

# I<sup>2</sup>CNER

International Institute for Carbon-Neutral Energy Research

## 2012 Annual Report



KYUSHU UNIVERSITY

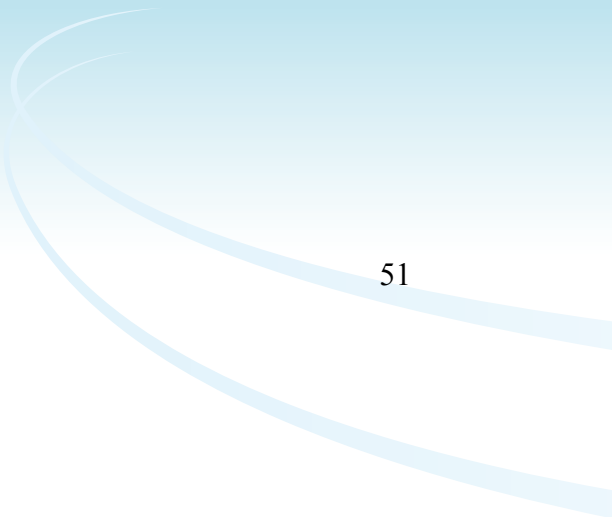
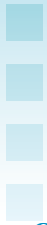




# Table of Contents

<b>World Premier International Research Center Initiative (WPI)</b>	4
▪ Background	
▪ Program Summary	
<hr/>	
<b>Message from the Director</b>	5
<hr/>	
<b>About ICNER</b>	6
▪ Mission	
▪ Science Organization	
<hr/>	
<b>Hydrogen Production</b>	8
▪ Executive Summary	
▪ Significant Publications	
▪ Relationship of significant publications to the targets and milestones of the Division's roadmap	
▪ Selected Publications	
<hr/>	
<b>Hydrogen Materials Compatibility</b>	14
▪ Executive Summary	
▪ Significant Publications	
▪ Relationship of significant publications to the targets and milestones of the Division's roadmap	
▪ Selected Publications	
<hr/>	
<b>Fuel Cells</b>	18
▪ Executive Summary	
▪ Significant Publications	
▪ Relationship of significant publications to the targets and milestones of the Division's roadmap	
▪ Selected Publications	
<hr/>	
<b>Thermal Science and Engineering</b>	22
▪ Executive Summary	
▪ Significant Publications	
▪ Relationship of significant publications to the targets and milestones of the Division's roadmap	
▪ Selected Publications	
<hr/>	
<b>Hydrogen Storage</b>	25
▪ Executive Summary	
▪ Significant Publications	
▪ Relationship of significant publications to the targets and milestones of the Division's roadmap	
▪ Selected Publications	

<b>Catalytic Materials Transformations</b>	28
<ul style="list-style-type: none"> <li>▪ Executive Summary</li> <li>▪ Significant Publications</li> <li>▪ Relationship of significant publications to the targets and milestones of the Division's roadmap</li> <li>▪ Selected Publications</li> </ul>	
<b>CO<sub>2</sub> Capture and Utilization</b>	31
<ul style="list-style-type: none"> <li>▪ Executive Summary</li> <li>▪ Significant Publications</li> <li>▪ Relationship of significant publications to the targets and milestones of the Division's roadmap</li> <li>▪ Selected Publications</li> </ul>	
<b>CO<sub>2</sub> Storage</b>	33
<ul style="list-style-type: none"> <li>▪ Executive Summary</li> <li>▪ Significant Publications</li> <li>▪ Relationship of significant publications to the targets and milestones of the Division's roadmap</li> <li>▪ Selected Publications</li> </ul>	
<b>Energy Analysis</b>	36
<ul style="list-style-type: none"> <li>▪ Executive Summary <ul style="list-style-type: none"> <li>- Technology Options for a Low Carbon and Carbon-neutral Energy Society in Japan</li> <li>- A Model Framework for Assessing Energy Technology Systems</li> <li>- Draft Roadmap</li> <li>- Future Directions</li> </ul> </li> <li>▪ Selected Publications</li> </ul>	
<b>Researchers &amp; Administrative Personnel</b>	40
<ul style="list-style-type: none"> <li>▪ I<sup>2</sup>CNER Organizational Structure</li> <li>▪ I<sup>2</sup>CNER Personnel</li> </ul>	
<b>I<sup>2</sup>CNER's Network of International Collaborations</b>	45
<b>International Engagement</b>	46
<ul style="list-style-type: none"> <li>▪ Visitors (I<sup>2</sup>CNER Principal Investigators from Overseas Collaborating Institutions)</li> <li>▪ Visitors (Researchers from Overseas Collaborating Institutions)</li> </ul>	
<b>Selected Awards</b>	49
<b>The New I<sup>2</sup>CNER Building</b>	50



**Outreach Activities**

51

- Symposia and Workshops
- Press Releases
- Publications
- I<sup>2</sup>CNER Seminar Series
- Institute Interest Seminar Series

---

**Finances**

64

---

**FY2013 Events Schedule**

65

---

**Access Map**

66

# World Premier International Research Center Initiative (WPI)



## Background

An intensifying global demand for talented researchers is accelerating the need among the world's nations to develop the best scientific minds. This trend has prompted Japan to establish new research centers that attract top-notch researchers from around the world so as to place itself within the "circle" of excellent human resources.

## Program Summary

The World Premier International Research Center Initiative (WPI) provides concentrated support to establish and operate research centers that have at their core a group of top-level investigators. The objective of these centers is to create a research environment of a sufficiently high standard to give them a very visible presence within the global scientific community—that is, to create a vibrant environment that will provide a strong incentive to frontline researchers around the world to want to work at these centers.

The WPI program has four basic objectives: advancing leading-edge research, creating interdisciplinary domains, establishing international research environments, and reforming research organizations. To achieve these objectives,

WPI research centers are required to tackle the following challenges:

### Critical Mass of Outstanding Researchers

- Bringing together top-level researchers within a host research institution
- Inviting top-notch researchers from around the world

### Attractive Research and Living Environment of Top International Standards

- Strong leadership by center director
- English as the primary language
- Rigorous system for evaluating research and system of merit-based compensation
- Strong support function
- Facilities and equipment appropriate to a top world-level research center
- Housing and support for daily living and education of dependent children

To assist the WPI research centers in carrying out this mandate, the Japanese government provides them with long-term, large-scale financial support.

## World Premier International Research Center Initiatives(as of April 1, 2013)

The World Premier International Research Center Initiative (WPI) is a project that was launched by the Ministry of Education, Culture, Sports, Science and Technology (MEXT) in 2007. The WPI seeks to form an ideal research environment within visible research centers that maintain high research standards, where leading researchers will be attracted from all over the world.

### Tohoku University

#### Advanced Institute for Materials Research (AIMR)

Integrating physics, chemistry, materials science, bioengineering, electronics and mechanical engineering, AIMR is striving to create innovative functional materials. A mathematical unit joined the team in 2011 to help establish a unified theory of materials science, aiming at the realization of a global materials research hub.



### Kyoto University

#### Institute for Integrated Cell-Material Sciences (iCeMS)

Established to integrate the cell and material sciences, the iCeMS combines the potential power of stem cells (e.g., ES/iPS cells) and of mesoscopic sciences to benefit medicine, pharmaceutical studies, the environment, and industry.



### Osaka University

#### Immunology Frontier Research Center (IFReC)

An innovative research center, which pursues the goal of comprehensive understanding of immune reactions through the fusion of immunology, various imaging technologies, and Bioinformatics.



### Kyushu University

#### International Institute for Carbon-Neutral Energy Research (I<sup>2</sup>CNER)

Toward the realization of a low-carbon society, I<sup>2</sup>CNER aims to resolve the challenges of the use of hydrogen energy and CO<sub>2</sub> capture and sequestration by fusing together sciences from an atomic level to a global scale.



### Nagoya University

#### Institute of Transformative Bio-Molecules (ITbM)

The goal of ITbM is to develop innovative functional molecules that make a marked change in the form and nature of biological science and technology (transformative bio-molecules). ITbM will connect molecules, create value, and change the world, one molecule at a time.



### National Institute for Materials Science International Center for Materials Nanoarchitectonics (MANA)

A major focus of our activities is the development of innovative materials on the basis of a new paradigm "nanoarchitectonics," ground-breaking innovation in nanotechnology.



### University of Tsukuba

#### International Institute for Integrative Sleep Medicine (IIIS)

IIIS seeks to elucidate the fundamental mechanism of sleep/wakefulness, to develop strategies to regulate sleep, and to contribute to the enhancement of world health by combatting sleep disorders and associated diseases.



### Tokyo Institute of Technology

#### EARTH-LIFE SCIENCE INSTITUTE (ELSI)

ELSI focuses the origins of Earth and life. Both studies are inseparable because life should have originated in unique environment on the early Earth. To accomplish our challenge, we establish a world-leading interdisciplinary research hub by gathering excellent researchers in Earth and planetary sciences, life science, and related fields.



### Kavli Institute for the Physics and Mathematics of the Universe (Kavli IPMU)

Today's Institutes for Advanced Study, The University of Tokyo

With accumulated research on mathematics, physics and astronomy, this research core works to bring light to the mysteries of the universe, such as its origin, and to provide an analysis of evolution.



Refer to: MEXT Website [http://www.mext.go.jp/english/research\\_promotion/1303822.htm](http://www.mext.go.jp/english/research_promotion/1303822.htm)  
JSPS Website <http://www.jsps.go.jp/english/e-toplevel/index.html>

## Message from the Director

I would call the International Institute for Carbon-Neutral Energy Research's (I<sup>2</sup>CNER's) third year the "transition year" because we initiated the process of transitioning to a steady state. Our primary achievement this year was the re-structuring and re-focusing of each research division, along with the creation of preliminary roadmaps which include research targets and milestones over short-, mid-, and long-term scenarios, both for the Divisions and for the Institute as whole, in collaboration with the Energy Analysis Research Division. The opening of the I<sup>2</sup>CNER building in January 2013 on Kyushu University's Ito Campus has allowed us to bring all of our researchers under one roof, which will promote synergy, collaboration, and ultimately, fusion research. A new initiative was introduced whereby programs which are advancing fusion research will be reinforced financially within the Institute. The personnel of the Institute have been greatly enriched over the last year with the addition of 13 new postdocs and 34 new graduate students, among others.



Some of the research highlights include: a significant discovery on energy efficiency for organic light-emitting diodes, which was published in *Nature* by the Adachi Group, and a potentially revolutionary approach to the understanding of functional [NiFe]hydrogenase in catalysis, which was published in *Science* by the Ogo group. Selected highlights of innovative ideas developed in the Institute include: how to load metal nanoparticles onto CNTs for use as electrocatalysts for fuel cells; the unveiling of the anisotropic heat conduction nature in the in- and out-of-shell thermal conductivities of multi-walled CNTs; new insights into the nature of cyclic deformation-induced microstructure evolution during hydrogen-accelerated fatigue crack growth; how severely strained TiFe readily absorbs and desorbs hydrogen without activation; the influence of electrolyte composition on the electrochemical reduction of CO<sub>2</sub> to CO; and the detection and monitoring of CO<sub>2</sub> leakage in sub-seabed storage using seafloor-based acoustic tomography and mapping the distribution of the leakage points using novel pH/pCO<sub>2</sub> sensors.

In summary, I<sup>2</sup>CNER, through its cutting-edge collaborative research, transformative research environment, engagement of premier international agencies, outreach programs, and the successful partnership between Kyushu University and the University of Illinois at Urbana-Champaign is transitioning not only to a steady state, but also to a symbolic presence of cooperation between Japan and the US on carbon-neutral energy.

A handwritten signature in black ink, appearing to read 'P. Sofronis'. The signature is stylized and written in a cursive-like font.

Professor Petros Sofronis, Ph.D.  
Director  
International Institute for Carbon-Neutral Energy Research (I<sup>2</sup>CNER)

# About I<sup>2</sup>CNER

## Mission

At I<sup>2</sup>CNER, our mission is to contribute to the creation of a sustainable and environmentally-friendly society by conducting fundamental research for the advancement of low carbon emission and cost effective energy systems, and improvement of energy efficiency. Amongst the array of technologies that I<sup>2</sup>CNER's research aims to enable is the innovative, safe, and reliable production, storage, and utilization of hydrogen as a fuel in a hydrogen-based economy. Our research also explores the underlying science of CO<sub>2</sub> capture and storage technology or the conversion of CO<sub>2</sub> to a useful product. Additionally, it is our mission to establish an international academic environment that fosters innovation through collaboration and interdisciplinary research (fusion).

## Science Organization

The Institute is organized into thematic research areas (Research Divisions) which address specific research objectives. Each division is led by a senior WPI Principal Investigator (Lead PI) of the Institute. Typically, there are several research groups within each division which focus on individual aspects of the primary division objectives.

