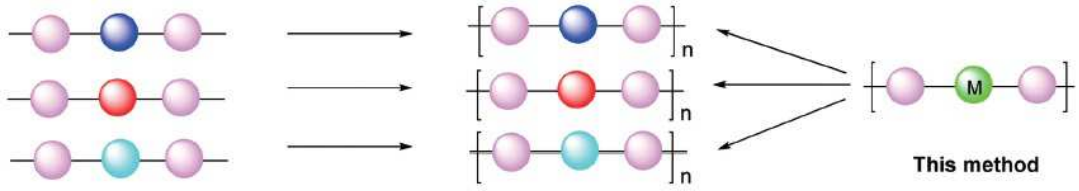


Fig. 2. Two-dimensional plot of catalytic activity for various dopant metal in metal-oxide.

Research Cluster	Abstract	Contacts
Acid-Base Catalysis	<p>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.</p> 	<p>Cluster Leader: Kiyotaka NAKAJIMA e-mail: nakajima phone: 9136</p>

Research Cluster	Abstract	Contacts
Functional Alloy Catalysts	<p>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:</p> <ol style="list-style-type: none"> (1) Achieving stereo and regioselective molecular transformations using specific atomic arrangements of ordered alloys. (2) Development of surface-modified intermetallics for efficient molecular conversion. (3) Synthesis and application of “intermetallic-soloid solution hybrid alloys” for well-controllable catalyst design. <div style="display: flex; justify-content: space-around; align-items: flex-start;"> <div style="text-align: center;">  <p>Fig. 1. Hydrogen-mediated stereoselective alkene isomerization using specific surface atomic arrangement of RhSb ordered alloys.</p> </div> <div style="text-align: center;">  <p>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.</p> </div> </div>	<p>Cluster Leader: Shinya FURUKAWA e-mail: furukawa phone: 9162</p>

Research Cluster	Abstract	Contacts
<p>Transition-metals-induced Synthesis and Transformation of Polymer</p>	<p>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.</p> <p>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.</p> 	<p>Cluster Leader: Zhiyi SONG e-mail: songzhiyi phone: 9153</p>