The research divisions are:

- Hydrogen Production
- Hydrogen Materials Compatibility
- Fuel Cells
- Thermal Science and Engineering
- Hydrogen Storage
- Catalytic Materials Transformations
- CO<sub>2</sub> Capture and Utilization
- CO<sub>2</sub> Storage
- Energy Analysis\*

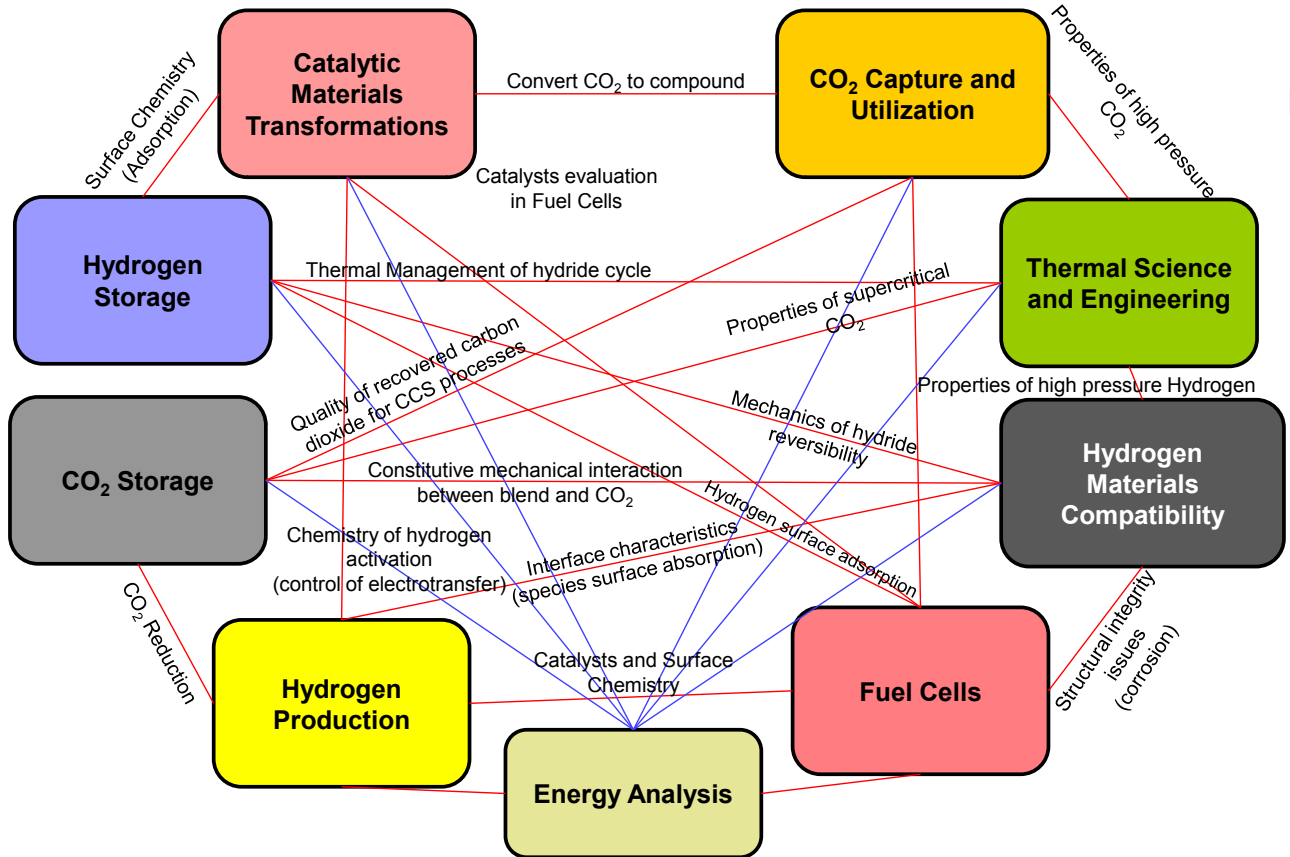
A schematic diagram of the interaction and interdisciplinary fusion among the technical divisions is shown in the figure on page 7.

Not only are I<sup>2</sup>CNER's researchers tasked with crossing the boundaries of various scientific disciplines, but they also must work hard to bridge the Pacific Ocean. The I<sup>2</sup>CNER project is highly unique, in that it has its main facility at Kyushu University (KU) in Japan and a Satellite facility at the University of Illinois at Urbana-Champaign (UIUC) in the United States. The research projects at UIUC are complementary to and integrated with those at KU. In addition, the Satellite Institute is a hub for identifying and engaging state of the art research programs and faculty at universities and other research institutions in the U.S. and internationally with which I<sup>2</sup>CNER can collaborate. These collaborations with first class international research centers, universities, and national laboratories help I<sup>2</sup>CNER to ensure that its mission has maximum impact in Japan and throughout the world. In order to sustain its fruitful international relationships, the I<sup>2</sup>CNER Administration encourages the Institute's researchers to engage in exchange visits with all its international partners, especially the Satellite Institute. The symbiotic relationship between KU and UIUC is exemplary of I<sup>2</sup>CNER's vision for the international collaborations necessary to achieve breakthroughs in fundamental science.

\* The goals of the Energy Analysis Research Division (EAD) are to ensure that I<sup>2</sup>CNER research is relevant to the future carbon-neutral energy infrastructure for Japan, to ensure that I<sup>2</sup>CNER research is informed of all relevant current and future energy options, and to help enable an I<sup>2</sup>CNER Vision and Roadmap for a low carbon energy infrastructure for Japan. All analyses of energy solution pathways include cost, energy use, greenhouse gas (GHG) emissions, and issues of national security. Analyses are done on a Well to Wheel (WTW)/Cradle to Grave (CTG) basis where all activities, costs, and energy flows are tracked throughout the energy pathway from the source of the primary energy (e.g. a natural gas well) through the final use of that energy (e.g. as electricity from a gas turbine for use in the residential market or hydrogen gas used in a fuel cell vehicle).



## Research Teams—Fusion of Disciplines





# HYDROGEN PRODUCTION

## EXECUTIVE SUMMARY

The efforts of the Hydrogen Production Research Division focus on the science and engineering of technologies to produce and conserve energy, and to use that energy to reduce hydrogen to a storable fuel. The Division is developing photoelectrochemical cells for direct conversion of sunlight to hydrogen and photovoltaics combined with steam electrolysis as a two-step hydrogen reduction process. As a complement to photovoltaics, organic light emitting devices are being developed both for high efficiency lighting to contribute to energy conservation and because the underlying science is very valuable to organic photovoltaics, an energy production method which is being studied. Research also includes use of microstructural characterization techniques for analysis of the interface structure of organic dye and inorganic semiconductors in photocatalysts.

The research in the division falls under the themes of energy production, conservation, and storage. The theme of energy production is based on conversion of solar to electric energy. The conservation theme is represented through enhanced lighting efficiency based on high efficiency solid state lighting. Finally, the theme of fuel production is represented through hydrogen reduction and advanced batteries. The work includes experimental materials synthesis, device fabrication and testing, and theory-based materials development. Projects encompass novel inorganic and organic photocatalysts and electrodes, synthesis of novel molecules for organic light emitters and photoelectrochemical and photovoltaic cells, and materials for high temperature electrochemical and electrolytic water reduction and electric energy storage.

## Significant Publications

### *Highly efficient organic light-emitting diodes from delayed fluorescence*

H. Uoyama, K. Goushi, K. Shizu, H. Nomura and C. Adachi  
Nature, 492(7428), 234-238, 2012

We have found a novel path to high organic light emitting diode (OLED) efficiency. We designed a class of organic molecules in which the energy difference between the singlet and triplet states is less than 100meV (compared to the more typical 0.5–1.0eV). Thermal energy can thus promote triplet-state molecules into the singlet state, resulting in thermally activated delayed fluorescence. We named this new efficient exciton harvesting mechanism as “Hyperfluorescence.” The thermally activated delayed fluorescence (TADF) OLEDs can be made to emit in a wide range of colors with nearly 100% internal electroluminescence (EL) efficiency using simple aromatic compounds. This is a significant breakthrough in light emitting devices, contributing for low cost and energy conservation devices. In the hydrogen production division, we focus on various high efficiency energy conversion devices including transformation of electricity into light, e.g. OLEDs. Improvement of the efficiency in light emitting devices is an important target for the division.

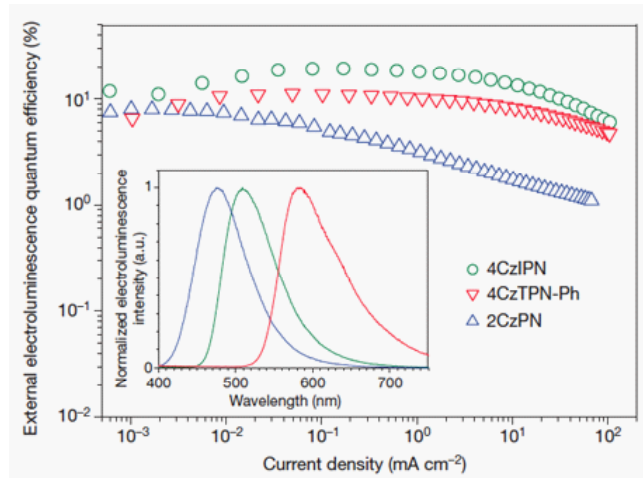


Fig. 1

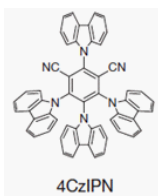


Fig. 2

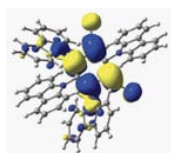


Fig. 3

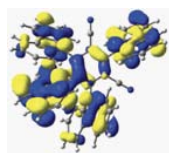


Fig. 4

Fig. 1 shows the external electroluminescence efficiency of OLEDs obtained with three different related carbazoyl dicyanobenzene molecules. Fig. 2 shows the structure of one of the new molecules created. Fig. 3 shows the lowest unoccupied molecular orbital. Fig. 4 shows the highest occupied molecular orbital of the molecule shown in Fig. 2.

### *Photoinduced Hydrogen Evolution from Water by a Simple Platinum(II) Terpyridine Derivative: A Z-Scheme Photosynthesis*

M. Kobayashi, S. Masaoka and K. Sakai

Angewandte Chemie-International Edition, 51(30), 7431-7434, 2012

This work is the first successful finding that a simple molecular system consisting of a platinum (II) coordination compound can demonstrate an artificial ‘Z-scheme’ photosynthesis to generate molecular hydrogen from water upon visible light irradiation. This is the first example which mimics the so-called ‘Z-scheme photosynthesis’ achieved in the natural photosynthesis of green plant. This provides a new strategy to develop solar light-induced water splitting systems which have the capability to generate hydrogen without forming CO<sub>2</sub>. Such water splitting systems are one of ICNER’s research targets.

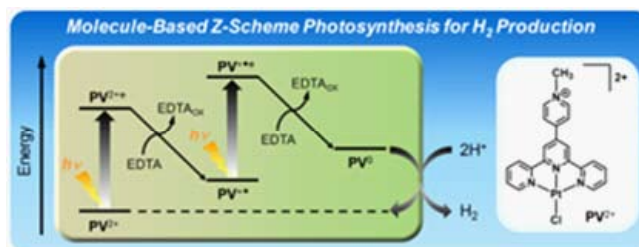


Fig. 5. Molecule-Based Z-Scheme Photosynthesis for H<sub>2</sub> Production

### *Electronic and oxide ion conductivity in $\text{Pr}_2\text{Ni}_{0.71}\text{Cu}_{0.24}\text{Ga}_{0.05}\text{O}_4/\text{Ce}_{0.8}\text{Sm}_{0.2}\text{O}_2$ (PNCG/SDC) laminated film*

J. Hyodo, S. Ida, J. A. Kilner and T. Ishihara  
Solid State Ionics, 230, 16-20, 2013

Dense and uniform PNCG-SDC film was successfully deposited on MgO substrate by laser ablation method. The electrical conductivity measurements were performed as a function of layer thickness of PNCG or SDC. The conductivity increased with decreasing SDC layer thickness. Since improved oxide ion conductivity can decrease the electricity for production of hydrogen in steam electrolysis, it is highly interesting that PNCG/SDC laminated film with nano size thickness shows the improved oxide ion conductivity and we expect that we can improve the efficiency of steam electrolysis at intermediate temperature. An electrolyzer with improved efficiency is an effective means of transforming solar energy into hydrogen, which is one of FCNER's research targets.

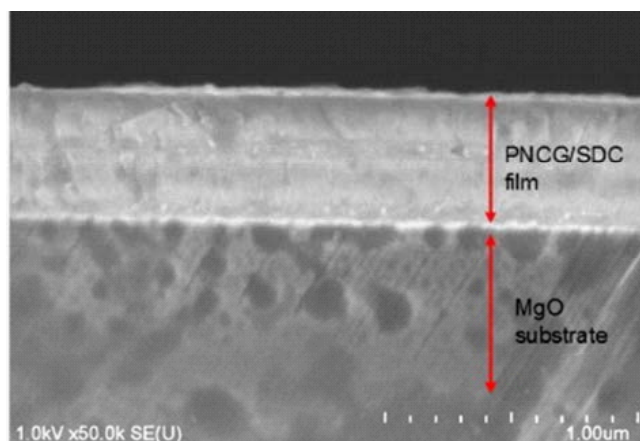


Fig. 6. SEM image of the PNCG/SDC laminated film with 100nm thickness for each layer. Since the film thickness of PNCG was kept at 100nm, increase in electrical conductivity could be assigned to the improved conductivity in SDC layer.

## Relationship of significant publications to the targets and milestones of the Division's roadmap

In the Hydrogen Production Research Division, our main objective is to convert solar energy to hydrogen. At present, two main approaches are explored; one is photocatalytic water splitting and the other is steam electrolysis combined with solar light. The objectives of this division have been expanded to include organic light emitting diodes (OLEDs) and batteries for energy conservation. The three above-listed papers are related to OLEDs, photocatalysts and new batteries. The first paper, reported by the Adachi group,

focuses on OLEDs, including a report on a new molecule for increasing the efficiency of OLEDs, which is useful from an energy conservation perspective. The second paper, reported by the Sakai group, outlines their attempt to achieve water splitting with a single molecule catalyst. The paper reported by the Ishihara group is related to novel oxygen diffusion materials, which are obtained by laminating two nano-sized materials. This material could be used as an electrolyte in the new concept of Fe-air batteries.

## Selected Publications

Arita, H., Mitamura, K., Kobayashi, M., Yamada, N. L., Jinnai, H. and Takahara, A. (2013), Chain-mixing behavior at interface between polystyrene brushes and polystyrene matrices, *Polymer Journal*, 45 (1), 117-123

Haraguchi, M., Hirai, T., Ozawa, M., Miyaji, K. and Tanaka, K. (2013), Hydrophobic acrylic hard coating by surface segregation of hyper-branched polymers, *Applied Surface Science*, 266, 235-238

Higaki, Y., Okazaki, R. and Takahara, A. (2012), Semirigid Biobased Polymer Brush: Poly( $\alpha$ -methylene- $\gamma$ -butyrolactone) Brushes, *ACS Macro Letters*, 1(9), 1124-1127

Hirai, T., Kawasaki, K. and Tanaka, K. (2012), Interfacial kinetics of a model epoxy-amine addition reaction, *Physical Chemistry Chemical Physics*, 14 (39), 13532-13534

Hori, K., Penaloza, D. P., Shundo, A. and Tanaka, K. (2012), Time-dependent heterogeneity in viscoelastic properties of worm-like micelle solutions, *Soft Matter*, 8 (28), 7361-7364

Horinouchi, A., Atarashi, H., Fujii, Y. and Tanaka, K. (2012), Dynamics of water-induced surface reorganization in poly(methyl methacrylate) films, *Macromolecules*, 45 (11), 4638-4642

- Hoshino, T., Murakami, D., Ito, K., Tanaka, Y., Sasaki, S., Takata, M., Jinnai, H. and Takahara, A. (2013), Thermal gradient effect on the dynamical behavior of nanoparticles observed using X-ray photon correlation spectroscopy, *Polymer Journal*, 45 (1), 94-99
- Hyodo, J., Ida, S., Kilner J. A. and Ishihara T. (2013), Electronic and oxide ion conductivity in  $\text{Pr}_2\text{Ni}_{0.71}\text{Cu}_{0.24}\text{Ga}_{0.05}\text{O}_4/\text{Ce}_{0.85}\text{Sm}_{0.2}\text{O}_2$  laminated film, *Solid State Ionics*, 230, 16-20
- Ida, S., Okamoto, Y., Matsuka, M., Hagiwara, H. and Ishihara, T. (2012), Preparation of Tantalum-Based Oxynitride Nanosheets by Exfoliation of a Layered Oxynitride,  $\text{CsCa}_2\text{Ta}_3\text{O}_{10-x}\text{N}_y$ , and Their Photocatalytic Activity, *Journal of the American Chemical Society*, 134 (38), 15773-15782
- Inoishi, A., Ida, S., Uratani, S., Okano, T. and Ishihara, T. (2013), Ni-Fe-Ce(Mn, Fe) $\text{O}_2$  cermet anode for rechargeable Fe-Air battery using  $\text{LaGaO}_3$  oxide ion conductor as electrolyte, *RSC Advances*, 3 (9), 3024-3030
- Inoishi, A., Ju, W. Y., Ida, S. and Ishihara, T. (2013), Fe-air rechargeable battery using oxide ion conducting electrolyte of  $\text{Y}_2\text{O}_3$  stabilized  $\text{ZrO}_2$ , *Journal of Power Sources*, 229, 12-15
- Ishihara, T., Matsushita, S., Sakai, T. and Matsumoto, H. (2012), Intermediate temperature solid oxide electrolysis cell using  $\text{LaGaO}_3$ -base oxide, *Solid State Ionics*, 225, 77-80
- Ishihara, T., Tominaga, K., Hyodo, J. and Matsuka, M. (2012), Improved electrical conductivity in  $\text{Pr}_2\text{Ni}(\text{Cu},\text{Ga})\text{O}_4$  film with nano thickness, *International Journal of Hydrogen Energy*, 37 (9), 8066-8072
- Jinnai, H., Tsuchiya, T., Motoki, S., Kaneko, T., Higuchi, T. and Takahara, A. (2012), Transmission electron microtomography in soft materials, *Journal of Electron Microscopy*, *Journal of Electron Microscopy*, 62 (2), 243-258
- Ju, Y. W., Ida, S. and Ishihara, T. (2012), Nickel-iron anode substrate for smart solid oxide fuel cells with a self-protecting function against reoxidation, *Fuel Cells*, 12 (6), 1064-1069
- Kim, S. J., Sakai, T., Oda, H., Hamagami, J., Okuyama, Y., Matsuka, M., Ohta, S., Shimizu, Y., Ishihara T. and Matsumoto, H. (2012), Water Electrolysis Using Water-Absorbing Porous Electrolyte Consisting of a Sulfonated Nanotitania Proton Conductor, *Electrochemistry*, 80 (4), 246-248
- Kim, S. J., Sakai, T., Oda, H., Okuyama, Y., Mizutani, Y., Hamagami, J., Matsuka, M., Ishihara, T. and Matsumoto, H. (2012), Long-term stability of sulfated hydrous titania-based electrolyte for water electrolysis, *Journal of Solid State Electrochemistry*, 16 (11), 3587-3592
- Kobayashi, M., Masaoka, S. and Sakai, K. (2012), Photoinduced Hydrogen Evolution from Water by a Simple Platinum (II) Terpyridine Derivative: A Z-Scheme Photosynthesis, *Angewandte Chemie-International Edition*, 51 (30) 7431-7434
- Kobayashi, M., Masaoka, S. and Sakai, K. (2012), Synthesis, crystal structure, spectroscopic and electrochemical properties, and H<sub>2</sub>-evolving activity of a new  $[\text{PtCl}(\text{terpyridine})](+)$  derivative with viologen-like redox properties, *Dalton Transactions*, 41 (16), 4903-4911
- Kobayashi, M., Matsugi, T., Saito, J., Imuta, J.-I., Kashiwa, N. and Takahara, A. (2013), Direct modification of polyolefin films by surface-initiated polymerization of a phosphobetaine monomer, *Polymer Chemistry*, 4(3), 731-739
- Li, X., Staykov, A. and Yoshizawa, K. (2012), Orbital Views on Electron-Transport Properties of Cyclophanes: Insight into Intermolecular Transport, *Bulletin of the Chemical Society of Japan*, 85 (2), 181-188
- Ma, W., Higaki, Y., Otsuka, H. and Takahara, A. (2013), Perfluoropolyether-infused nano-texture: a versatile approach to omniphobic coatings with low hysteresis and high transparency, *Chemical Communications*, 49 (6), 597-599
- Ma, W., Wu, H., Higaki, Y., Otsuka, H. and Takahara, A. (2012), A "non-sticky" superhydrophobic surface prepared by self-assembly of fluoroalkyl phosphonic acid on a hierarchically micro/nanostructured alumina gel film, *Chemical Communications*, 48 (54), 6824-6826

- Ma, W., Yah, W. O., Otsuka, H. and Takahara, A. (2012), Application of imogolite clay nanotubes in organic-inorganic nanohybrid materials, *Journal of Materials Chemistry*, 22 (24), 11887-11892
- Matsubayashi, A., Fukunaga, K. and Tanaka, K. (2012), Metal ions/ion clusters transport in glassy polymer films: construction of multi-layered polymer and metal composite films, *Journal of Materials Chemistry*, 22 (31), 15578-15585
- Matsumoto, H., Sakai, T. and Okuyama, Y. (2013), Proton-conducting oxide and applications to hydrogen energy devices, *Pure and Applied Chemistry*, 85 (2), 427-435
- Mitamura, K., Yamada, N. L., Sagehashi, H., Torikai, N., Arita, H., Terada, M., Kobayashi, M., Sato, S., Seto, H., Goko, S., Furusaka, M., Oda, T., Hino, M., Jinnai, H. and Takahara, A. (2013), Novel neutron reflectometer SOFIA at J-PARC/MLF for in-situ soft-interface characterization, *Polymer Journal*, 45 (1), 100-108
- Nishida, J., Kobayashi, M. and Takahara, A. (2013), Gelation and Adhesion Behavior of Mussel Adhesive Protein Mimetic Polymer, *Journal of Polymer Science, Part A: Polymer Chemistry*, 51 (5), 1058-1065
- Okamura, M., Yoshida, M., Kuga, R., Sakai, K., Kondo, M. and Masaoka, S. (2012), A Mononuclear Ruthenium Complex Showing Multiple Proton-Coupled Electron Transfer toward Multi-electron Transfer Reactions, *Dalton Transactions*, 41 (42), 13081-13089
- Penalzoza, D. P., Hori, K., Shundo, A. and Takai, K. (2012), Spatial heterogeneity in a lyotropic liquid crystal with hexagonal phase, *Physical Chemistry Chemical Physics*, 14 (15), 5247-5250
- Sakai, T., Matsushita, S., Hyodo, J., Okumura, Y., Matsuka, M., Ishihara, T. and Matsumoto, H. (2012), Effect of doped ceria interlayer on cathode performance of the electrochemical cell using proton conducting oxide, *Electrochimica Acta*, 75, 179-184
- Schacher, F. H., Sugimori, H., Hong, S., Jinnai, H. and Müller, A. H. E. (2012), Tetragonally Perforated Lamellae of Polybutadiene-block-poly(2-vinylpyridine)-block-poly(tert-butyl methacrylate)(BVT) Triblock Terpolymers in the Bulk: Preparation, Cross-Linking, and Dissolution, *Macromolecules*, 45 (19), 7956-7963
- Shin, T. H., Okamoto, Y., Ida, S. and Ishihara, T. (2012), Self-recovery of Pd Nanoparticles That were Dispersed over La(Sr) Fe(Mn)O<sub>3</sub> for Intelligent Oxide Anodes of Solid-Oxide Fuel Cells, *Chemistry - A European Journal*, 18 (37), 11695-11702
- Shinohara, T., Shirahase, T., Murakami, D., Hoshino, T., Kikuchi, M., Joike, J.-I., Horigome, M., Masunaga, H., Ogawa, H. and Takahara, A. (2012), Precise and Non-destructive Characterization of 'Buried' Nano-structure in Polymer Thin Film by Synchrotron Radiation Ultra-Small Angle X-ray Scattering, *Polymer Journal*, 45 (3), 307-312
- Staykov, A., Li, X., Tsuji, Y. and Yoshizawa K. (2012), Current Rectification in Nitrogen- and Boron-Doped Nanographenes and Cyclophanes, *Journal of Physical Chemistry C*, 116(34), 18451-18459
- Staykov, A., Nishimi, T., Yoshizawa, K. and Ishihara, T. (2012), Oxygen Activation on Nanometer-Size Gold Nanoparticles, *Journal of Physical Chemistry C*, 116 (30), 15992-16000
- Tsuji, Y., Staykov, A. and Yoshizawa, K. (2012), Orbital Determining Spintronic Properties of a  $\pi$ -Conjugated System, *Journal of Physical Chemistry C*, 116 (30), 16325-16332
- Tsuruta, H., Fujii, Y., Kai, N., Kataoka, H., Ishizoe, T., Doi, M., Morita, H. and Tanaka, K. (2012), Local conformation and relaxation of polystyrene at substrate interface, *Macromolecules*, 45 (11) 4643-4649
- Tsuruta, H., Ikinaga, Y., Fujii, Y. and Tanaka, K. (2013), A simple approach for surface hardening of polystyrene, *Applied Surface Science*, 264, 589-592
- Uoyama, H., Goushi, K., Shizu, K., Nomura H. and Adachi, C. (2012), Highly efficient organic light-emitting diodes from delayed fluorescence, *Nature*, 492 (7428), 234-238

- Wu, H., Su, Z. and Takahara, A. (2012), Isotactic polystyrene nanorods with gradient crystallite states, *Soft Matter*, 8 (11), 3180-3184
- Xie, J., Ju, Y. W., Matsuka, M., Ida, S. and Ishihara, T. (2013), Synergy effects of  $\text{Pr}_{1.91}\text{Ni}_{0.71}\text{Cu}_{0.24}\text{Ga}_{0.05}\text{O}_4$  and  $\text{Ba}_{0.5}\text{La}_{0.5}\text{CoO}_3$  composite on cathodic activity for intermediate temperature solid oxide fuel cells, *Journal of Power Sources*, 228, 229-236
- Xu, H., Nishida, J., Wu, H., Higaki, Y., Otsuka, H., Ohta, N. and Takahara, A. (2013), Structural effects of catechol-containing polystyrene gels based on a dual cross-linking approach, *Soft Matter*, 9 (6), 1967-1974
- Yah, W. O., Xu, H., Soejima, H., Ma, W., Lvov, Y. And Takahara, A. (2012), Biomimetic Dopamine Derivative for Selective Polymer Modification of Halloysite Nanotube Lumen, *Journal of the American Chemical Society*, 134 (29), 12134-12137
- Yamaguchi, H., Kikuchi, M., Kobayashi, M., Ogawa, H., Masunaga, H., Sakata, O. and Takahara, A. (2012), Influence of Molecular Weight Dispersity of Poly{2-(perfluorooctyl)ethyl acrylate} Brushes on Their Molecular Aggregation States and Wetting Behavior, *Macromolecules*, 45 (3), 1509-1516
- Yashima, M., Yamada, H., Nuansaeng, S. and Ishihara, T. (2012), Role of  $\text{Ga}^{3+}$  and  $\text{Cu}^{2+}$  in the High Interstitial Oxide-Ion Diffusivity of  $\text{Pr}_2\text{NiO}_4$ -Based Oxides: Design Concept of Interstitial Ion Conductors through the Higher-Valence  $d^{10}$  Dopant and Jahn-Teller Effect, *Chemistry of Materials*, 24 (21), 4100-4113
- Zhang, C., Fujii, Y. and Tanaka, K. (2012), Effect of Long Range Interactions on the Glass Transition Temperature of Thin Polystyrene Films, *ASC Macro Letters*, 1(11), 1317-1320



# HYDROGEN MATERIALS COMPATIBILITY

## EXECUTIVE SUMMARY

Deployment of hydrogen fuel-based technologies requires that high-pressure hydrogen storage and distribution systems are safe, reliable, structurally efficient, and cost-effective. One safety and reliability consideration for hydrogen containment systems is the effect of hydrogen on material degradation (e.g., hydrogen embrittlement). Hydrogen-material interactions can accelerate fatigue crack propagation, reduce fracture toughness, and enhance wear of structural components, which can lead to unexpected and catastrophic failures unless the related material degradation phenomena are understood and accommodated.

The objective of the research in this division is to establish the fundamental knowledge that enables the development of new tools and technology: reliable and efficient test methods for measuring the effects of hydrogen on the fatigue, fracture, and wear properties of materials; models of hydrogen-assisted fatigue, fracture, and wear that include the detailed physics of hydrogen uptake, hydrogen-defect interactions, and material degradation; and next-generation materials having lower cost and improved performance (e.g., higher strength) without compromising resistance to hydrogen-induced degradation. This fundamental knowledge is attained by conducting complex mechanical property measurements on materials in challenging environments that include both high-pressure hydrogen and low temperature. In addition, physical models of hydrogen-induced material degradation derived from the mechanistic studies serve as the foundation for developing predictive model frameworks. The research activities in this division will ultimately lead to hydrogen containment systems that are optimized in terms of cost, performance, and safety.



## Significant Publications

### *A microstructural based understanding of hydrogen-enhanced fatigue of stainless steels*

M. L. Martin, P. Sofronis, I. M. Robertson, T. Awane and Y. Murakami  
International Journal of Fatigue, DOI:10.1016/j.ijfatigue.2012.08.009, 2012

We have developed the capability to extract using the focused-ion beam (FIB) lift-out technique, transmission electron microscopy (TEM) samples from site-specific locations on fracture surfaces with irregular topography. This new technique has led to a significant advance in our understanding of microstructure evolution under fatigue loading in both 304 and 316 stainless steel in the presence and absence of hydrogen as it makes it possible for the first time to observe the microstructure immediately beneath the fracture surface. Most notably, we have discovered that the microstructure developed beneath striations consists of a layered structure with the complexity decreasing with distance from the fracture surface. The uniqueness of these results is that they demonstrate that the microstructure beneath striations has evolved to an unanticipated state and the presence of hydrogen induces refinement, but of a different nature. These results emphasize the need to understand the degree of microstructure development during fatigue loading but prior to crack propagation, as this microstructure determines and dictates crack propagation and growth.

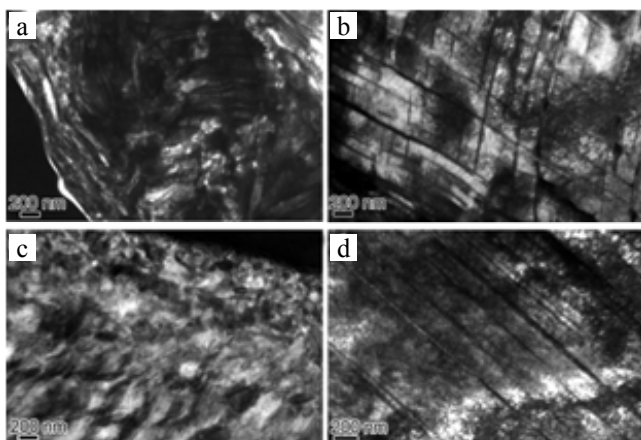


Fig. 1. Microstructures immediately beneath the fatigue fracture surfaces of 316 stainless steel fractured in both the absence (a-b) and the presence (c-d) of hydrogen. a) Microstructure immediately beneath the fracture surface (left side) produced in air consisting of a banded structure indicative of high levels of strain. b) Microstructure 5 $\mu$ m from the fracture surface produced in air consisting of an array of planar structures (twins). c) Microstructure immediately beneath the fracture (top side) produced after hydrogen charging consisting of fine grains. d) Microstructure 5 $\mu$ m from the fracture surface produced after hydrogen charging consisting of planar structures (twins).

### *Surface-layer microstructure control for metastable austenitic stainless steel plate to improve hydrogen embrittlement resistance*

K. Tsuboi, A. Macadre, T. Tsuchiyama and S. Takaki  
CAMP-ISIJ, 25, 1185, 2012

A central goal is to develop lower-cost and higher-strength steels with excellent hydrogen embrittlement resistance. Through solution nitriding of metastable type 304 austenitic stainless steel, we managed to fully stabilize an austenite surface layer that hinders hydrogen ingress. Underneath this layer an almost 80% of austenite transformed to martensite at each position below the surface in non-nitrided material. The effectiveness of such an austenite surface layer (10 $\mu$ m thick) against hydrogen embrittlement was measured. The material's response in uniaxial tension in the presence of hydrogen is almost identical to that in the absence of hydrogen. A patent has already been obtained on this technology.

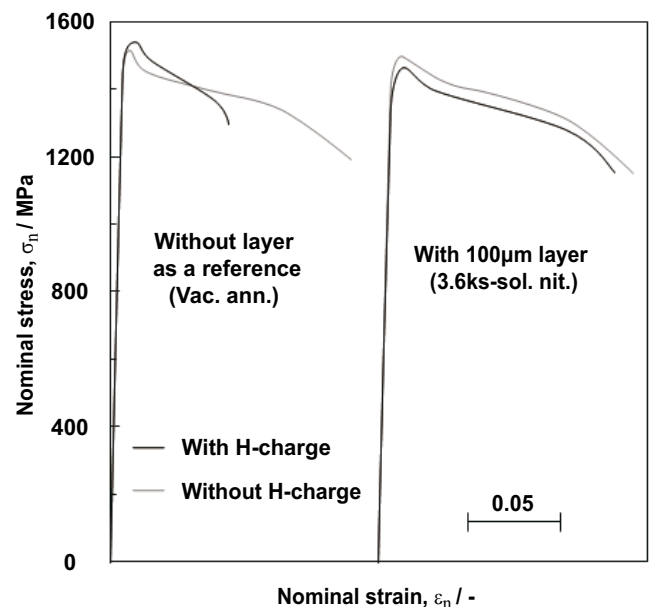


Fig. 2. Comparison of nominal stress-strain curves for hydrogen-charged and non-charged solution-nitrided (3.6ks) and 60% cold-rolled SUS304 steel sheets (100 $\mu$ m austenite phase layer).

### *Hydrogen-Induced Intergranular Failure in Nickel Revisited*

M. L. Martin, B. P. Somerday, R. O. Ritchie, P. Sofronis and I. M. Robertson  
Acta Materialia, 60(6-7), 2739-2745, 2012

The basic mechanisms of hydrogen-induced intergranular fracture in nickel have been identified. Evidence of copious plasticity was confirmed underneath the fracture surface; immediately beneath it, an extensive dislocation defect substructure exists. These findings raise interesting questions about the role of plasticity in establishing the conditions for hydrogen-induced crack initiation and propagation along a grain boundary. In fact, the mechanisms of hydrogen embrittlement are re-examined in light of these new results.

## Relationship of significant publications to the targets and milestones of the Division's roadmap

The significant publications for the Hydrogen Materials Compatibility Research Division address both short- and mid-term research objectives. Specifically, the publications “A microstructural based understanding of hydrogen-enhanced fatigue of stainless steels” and “Hydrogen-induced intergranular failure in nickel revisited” represent progress toward the short-term research objective of elucidating salient mechanisms governing hydrogen-induced degradation in structural metals. Both publications reveal a key insight that plastic deformation plays an essential role in the hydrogen-induced degradation mechanism of low-strength engineering alloys relevant to hydrogen containment components. In

addition, the publication “Surface-layer microstructure control for metastable austenitic stainless steel plate to improve hydrogen embrittlement resistance” satisfies the mid-term research objective of employing mechanistic understanding to selectively create next-generation materials. This publication demonstrates that by recognizing the mechanistic importance of strain-induced martensite in hydrogen-induced degradation of stainless steels, the surface composition of these steels can be modified by nitrogen to suppress the formation of strain-induced martensite. This relatively simple modification can be applied to lower-cost stainless steels such as 304 to improve their hydrogen compatibility.

## Selected Publications

Deutges, M., Knorr, I., Borchers, C., Volkert, C. A. and Kirchheim, R. (2013), Influence of hydrogen on the deformation morphology of vanadium (100) micropillars in the  $\alpha$ -phase of the vanadium–hydrogen system, *Scripta Materialia*, 68 (1), 71-74

Fujita, S. and Murakami, Y. (2013), A New Nonmetallic Inclusion Rating Method by Positive Use of Hydrogen Embrittlement Phenomenon, *Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science*, 44 (1), 303-322

Kimimura, S., Yamada, H. and Xu, C.N. (2012), Strong reddish-orange light emission from stress-activated  $\text{Sr}_{n+1}\text{Sn}_n\text{O}_{3n+1}:\text{Sm}^{3+}$  ( $n=1, 2, \text{infinity}$ ) with perovskite-related structures, *Applied Physics Letters*, 101, 091113

Kirchheim, R. (2012), Solid solution softening and hardening by mobile solute atoms with special focus on hydrogen, *Scripta Materialia*, 67 (9), 767-770

Martin, M. L., Sofronis, P., Robertson, I. M., Awane, T. and Murakami, Y. (2012), A microstructural based understanding of hydrogen-enhanced fatigue of stainless steels, *International Journal of Fatigue*, DOI: 10.1016/j.ijfatigue.2012.08.009

Martin, M. L., Somerday, B. P., Ritchie, R. O., Sofronis, P. and Robertson, I. M. (2012), Hydrogen-induced intergranular failure in nickel revisited, *Acta Materialia*, 60 (6-7), 2739-2745

Murakami, Y. (2012), Material defects as the basis of fatigue design, *International Journal of Fatigue*, 41, 2-10

Murakami, Y., Kanezaki, T. and Sofronis, P. (2013), Hydrogen embrittlement of high strength steels: Determination of the threshold stress intensity for small cracks nucleating at nonmetallic inclusions, *Engineering Fracture Mechanics*, 97 (1), 227-243

Nagao, A., Smith, C.D., Dadfarnia, M., Sofronis, P. and Robertson, I. M. (2012), The role of hydrogen in hydrogen embrittlement fracture of lath martensitic steel, *Acta Materialia*, 60 (13-14), 5182-5189

Nibur, K. A., Somerday, B. P., Marchi, C. S., Foulk III, J. W., Dadfarnia, M. and Sofronis, P. (2013), The Relationship Between Crack-Tip Strain and Subcritical Cracking Thresholds for Steels in High-Pressure Hydrogen Gas, *Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science*, 44 (1), 248-269

Onoue, K., Murakami, Y. and Sofronis, P. (2012), Japan's energy supply: Mid-to-long-term scenario - A proposal for a new energy supply system in the aftermath of the March 11 earthquake, *International Journal of Hydrogen Energy*, 37 (10), 8123-8132

Roiko, A. and Murakami, Y. (2012), A design approach for components in ultralong fatigue life with step loading, *International Journal of Fatigue*, 41, 140-149

Tsuboi, K., Tsuchiyama, T., Takaki, S. and Tsutsumi, S. (2012), Mechanical Properties of Strength-Gradient Steel Sheets Produced by Solution Nitriding, *ISIJ, International*, 52 (10), 1872-1878

Wu, H., Hamada, S. and Noguchi, S. (2013), Fatigue strength prediction for inhomogeneous face-centered cubic metal based on Vickers hardness, *International Journal of Fatigue*, 48, 48-54

Yamabe, J., Matsumoto, T., Matsuoka, S. and Murakami, Y. (2012), A new mechanism in hydrogen-enhanced fatigue crack growth behavior of a 1900-MPa-class high-strength steel, *International Journal of Fracture*, 177 (2), 141-162

Zhan, T. Z., Xu, C. N., Yamada, H., Terasawa, Y., Zhang, L., Iwase, H. and Kawai, M. (2012), Beam profile indicator for swift heavy ions using phosphor afterglow, *AIP Advances*, 2 (3), 032116



# FUEL CELLS

## EXECUTIVE SUMMARY

The goal of the Fuel Cells Research Division is to develop efficient, cost-effective, and stable methods to convert hydrogen and other fuels into electricity using a fuel cell. Both high temperature (HT) and low temperature (LT) solid oxide fuel cells (SOFC) and low temperature polymer electrolyte membrane fuel cells (PEFC) are examined, as shown in the roadmap figure. For the former, efforts are directed at developing lower temperature conductors, higher durability materials, and more effective electrode materials (catalysts). In the latter, efforts are directed at developing more durable and effective catalyst supports, more efficient and cheaper catalysts, and ionic membranes which can function at high temperatures. While a practical focus on new systems remains at the forefront of this effort, more fundamental studies provide insight to inform future directions.

## Significant Publications

### Fuel cell electrocatalyst using polybenzimidazole-modified carbon nanotubes as support materials

T. Fujigaya and N. Nakashima

Advanced Materials, 25 (12), 1666-1681, 2013

In this paper, we summarize the fundamental properties of the carbon nanotubes(CNTs)/polybenzimidazoles(PBIs)/ Pt and discuss their potential as a new electrocatalyst for PEFCs in comparison with the conventional ones. Furthermore, potential applications of CNT/PBIs including use of the materials for oxygen reduction catalysts and reinforcement of PBI films are summarized.

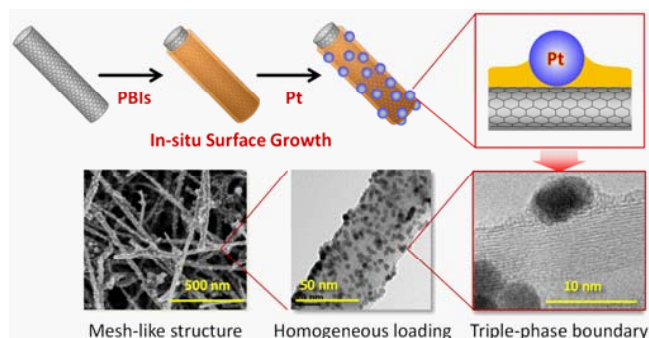


Fig 1. (Above) Schematic diagram of platinum nanoparticles decorated on PBI-coated carbon nanotubes. (Below) Electron microscopy of this same CNT-PBI-Pt electrocatalyst system

### Extremely high thermal resistive poly (*p*-phenylene benzobisoxazole) with desired shape and form from a newly synthesized soluble precursor

T. Fukumaru, T. Fujigaya and N. Nakashima

Macromolecules, 45(10), 4247-4253, 2012

The poly (*p*-phenylene benzobisoxazole) (PPBO) fiber has a very high thermal stability as well as mechanical strength when compared to any other polymers. However, one of the critical drawbacks of the polymer is its insolubility in organic solvents. To overcome this problem, we synthesized a soluble PPBO precursor that is soluble in common organic solvents, and the films made by the solution-cast method provided PPBO films after thermal treatment at 500°C. The result indicates that we now readily fabricate extremely high thermal resistive PPBO materials with desired shape and form.

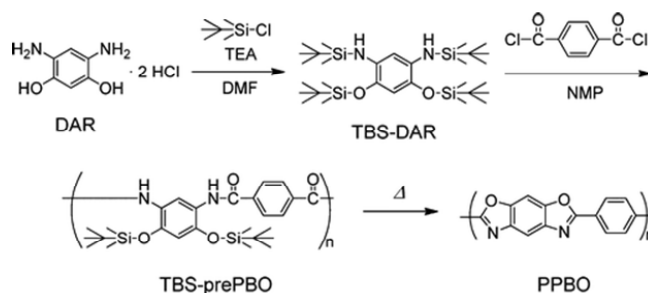


Fig. 2. In this study, we describe the design and synthesis of a soluble PPBO precursor followed by the fabrication of PPBO films as shown in this figure. This is the first report describing the fabrication of PPBO films with extremely high thermal stability (decomposition temperature, 670°C) without using a strong acid solvent.

### Reducing the chemical expansion coefficient in ceria by addition of zirconia

S. R. Bishop, D. Marrocchelli, W. Fang, K. Amezawa, K. Yashiro and

G. W. Watson

Energy and Environmental Science, 6 (4), 1142-1146, 2013

In many advanced electrodes for low temperature SOFCs, changes in oxygen content (“breathing”) of the electrode result in chemical expansion and consequent large stresses during operation, often resulting in mechanical failure. We demonstrated for the first time a method to reduce the chemical expansion by controlling lattice relaxation around oxygen vacancies. A 54% decrease in chemical expansion coefficient was observed, and this discovery has strong implications for increasing SOFC durability.

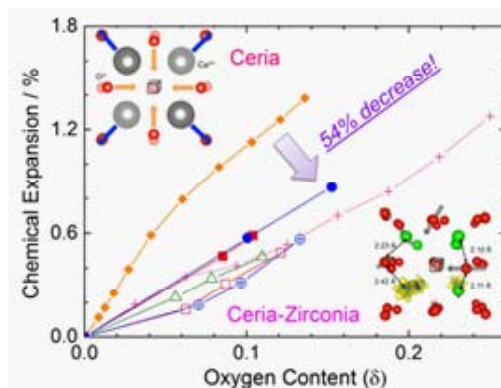
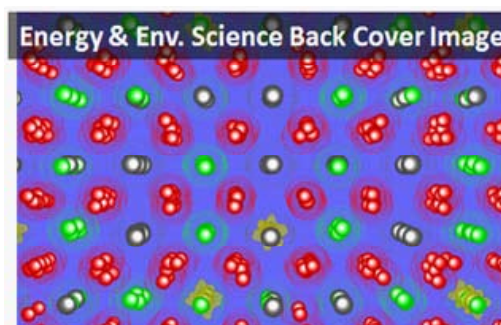


Fig. 3. By tailoring the lattice relaxation around oxygen vacancies by adding Zr to  $\text{CeO}_2$ , the chemical expansion was significantly reduced as computationally predicted by our group.

## Relationship of significant publications to the targets and milestones of the Division's roadmap

The roadmap of the Fuel Cell Research Division is focused on targets for efficient durable fuel cells, namely (i) high-temperature polymer electrolyte fuel cell (HT-PEFC) and (ii) durable solid oxide fuel cells (SOFC). The first paper (Nakashima et al.) contributes to the HT-PEFC target where the use of polybenzimidazoles (PBI) makes HT-PEFC operation beyond 100°C possible and carbon nanotubes (CNT) can contribute to realize stable electrocatalyst under severe corrosive operational conditions. The conventional Nafion membrane and the conventional carbon black catalyst

support cannot be used under such conditions for a long time, which makes this a significant breakthrough in PEFC research. The second paper (Fukumaru et al.) offers thermal stability of these new materials systems to improve the durability of HT-PEFC. The third paper (Bishop et al.) deals with an important milestone to develop oxide-based redox-tolerant alternative SOFC anode materials. The control of their chemical expansion is one of the essential steps for our long-term target to realize durable SOFCs.

## Selected Publications

Akazaki, K., Toshimitsu, F., Ozawa, H., Fujigaya, T. and Nakashima, N. (2012), Recognition and One-pot Extraction of Right- and Left-handed Semi-conducting Single-Walled Carbon Nanotube Enantiomers Using Fluorene-Binaphthol Chiral Copolymers, *Journal of the American Chemical Society*, 134 (30), 12700-12707

Bishop, S. R., Stefanik, T. S. and Tuller, H. L. (2012), Defects and transport in  $\text{Pr}_x\text{Ce}_{1-x}\text{O}_{2-\delta}$ : Composition trends, *Journal of Materials Research*, 27 (15), 2009-2016

Chen, D., Bishop, S. R. and Tuller, H. L. (2012), Non-stoichiometry in Oxide Thin Films: A Chemical Capacitance Study of the Praseodymium-Cerium Oxide System, *Advanced Functional Materials*, 23 (17), 2168-2174

Chen, D., Bishop, S. R. and Tuller, H. L. (2012), Praseodymium-Cerium Oxide Thin Film Cathodes: Study of Oxygen Reduction Reaction Kinetics, *Journal of Electroceramics*, 28 (1), 62-69

Cortie, M. B., Liu, F., Arnold, M. D. and Niidome, Y. (2012), Multimode Resonances in Silver Nanocuboids, *Langmuir*, 28 (24), 9103-9112

Frison, R., Heiroth, S., Rupp, J. L. M., Conder, K., Barthazy, E. J., Müller, E., Horisberger, M., Döbeli, M. and Gauckler, L. J. (2013), Crystallization of 8 Mol% Ytria-Stabilized Zirconia Thin-Films Deposited by Rf-Sputtering, *Solid State Ionics*, 232, 29-36

Fujigaya, T., Kim, C., Matsumoto, K. and Nakashima, K. (2013), Effective Anchoring of Pt-Nanoparticles onto Sulfonated Polyelectrolyte-Wrapped Carbon Nanotubes for Use as a Fuel Cell Electrocatalyst, *Polymer Journal*, 45 (3), 326-330

Fukumaru, T., Fujigaya, T. and Nakashima, N. (2012), Extremely High Thermal Resistive Poly(p-phenylene benzobisoxazole) with Desired Shape and Form from a Newly Synthesized Soluble Precursor, *Macromolecules*, 45 (10), 4247-4253

Hamasaki, Y., Nakashima, N. and Niidome, Y. (2013), Effects of Anions on Electrochemical Reactions of Silver Shells on Gold Nanorod, *Journal of Physical Chemistry C*, 117 (6), 2521-2530

Hamasaki, Y., Nakashima, N. and Niidome, Y. (2012), Electrochemical Deposition of Silver on Gold Electrodes in the Presence of Halogen Ions, *Chemistry Letters*, 41 (9), 962-964

Hirana, Y., Niidome, Y. and Nakashima, N. (2012), Effect of Charge of a Matrix Polymer on the Electronic States of Single-Walled Carbon Nanotubes, *Bulletin of the Chemical Society of Japan*, 85 (12), 1262-1267

Itoh, T., Hoshikawa, Y., Matsuura, S.-I., Mizuguchi, J., Arafune, H., Hanaoka, T., Mizukami, F., Hayashi, A., Nishihara, H. and Kyotani, T. (2012), Production of L-theanine using glutaminase encapsulated in carbon-coated mesoporous silica with high pH stability, *Biochemical Engineering Journal*, 68, 207-214

Kato, Y., Inoue, A., Niidome, Y. and Nakashima, N. (2012), Thermodynamics on Soluble Carbon Nanotubes: How Do DNA Molecules Replace Surfactants on Carbon Nanotubes?, *Scientific Reports*, 2, 733

- Kim, J. J., Bishop, S. R., Thompson, N., Kuru, Y. and Tuller, H. (2012), Optically derived energy band gap states of Pr in ceria, *Solid State Ionics*, 225, 198-200
- Kim, J. J., Kuhn, M., Bishop, S. R. and Tuller, H. L. (2013), Cathodic and defect properties of  $\text{Ba}_x\text{Sr}_{1-x}\text{Ti}_{1-y}\text{Fe}_y\text{O}_{3-y/2+\delta}$  mixed conducting oxides, *Solid State Ionics*, 230, 2-6
- Kuru, Y., Marrocchelli, D., Bishop, S. R., Chen, D., Yildiz, B. and Tuller, H. L. (2012), Anomalous Chemical Expansion Behavior of  $\text{Pr}_{0.2}\text{Ce}_{0.8}\text{O}_{2-\delta}$  Thin Films Grown by Pulsed Laser Deposition, *Journal of Electrochemical Society*, 159 (11), F799-F803
- Liu, C., Noda, Z., Sasaki, K. and Hayashi, K. (2012), Development of a Polyaniline Nanofiber-based Carbon Monoxide Sensor for Hydrogen Fuel Cell Application, *International Journal of Hydrogen Energy*, 37 (18), 13529-13535
- Liu, Q., Fujigaya, T. and Nakashima, N. (2012), Graphene unrolled from 'cup-stacked' carbon nanotubes, *Carbon*, 50 (15), 5421-5428
- Marrocchelli, D., Bishop, S. R., Tuller, H. L., Watson, G. W. and Yildiz, B. (2012), Charge localization increases chemical expansion in cerium-based oxides, *Physical Chemistry Chemistry Physics*, 14 (35), 12070-12074
- Marrocchelli, D., Bishop, S. R., Tuller, H. L. and Yildiz, B. (2012), Understanding chemical expansion in non-stoichiometric oxides: ceria and zirconia case studies, *Advanced Functional Materials*, 22 (9), 1958-1965
- Masuda, Y., Kugimiya, S., Murai, K., Hayashi, A. and Kato, K. (2013), Enhancement of activity and stability of the formaldehyde dehydrogenase by immobilizing onto phenyl-functionalized mesoporous silica, *Colloids and Surfaces B: Biointerfaces*, 101, 26-33
- Noda, Z., Hirata, K., Hayashi, A., Taniguchi, S., Nakazato, N., Seo, A., Yasuda, I., Ariura, S., Shinkai, H. and Sasaki, K. (2012), PEFC-type Impurity Sensors for Hydrogen Fuels, *International Journal of Hydrogen Energy*, 37 (21), 16256-16263
- Park, J. S., Hirana, Y., Mouri, S., Miyauchi, Y., Nakashima, N. and Matsuda, K. (2012), Observation of Negative and Positive Triions in the Electrochemically Carrier-doped Single-walled Carbon Nanotubes, *Journal of the American Chemical Society*, 134 (35), 14461-14466
- Quang-Tuyen, T., Shiratori, Y. and Sasaki, K. (2013), Feasibility of palm-biodiesel fuel for a direct internal reforming solid oxide fuel cell, *International Journal of Energy Research*, 37 (6), 609-616
- Schlupp, M. V. F., Binder, S., Martynczuk, J., Prestat, M. and Gauckler, L. J. (2012), Crack-free yttria stabilized zirconia thin films by aerosol assisted chemical vapor deposition: Influence of water and carrier gas, *Thin Solid Films*, 522 58-65
- Schlupp, M. V. F., Martynczuk, J., Prestat, M. and Gauckler, L. J. (2012), Precursor Decomposition, Microstructure, and Porosity of Yttria Stabilized Zirconia Thin Films Prepared by Aerosol-Assisted Chemical Vapor Deposition, *Advanced Energy Materials*, 3(3), 375-385
- Takahashi, Y., Shiratori, Y., Furuta, S. and Sasaki, K. (2012), Thermo-mechanical reliability and catalytic activity of Ni-Zirconia anode supports in internal reforming SOFC running on biogas, 225, 113-117
- Tornow, C. E., Thorson, M. R., Ma, S., Gewirth, A. A. and Kenis Paul J.A. (2012), Nitrogen-based Catalysts for the Electrochemical Reduction of  $\text{CO}_2$  to CO, *Journal of the American Chemical Society*, 134 (48), 19520-19523
- Tsuru, Y., Nakashima, N. and Niidome, Y. (2012), Optical properties of Au-Ag core-shell nanorods on glass and ITO substrates, *Optics Communications*, 285(16), 3419-3422
- Watari, R., Nishihara, M., Tajiri, H., Otsuka, H. and Takahara, A. (2012), Preparation of novel polyimide hybrid materials by multi-layered charge-transfer complex formation, *Polymer Journal*, 1-6
- Yoshizumi, T., Taniguchi, S., Shiratori, Y. and Sasaki, K. (2012), Sulfur Poisoning of SOFCs: Voltage Oscillation and Ni Oxidation, *Journal of Electrochemical Society*, 159 (11), F693-F701



# THERMAL SCIENCE AND ENGINEERING

## EXECUTIVE SUMMARY

In consultation with the Energy Analysis Research Division, the Thermal Science and Engineering (TSE) Research Division's research objectives now cover the broader area of thermal science and engineering. The overarching objective is the reduction of CO<sub>2</sub> emissions through efficient use of thermal energy. Moreover, almost all energy conversion processes suffer from losses associated with the transfer of thermal energy (heat) from higher to lower temperatures. Fundamental progress towards more intelligent and efficient energy utilization could be made if heat is transferred with the smallest possible temperature difference. For instance, thermoelectrics, the direct thermal-to-electrical energy conversion systems, which could operate at lower temperatures (100–700°C), will significantly expand the possibilities for waste heat recovery applications.

Further advancement and optimization of new energy technologies will be inhibited without an expansion of our knowledge base of the thermophysical properties of key substances projected for widespread use in the future low-carbon emission society. To lay the foundation for a wide range of low-emission technologies, in this regard, we need to expand the thermal properties database of relevant substances to a wider range of conditions and we need to generate data to understand the mechanisms of heat and mass transfer associated with material interfaces, phase-change phenomena, surface phenomena and thin films relevant for developing new high-efficiency energy conversion technologies.



## Significant Publications

### *A compact curved vibrating wire technique for measurement of hydrogen gas viscosity*

E. Yusibani, P. L. Woodfield, K. Shinzato, Y. Takata and M. Kohno  
Experimental Thermal and Fluid Science, 47, 1-5, 2013

Studies of the application of a curved vibrating wire method to measure hydrogen gas viscosity have been done. A fine tungsten wire with a nominal diameter of 50 $\mu$ m is bent into a semi-circular shape and arranged symmetrically in a magnetic field. The frequency domain response for forced oscillation of the wire is used for calculating the viscosity. Argon, nitrogen, helium and hydrogen viscosities have been measured at room temperature up to 0.7MPa. The deviations with respect to existing equations suggest that with more refinements, it may be possible to take gas viscosity measurements with a precision of less than 1%. The developed method will be applied to measure viscosity of high pressure hydrogen, which was not successfully measured by the capillary methods. In the future, measured viscosity data will be compiled into a prediction equation and implemented into the thermophysical property database for a wide range of hydrogen.

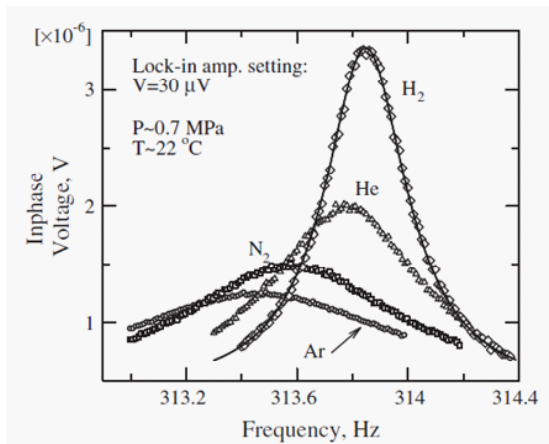


Fig. 1. Typical measurement and the corresponding least squares fit to the measured data with a 10mHz/step at 0.7MPa

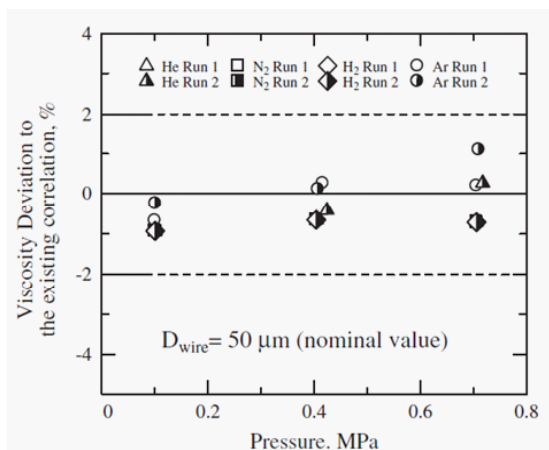


Fig. 2. Viscosity deviations versus pressure at room temperature

### *Enhanced anisotropic heat conduction in multi-walled carbon nanotubes*

H. Hayashi, T. Ikuta, T. Nishiyama and K. Takahashi  
Journal of Applied Physics, 113(1), 014301, 2013

The carbon nanotube is a promising candidate as a supporting material for fuel cell catalyst. However, its thermophysical property is still veiled, especially for multi-walled carbon nanotubes (MWNTs). Here, anisotropy of heat conduction in MWNTs is investigated by measuring heat flows in a pristine MWNT and in a MWNT with defects, which enables us to determine the in- and out-of-shell thermal conductivities of each MWNT graphite shell. Current results contribute to understanding not only MWNT but a variety of carbon-based materials including gas diffusion layer.

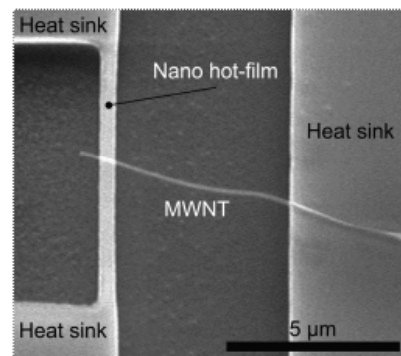


Fig. 3. SEM image of measurement of thermal conductivity of an individual CNT

### *Entropy generation minimization: A practical approach for performance evaluation of temperature cascaded co-generation plants*

A. Myat, K. Thu, Y. D. Kim, B. B. Saha and K. C. Ng  
Energy, 46(1), 493-521, 2012

The paper presents a practical tool that employs the entropy generation minimization (EGM) approach for an in-depth performance evaluation of a co-generation plant with a temperature-cascaded concept. Results showed that the temperature cascaded arrangement of a cogeneration plant yields an overall efficiency as high as 67%, whilst the specific entropy generation of 1.72W/K-kW and thus, can significantly contribute to achieving a low carbon society.

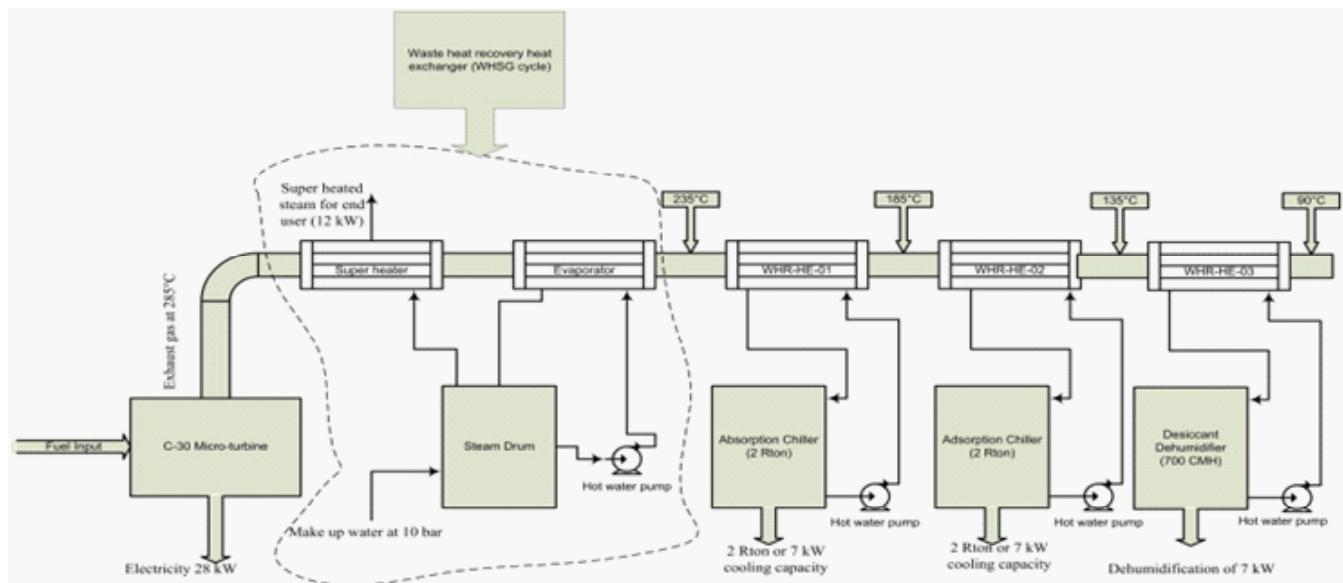


Fig. 4. The schematic layout diagram of temperature cascaded cogeneration system

## Relationship of significant publications to the targets and milestones of the Division's roadmap

The Thermal Science and Engineering (TSE) Research Division covers wide range of research fields related to thermophysical properties and heat transfer of various substances, and applications for high-efficiency use of thermal energy. The work of Yusibani et al. (2013) describes the development of a new measurement method for hydrogen viscosity at high pressure and high temperature region. The study on thermophysical property measurements for hydrogen was set as a short-term target in the Division's roadmap. The work of Myat et al (2012) presents a practical tool for high-

efficiency use of thermal energy by the entropy generation minimization (EGM) method. The work is an essential part of the applications of waste heat- powered air conditioning and refrigeration systems, which are the Division's mid- and long-term goals.

The work of Hayashi et al. (2013) describes the state-of-the-art thermal conductivity measurement of carbon nanotubes (CNT). The CNT is a promising material for various energy systems. Understanding of its thermophysical properties is one of the Division's long-term goals.

## Selected Publications

Askalany, A. A., Saha, B. B., Ahmed, M. S. and Ismail, I. M. (2013), Adsorption cooling system employing granular activated carbon-R134a pair for renewable energy applications, *International Journal of Refrigeration*, 36 (3), 1037-1044

Askalany, A. A., Saha, B. B., Kariya, K., Ismail, I. M., Salem, M., Ahmed, H. H. and Morsy, M. G. (2012), Hybrid adsorption cooling systems-An overview, *Renewable and Sustainable Energy Reviews*, 16 (8), 5758-5801

Askalany, A. A., Salem, M., Ismael, I. M., Ali, A. H. H., Morsy, M. G. and Saha, B. B. (2013), An overview on adsorption pairs for cooling, *Renewable and Sustainable Energy Reviews*, 19, 565-572

Choudhury, B., Saha, B. B., Chatterjee, P. K. and Sarkar, J. P. (2013), An overview of developments in adsorption refrigeration systems towards a sustainable way of cooling, *Applied Energy*, 104, 554-567

Hirotsu, J., Ikuta, T., Nishiyama, T. and Takahashi, K. (2013), Measuring the thermal boundary resistance of van der Waals contacts using an individual carbon nanotube, *Journal of Physics Condensed Matter*, 25(2), 025301

Myat, A., Thu, K., Kim, Y. D., Saha, B. B., and Ng, K. C. (2012), Entropy generation minimization: A practical approach for performance evaluation of temperature cascaded co-generation plants, *Energy*, 46(1), 493-521

Srinivasan, K., Dutta, P., Ng, K. C. and Saha, B. B. (2012), Calculation of Heat of Adsorption of Gases and Refrigerants on Activated Carbons from Direct Measurements Fitted to the Dubinin-Astakhov Equation, *Adsorption Science and Technology*, 30(7), 549-565

Srinivasan, K., Dutta, P., Saha, B. B., Ng, K. C. and Prasad, M. (2013), Realistic minimum desorption temperatures and compressor sizing for activated carbon + HFC 134a adsorption coolers, *Applied Thermal Engineering*, 51(1-2), 551-559



# HYDROGEN STORAGE

## EXECUTIVE SUMMARY

The mission of the Hydrogen Storage Research Division is to carry out basic science research for the development of hydrogen storage materials for technology options that can significantly advance the realization of a carbon-neutral energy society. Applications include onboard hydrogen storage, stationary energy storage in wide range of usage and capacity, electrochemical applications, such as the Ni-hydrogen battery, and others.

In the area of mobile applications, especially onboard hydrogen storage for fuel cell vehicles, recent discussions with the Japanese automotive industry have guided the Division to focus on weight density, volume density, cost, and shape—Lead Principal Investigator (PI) Professor Akiba is the chairperson of the national committee to revise the national hydrogen storage roadmap.

For stationary applications, after the East-Japan earthquake, compact, stable energy storage for fluctuating renewable energy sources over short- to long-term scenarios has become increasingly important. Storage of electricity in the form of hydrogen is a promising solution pathway. The volume energy density of hydrogen is higher than existing batteries by more than one order. Also, hydrogen storage materials can store hydrogen at much higher density than compressed gas of 70MPa and liquefied hydrogen. For stationary applications, there are no Japanese national targets at present. One of the reasons is that this application is dispersed in scale, purpose, location of installation, etc. The Division's research is focused on volume density, cycle ability, and cost, as they all constitute key targets for the development of materials for stationary usage.

## Significant Publications

### *High-pressure torsion of TiFe intermetallics for activation of hydrogen storage at room temperature with heterogeneous nanostructure*

K. Edalati, J. Matsuda, H. Iwaoka, S. Toh, E. Akiba and Z. Horita  
International Journal of Hydrogen Energy, 38 (11), 4622-4627, 2013

An intermetallic alloy of TiFe, which is free from rare earth elements, is a promising candidate for a stationary hydrogen storage system. However, a major drawback is the requirement for initial activation before the use for hydrogen storage. In this study, we have shown that TiFe becomes activated using the process of severe plastic deformation through high-pressure torsion (HPT) which allows plastic deformation into hard and brittle materials such as TiFe. With the HPT-processed TiFe, we expect a significant reduction of the cost with safety handling for the stationary hydrogen storage system.

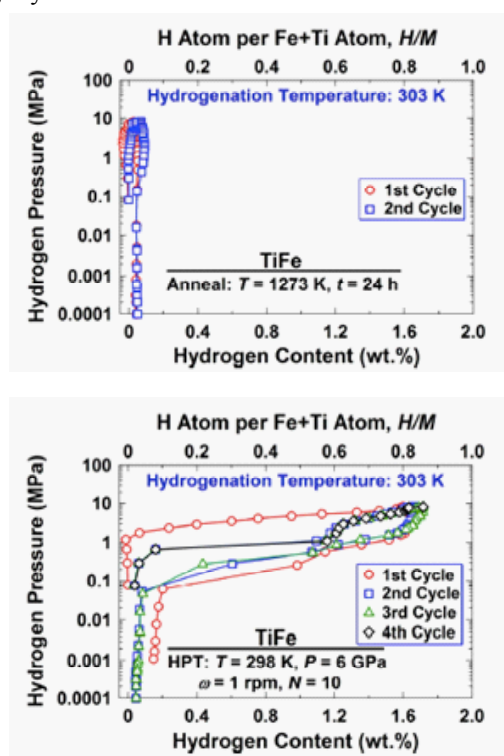


Fig. 1. (Above) Hydrogen absorption without straining (Below) Hydrogen Absorption after severe straining

## Relationship of significant publications to the targets and milestones of the Division's roadmap

Hydrogen exists in a gas phase under ambient conditions. The volume energy density of hydrogen is usually less than that for conventional fuels such as gasoline. To realize the hydrogen economy, hydrogen storage/transport in a compact, light-weight, energy-efficient, and safe way is indispensable. Hydrogen storage materials contain hydrogen much denser than physical hydrogen storage, such as compressed gas and liquefied hydrogen. There are two applications for hydrogen

### *Effect of Rare Earth Elements and Alloy Composition on Hydrogenation Properties and Crystal Structures of Hydrides in $Mg_{2-x}RE_xNi_4$*

K. Sakaki, N. Terashita, S. Tsunokake, Y. Nakamura and E. Akiba  
Journal of Physical Chemistry C, 116 (36), 19156-19163, 2012

Mg based hydrogen absorbing alloys usually work at temperature above 673 K but  $Mg_{2-x}RE_xNi_4$  absorb and desorb hydrogen at room temperatures under moderate conditions. It was found that hydrogenation properties and crystal structure of the hydrides in  $Mg_{2-x}RE_xNi_4$  depend on the alloy composition but not the choice of rare earth element.

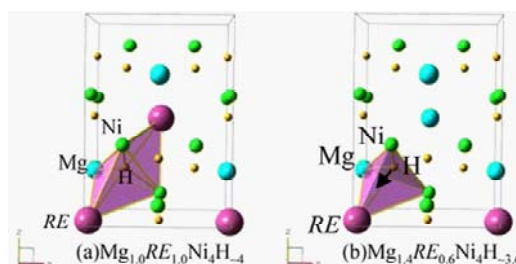


Fig. 2. Atomic coordinates of triangular bipyramid in  $Mg_{2-x}RE_xNi_4H_{4-x}$  for (a) stoichiometric and (b) Mg-rich compounds.

### *Nanotechnology in Mg-based materials for hydrogen storage*

H. Shao, G. Xin, J. Zheng, X. Li and E. Akiba  
Nano Energy, 1(4), 590-601, 2012

Mg-based materials are very promising for hydrogen storage applications. However, both the kinetic and thermodynamic problems remain for these applications. Here we review the methods used by the authors to synthesize Mg-based hydrogen storage materials with nanostructure as well as some novel techniques by other researchers. The focus is on how these nanotechnology processing methods could change the kinetics and thermodynamics in Mg-based materials for hydrogen storage. These methods include ball milling (mechanical grinding, mechanical alloying, reactive ball milling), thin film synthesis, hydrogen plasma metal reaction, and catalyzed solution synthesis.

storage materials: mobile and stationary. In the Division's roadmap, TiFe alloys and Mg-based materials are clearly shown as two of the strongest candidates for stationary applications. TiFe is a very significant low cost material that is a short-term research target in the Division's roadmap, while Mg-based materials are targeted for energy storage in the 2020s.

## Selected Publications

- Ashida, M. and Horita, Z. (2012), Effects of ball milling and high-pressure torsion for improving mechanical properties of Al-Al<sub>2</sub>O<sub>3</sub> nanocomposites, *Journal of Materials Science*, 47 (22), 7821-7827
- Cao, H., Zhang, Y., Wang, J., Xiong, Z., Wu, G. and Chen, P. (2012), Materials design and modification on amide-based composites for hydrogen storage, *Progress in Natural Science: Materials International*, 22 (6), 550-560
- Cubero-Sesin, J. M. and Horita, Z. (2012), Mechanical Properties and Microstructures of Al-Fe Alloys processed by High-Pressure Torsion, *Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science*, 43(13), 5182-5192
- Cubero-Sesin, J. M. and Horita, Z. (2012), Powder consolidation of Al-10 wt% Fe alloy by High-Pressure Torsion, *Materials Science and Engineering: A*, 558, 462-471
- Cubero-Sesin J. M., and Horita, Z. (2013), Strengthening of Al through addition of Fe and by processing with High-Pressure Torsion, *Journal of Materials Science*, 48, 4713-4722
- Edalati, K. and Horita, Z. (2012), Processing Sheets and Wires by Continuous High-Pressure Torsion, *Reviews on Advanced Materials Science*, 31 (1), 5-11
- Edalati, K., Horita, Z., Furuta, T. and Kuramoto, S. (2013), Dynamic Recrystallization and Recovery during High-Pressure Torsion: Experimental Evidence by Torque Measurement Using Ring Specimens, *Materials Science and Engineering: A*, 559, 506-509
- Edalati, K., Toh, S., Furuta, T., Kuramoto, S., Watanabe, M. and Horita, Z. (2012), Development of ultrahigh strength and high ductility in nanostructured iron alloys with lattice softening and nanotwins, *Scripta Materialia*, 67 (5), 511-514
- Edalati, K., Toh, S., Iwaoka, H. and Horita, Z. (2012), Microstructural Characteristics of Tungsten-Base Nanocomposites Produced from Micropowders by High-Pressure Torsion, *Acta Materialia*, 60 (9), 3885-3893
- Edalati, K., Toh, S., Iwaoka, H., Watanabe, M., Horita, Z., Kashioka, D., Kishida, K. and Inui, H. (2012), Ultrahigh strength and high plasticity in TiAl intermetallics with bimodal grain structure and nanotwins, *Scripta Materialia*, 67 (10), 814-817
- Ikoma, Y., Hayano, K., Edalati, K., Saito, K., Guo, Q. and Horita, Z. (2012), Phase transformation and nanograin refinement of silicon by processing through high-pressure torsion, *Applied Physics Letters*, 101 (12), 121908
- Kim, H., Nakamura, J., Shao, H., Nakamura, Y., Akiba, E., Chapman, K. W., Chupas, P. J. and Proffen, T. (2012), Variation in the ratio of Mg<sub>2</sub>Co and MgCo<sub>2</sub> in amorphous-like mechanically alloyed Mg<sub>x</sub>Co<sub>100-x</sub> using the atomic pair distribution function analysis, *Zeitschrift fuer Kristallographie*, 227 (5), 299-303
- Lee, S., Horita, Z., Hirotsawa, S. and Matsuda, K. (2012), Age-Hardening of Al-Li-Cu-Mg Alloy (2091) Processed by High-Pressure Torsion, *Materials Science and Engineering: A*, 546, 82-89
- Sakaki, K., Nakamura, Y. and Akiba, E. (2012), Identification of Vacancy Formation Sites in LaNi<sub>5</sub>Cu During Hydrogenation Using in Situ Coincidence Doppler Broadening Technique," *Journal of Physical Chemistry C*, 116(42), 22238-22244
- Sakaki, K., Terashita, N., Tsunokake, S., Nakamura, Y. and Akiba, E. (2012), Effect of Rare Earth Elements and Alloy Composition on Hydrogenation Properties and Crystal Structures of Hydrides in Mg<sub>2-x</sub>RE<sub>x</sub>Ni<sub>4</sub>, *Journal of Physical Chemistry C*, 116 (36), 19156-19163
- Shao, H., Xin, G., Zheng, J., Li, X. and Akiba, E. (2012), Nanotechnology in Mg-based materials for hydrogen storage, *Nano Energy*, 1, 590-601
- Yan, Y., Remhof, A., Hwang, S.-J., Li, H.-W., Mauron, P., Orimo, S. and Züttel, A. (2012), Pressure and temperature dependence of the decomposition pathway of LiBH<sub>4</sub>, *Physical Chemistry Chemical Physics*, 14(18), 6514-6519



# CATALYTIC MATERIALS TRANSFORMATIONS

## EXECUTIVE SUMMARY

The mission of the Catalytic Materials Transformations Research Division is to contribute to the creation of innovative carbon-neutral technology by developing novel catalysts, underlining both aspects of basic science and engineering. The activities are focused on investigations of catalysis-related “New energy and Energy conservation,” all of which will make a dramatic impact on the hydrogen-based carbon-neutral technology. The Division’s work is classified into three major research areas.

1. The sub-groups of S. Ogo and T. Rauchfuss are concentrated in basic research for understanding catalytic mechanism and exploring “novel catalysts for hydrogen activation and production.” Subsequently, the research will advance the ultimate goal for conducting artificial photosynthesis, extracting electrons from water to produce fuels (hydrogen, methane, or formate, etc) for a Carbon-Neutral Economy.
2. The sub-group of T. Katsuki explores effective “asymmetric catalysts for energy-conservation and waste-free materials transformations.”
3. The sub-group of M. Yamauchi is focused on developing “nanoalloy catalysts for a carbon-neutral energy cycle.”

In short, research in this Division focuses on exploring “novel catalysts” that underlie two important research objectives of Energy Conservation and Renewable Energy.

## Significant Publications

### *A Functional [NiFe]Hydrogenase Mimic That Catalyzes Electron and Hydride Transfer from H<sub>2</sub>*

S. Ogo, K. Ichikawa, T. Kishima, T. Matsumoto, H. Nakai, K. Kusaka and T. Ohhara

Science, 339(6120), 682-684, 2013

This paper reports the first elucidation of hydrogen activation using a functional [NiFe]-based model complex inspired from natural [NiFe]hydrogenase. This complex heterolytically activates hydrogen to form a hydride complex that is capable of reducing substrates by either hydride ion or electron transfer. The results will help to accelerate hydrogen fuel cell technology, representing the dramatic progress of hydrogen activation using a non-precious metal catalyst leading the way towards low-cost hydrogen fuel cells.

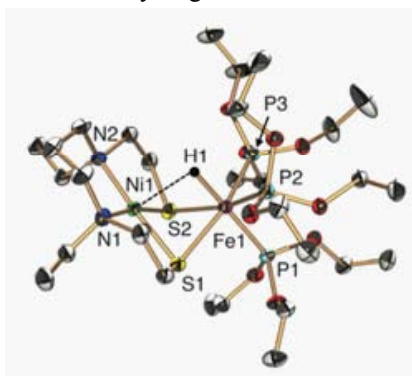


Fig. 1. Structure of the synthetic nickel-iron catalyst reported by Ogo et al.

### *Asymmetric Epoxidation of Conjugated Olefins with Dioxygen*

S. Koya, Y. Nishioka, H. Mizoguchi, T. Uchida and T. Katsuki  
Angewandte Chemie - International Edition, 51 (33), 8243-8246, 2012

Use of ubiquitous matters such as atmospheric heat and air is of importance for energy conservation for material transformations. In this report, desired epoxides, versatile

synthetic intermediates, were smoothly transformed in air at 25°C from conjugated olefins by using a newly designed (aqua) ruthenium(salen) complex as a catalyst and this oxidation has two remarkable advantages for energy conservation: 1. no waste, 2. no additive.

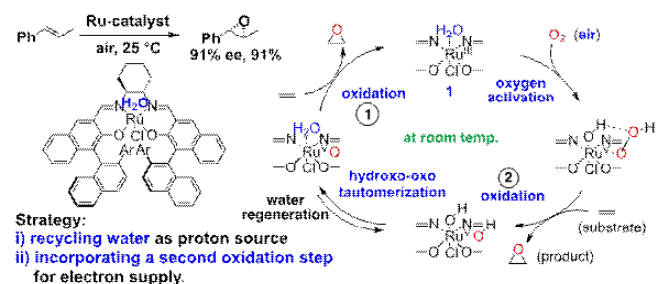


Fig. 2. Asymmetric epoxidation using air at room temperature and the mechanism proposed for this biological-like oxidation

### *Iron-catalyzed dioxygen-driven C-C bond formation: Oxidative dearomatization of 2-naphthols with construction of a chiral quaternary stereocenter*

T. Oguma and T. Katsuki  
Journal of the American Chemical Society, 134(49), 20017-20020, 2012

Hydroxyaromatic compounds are abundant natural products, but their conversion to useful intermediates requires an amount of energy and highly active reagents. In this report, a novel iron (salan) complex transforms fairly unreactive compounds to versatile intermediates using ubiquitous air under mild conditions. This method paves the way for carbon-neutral and clean material transformation in terms of 1) use of natural resources and 2) use of less toxic and abundant iron.

## Relationship of significant publications to the targets and milestones of the Division's roadmap

The Catalytic Materials Transformations Research Division is focused on the investigation of catalysis-related “New Energy” and “Energy Conservation.” The S. Ogo group synthesized a functional [NiFe]-based model complex for hydrogen activation, which was a major research accomplishment. This breakthrough study is completely on the course of the short-term target in the roadmap for H<sub>2</sub>-activation: synthetic H<sub>2</sub>ase, involving the theme of “New Energy.” The significant publication by the T. Katsuki group involves the

development of two novel catalysts, (aqua)ruthenium(salen) and iron(salan) complexes, which transform olefins to desired epoxides, versatile intermediates, and abundant but fairly unreactive hydroxyaromatic compounds to useful intermediates in air and under mild reaction conditions, respectively. This fundamental research of the waste-free asymmetric epoxidation is well established the short-term target of “the Methodologies for Energy Conservation.”

## Selected Publications

Eguchi, S., Yoon, K.-S. and Ogo, S. (2012), O<sub>2</sub>-stable Membrane-bound [NiFe]hydrogenase from a Newly Isolated *Citrobacter* sp. S-77. *J. Biosci. Bioeng.*, 114(5), 479-484

Fukunaga, Y., Uchida, T., Ito, Y., Matsumoto, K. and Katsuki, T. (2012), Ru(CO)-salen-Catalyzed Synthesis of Enantiopure aziridinyl ketones and Formal Asymmetric Synthesis of (+)-PD 128907, *Organic Letters*, 14 (17), 4658-4661

Inoki, D., Matsumoto, T., Nakai, H. and Ogo, S. (2012), Experimental Study of Reductive Elimination of H<sub>2</sub> from Rhodium Hydride Species, *Organometallics*, 31(8), 2996-3001

Ishida, M., Lim, J. M., Lee, B. S., Tani, F., Sessler, J. L., Kim D. and Naruta, Y. (2012), Photophysical Analysis of 1,10-Phenanthroline-Embedded Porphyrin Analogues and Their Magnesium(II) Complexes, *Chemistry - A European Journal*, 18 (45), 14329-14341

Jeong, K., Nakamori, H., Imai, S., Matsumoto, T., Ogo, S. and Nakai, H. (2012), A Neutral Five-coordinated Organoruthenium(0) Complex: X-ray Structure and Unique Solvatochromism, *Chemistry Letters*, 41(6), 650-651

Kim, C., Uchida, T. and Katsuki, T. (2012), Asymmetric Olefin Aziridination Using a Newly Designed Ru(CO)(salen) Complex as Catalyst, *Chemical Communications*, 48 (57), 7188-7190

Kim, K., Kishima, T., Matsumoto, T., Nakai, H. and Ogo, S. (2013), Selective Redox Activation of H<sub>2</sub> or O<sub>2</sub> in a [NiRu] Complex by Aromatic Ligand Effects, *Organometallics* 32(1), 79-87

Kim, K., Matsumoto, T., Robertson, A., Nakai, H. and Ogo, S. (2012), Simple Ligand Effects Switch a Hydrogenase Mimic between H<sub>2</sub> and O<sub>2</sub> Activation, *Chemistry - An Asian Journal*, 7(6), 1394-1400

Kobayashi, H., Morita, H., Yamauchi, M., Ikeda, R., Kitagawa, H., Kubota, Y., Kato, K., Takata, M., Toh, S. and Matsumura, S. (2012), Nanosize-Induced Drastic Drop in Equilibrium Hydrogen Pressure for Hydride Formation and Structural Stabilization in Pd-Rh Solid-Solution Alloys, *Journal of the American Chemical Society*, 134 (30), 12390-12393

Kobayashi, H., Yamauchi, M. and Kitagawa, H. (2012), Finding Hydrogen-Storage Capability in Iridium Induced by the Nanosize Effect, *Journal of the American Chemical Society*, 123 (16), 6893-6895

Koya, S., Nishioka, Y., Mizoguchi, H., Uchida, T. and Katsuki, T. (2012), Asymmetric Epoxidation of Conjugated Olefins with Dioxxygen, *Angewandte Chemie - International Edition*, 51 (33), 8243-8246

Liu, B., Liu, Q., You, D., Li, X., Naruta, Y. and Zhu, W. (2012), Molecular engineering of indoline based organic sensitizers for highly efficient dye-sensitized solar cells, *Journal of Materials Chemistry*, 22 (26), 13348-13356

Maity, P., Xie, S., Yamauchi, M. and Tsukuda, T. (2012), Stabilized gold clusters: from isolation toward controlled synthesis, *Nanoscale*, 4 (14), 4027-4037

Matsumoto, K., Egami, H., Oguma, T. and Katsuki, T. (2012), What Factors Influence the Catalytic Activity of Iron-salan Complexes for Aerobic Oxidative Coupling of 2-Naphthols?, *Chemical Communications*, 48 (44), 5823-5825

Nonaka, K., Nguyen, N. T., Yoon, K.-S. and Ogo, S. (2013), Novel "H<sub>2</sub>-oxidizing" [NiFeSe]hydrogenase from *Desulfovibrio vulgaris* Miyazaki F, *Journal of Bioscience and Bioengineering*, 115(4), 366-371

Oguma, T., and Katsuki T. (2012), Iron-Catalyzed Dioxxygen-Driven C-C Bond Formation: Oxidative Dearomatization of 2-Naphthols with Construction of a Chiral Quaternary Stereocenter, *Journal of the American Chemical Society*, 134(49), 20017-20020

Ohta, T., Liu, J. and Naruta, Y. (2013), Resonance Raman characterization of mononuclear heme-peroxo intermediate models, *Coordination Chemistry Reviews*, 257 (2), 407-413

Ohta, T., Liu, J., Saito, M., Kobayashi, Y., Yoda, Y., Seto, M. and Naruta, Y. (2012), Axial Ligand Effects on Vibrational Dynamics of Iron in Heme Carbonyl Studied by Nuclear Resonance Vibrational Spectroscopy, *Journal of Physical Chemistry B*, 116(47), 13831-1383





# CO<sub>2</sub> CAPTURE AND UTILIZATION

## EXECUTIVE SUMMARY

To contribute to the mitigation of CO<sub>2</sub> emissions, the CO<sub>2</sub> Capture and Utilization Research Division focuses on the fundamental science underlying the development of effective CO<sub>2</sub> separation and concentration technologies. In addition, since CO<sub>2</sub> is a by-product in current industrial H<sub>2</sub> generation, the Division's research efforts on separation technologies are important for establishing a carbon-neutral hydrogen-powered society. Lastly, the conversion of CO<sub>2</sub> to various value-added compounds, such as methanol, is also central to the Division's research objectives.

## Significant Publications

### *Nitrogen-based catalysts for the electrochemical reduction of CO<sub>2</sub> to CO*

C. E. Tornow, M. R. Thorson, S. Ma, A. A. Gewirth and P. J. A. Kenis  
Journal of the American Chemical Society, 134(48), 19520-19523, 2012

This paper reports the first example of a carbon-supported, nitrogen-based organometallic silver catalysts for the reduction of CO<sub>2</sub>. Their performance toward the selective formation of CO is similar to the performance achieved when using Ag as the catalyst (the typical nanoparticle-based catalyst used for this conversion), but comparatively at much lower silver loading. The paper also suggests possible mechanisms for this catalytic process. Performance data: Current Density (a measure of product conversion) >100mA/cm<sup>2</sup> and Faradaic Efficiency (a measure of selectivity for the desired product) >90%.

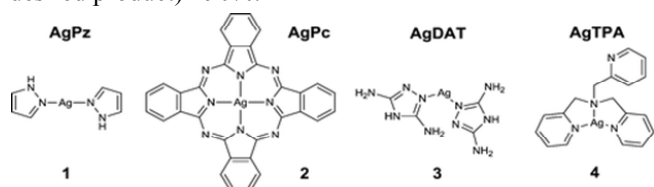


Fig. 1. Silver pyrazole supported on carbon (AgPz/C)

Fig. 2. Silver phthalocyanine supported on carbon (AgPc/C)

Fig. 3. Silver 3,5-diamino-1,2,4-triazole supported on carbon (AgDAT/C)

Fig. 4. Silver tris[(2-pyridyl)methyl]amine supported on carbon (AgTPA/C)

### *Effect of cations on the electrochemical conversion of CO<sub>2</sub> to CO*

M. R. Thorson, K. I. Siil and P. J. A. Kenis  
Journal of The Electrochemical Society, 160 (1), F69-F74, 2013

This paper reports the effect of electrolyte composition on the electrochemical reduction of CO<sub>2</sub> to CO. We observe that large alkali cations (cesium and rubidium) improve the current density (so conversion) by about 50%, while they suppress evolution of unwanted hydrogen, so the process becomes more selective for CO (Faradaic Efficiency >95%). We explain the effect of cation size on selectivity for CO by the interplay between the level of cation hydration and the extent of cation adsorption on Ag electrodes. Best Performance: Current Density (conversion) 80mA/cm<sup>2</sup>, Faradaic Efficiency (selectivity for CO<sub>2</sub>) 98%, and energetic efficiency of 65% (=very good!).

## Relationship of significant publications to the targets and milestones of the Division's roadmap

The work by Tornow et al. (2012) reports a new catalyst for CO<sub>2</sub> reduction by electrochemistry which performs at a Current Density (a measure of product conversion) level >100mA/cm<sup>2</sup> and a Faradaic Efficiency (a measure of selectivity for the desired product) level >90%. These numbers meet the target values for this year. The paper by Thorson et al. (2013) reports the effect of a counter cation in the electrochemical reduction

of CO<sub>2</sub>. We found that the counter cation, especially its size, has a large role in the improvement of selectivity of CO reduction. These accomplishments meet the Division's short term targets, namely the achieved energy efficiency of 65 % is in line with the short term target (>60%).

## Selected Publications

Maeda, E., Lee, Y., Kobayashi, Y., Taino, A., Koizumi, M., Fujikawa, S. and Delaunay, J. J. (2012), Sensitivity to refractive index of high-aspect-ratio nanofins with optical vortex, *Nanotechnology*, 23 (50), 505502

Thorson, M. R., Siil, K. I. and Kenis, P. J. A. (2013), Effect of cations on the electrochemical conversion of CO<sub>2</sub> to CO, *Journal of The Electrochemical Society*, 160 (1), F69-F74

# CO<sub>2</sub> STORAGE

## Executive Summary

The CO<sub>2</sub> Storage Research Division of I<sup>2</sup>CNER addresses the underlying science associated with the roadblocks for large-scale implementation of CO<sub>2</sub> storage, including risk of CO<sub>2</sub> leakage, risk of induced seismicity, and high-cost, all of which are closely related to the highly uncertain local geological characteristics of potential storage sites. The relevant carbon capture and storage (CCS) technologies and research target areas are depicted in the Division's roadmap. Thus, **reservoir characterization** as well as **monitoring and modeling of injected and leaked CO<sub>2</sub>** are crucial steps in the development of CCS relevant to I<sup>2</sup>CNER's short-term CCS objectives, as developed in parallel with the Energy Analysis Division, and have therefore received considerable research focus during FY 2012, with particular attention on the goal of monitoring and modeling of injected and leaked CO<sub>2</sub> in geological structures typical of Japan.

With respect to **reservoir characterization**, efforts are directed at understanding rock heterogeneity in constructing geological models and toward designing monitoring surveys, owing to the complicated nature of such formations in Japan compared to that in other countries (e.g., Australia). Furthermore, since it is difficult to find structural closure for CO<sub>2</sub> injection in the Japanese islands and around their continental margins (i.e., anticline structure), substantial research effort is focused on uncovering the physical mechanisms responsible for residual, dissolution, and mineralogical trapping of CO<sub>2</sub> in porous formations. The current efforts involve collaborative experimental, modeling, and simulation efforts to develop a comprehensive suite of tools that can be utilized in the future for robust prediction of CO<sub>2</sub> migration fate in the heterogeneous rock structure typical of Japan. An additional key focus area in this regard is the development of experimental capabilities that provide venues for studying the behavior of CO<sub>2</sub> in a range of contexts at pressures and temperatures relevant to actual CCS applications, including liquid CO<sub>2</sub> behavior in model and actual rock structures, as well as CO<sub>2</sub> fate upon leakage into the ocean through compromised cap rock (using a new high-pressure water tunnel to be installed at Kyushu

in FY2013). Finally, effort is directed toward developing reservoir characterization methods to construct geological models from limited geophysical/geological data.

With regard to **monitoring and modeling of injected and leaked CO<sub>2</sub>**, efforts are directed to the development and deployment of monitoring methods that can address the very long time scales associated with permanent trapping of CO<sub>2</sub> in geological formations (which are much different than those utilized in CO<sub>2</sub>-based enhanced oil recovery, for example). We are therefore developing a geophysical monitoring technique using the noise signal of ground tremors. To address potential leakage from sub-seabed storage sites, we are also developing monitoring techniques using seafloor-based acoustic tomography and pH/pCO<sub>2</sub> sensors mounted on an autonomous underwater vehicle (AUV) as well as on a remotely-operated underwater vehicle (ROV). Finally, since the aquifer water in many Japanese geological formations has low salinity, the dissolution rate, as well as chemical reaction rates, of injected CO<sub>2</sub> are being studied for successful prediction of CO<sub>2</sub> dispersion.

## Significant Publications

### *Development of detection and monitoring techniques of CO<sub>2</sub> leakage from seafloor in sub-seabed CO<sub>2</sub> storage*

K. Shitashima, Y. Maeda and T. Ohsumi  
Applied Geochemistry, 30, 114-124, 2013

This paper outlines the development of several instruments to observe the leaked CO<sub>2</sub> behavior in sea water, and testing and confirmation of their performance through a large number of in situ experiments in the open oceans. In addition, this paper proposes detection and monitoring strategies for CO<sub>2</sub> leakage from the seafloor in sub-seabed Carbon Capture and Storage (CCS) for the first time worldwide. Development of monitoring methods for leaked CO<sub>2</sub> is one of the main objectives of the I<sup>2</sup>CNER CO<sub>2</sub> Storage Research Division. These techniques can be applied to CO<sub>2</sub> injection experiments and/or natural analogue studies of hydrothermal systems to obtain data for understanding of the environmental impact of leaked CO<sub>2</sub>. These techniques contribute to increasing the public understanding of issues related to near-shore/off-shore sub-seabed CCS.

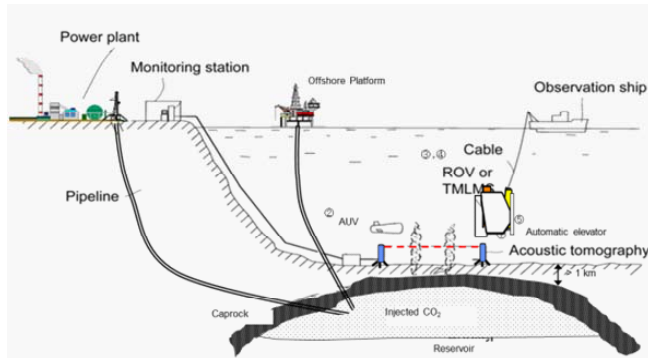
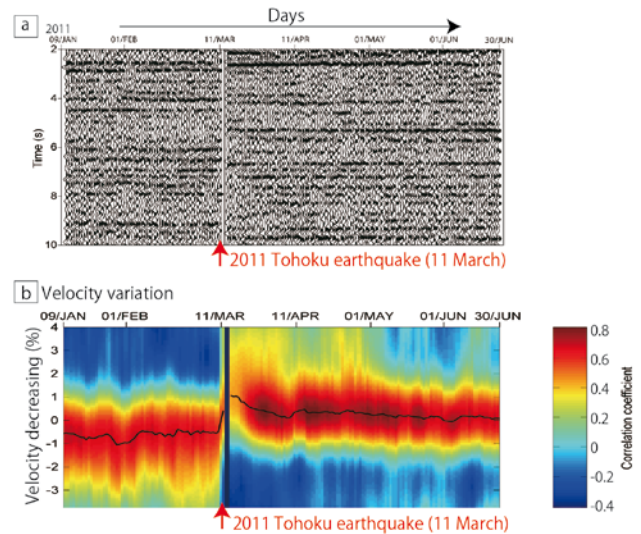


Fig. 1. Strategy for detection and monitoring of CO<sub>2</sub> leakage in sub-seabed CCS.

### *Monitoring seismic velocity change caused by the 2011 Tohoku-oki earthquake using ambient noise records*

S. Minato, T. Tsuji, S. Ohmi and T. Matsuoka  
Geophysical Research Letters, 39(9), L09309, 2012

This paper describes the development of a monitoring method to extract variation of seismic velocity using ambient noise. Development of monitoring methods for injected CO<sub>2</sub> is one of the main objectives of the I<sup>2</sup>CNER CO<sub>2</sub> Storage Research Division. Since the presented method constructs virtual signals from noise, we can continuously monitor the reservoir using only passive seismometer data. The low cost of this approach makes it particularly attractive for long-term monitoring in CCS projects. When we applied this method to the 2011 Tohoku earthquake, we successfully monitored the dynamic change of subsurface crustal stress. This method has the potential to predict aftershock distribution, because we can map the stress heterogeneity after the main shock. We further applied this method to the fluid injection experiment and successfully extracted the injected fluid distribution.



[a] Time-variation of virtual seismic traces. The reflection signal should be the same for horizontal direction, if no change was occurred beneath the seismometer. At the 2011 Tohoku earthquake, however, the seismic trace was significantly changed (red arrow). In CCS projects, the seismic traces are also changed, because the injected CO<sub>2</sub> changes subsurface conditions as in the case of the earthquake.

[b] Variation of P-wave velocity estimated from seismic traces displayed in panel (a). The P-wave velocity beneath the seismometer was decreased ~2% at the Tohoku earthquake. Even in CCS projects, P-wave velocity is also decreased due to the injected CO<sub>2</sub>. We can estimate CO<sub>2</sub> saturation within reservoir from the degree of velocity decreasing.

## Relationship of significant publications to the targets and milestones of the Division's roadmap

Development of monitoring methods for injected and leaked CO<sub>2</sub> is one of the main objectives of the ICNER CO<sub>2</sub> Storage Research Division. The work of Shitashima et al. (2012) outlines the development of several instruments to observe the leaked CO<sub>2</sub> behavior in sea water, and testing and confirmation of their performance through a large number of in situ experiments in the open oceans. In addition, this paper proposes detection and monitoring strategies for CO<sub>2</sub> leakage from the seafloor in sub-seabed CCS for the first time. These

techniques contribute to increasing the public understanding of issues related to near-shore/off-shore sub-seabed CCS. The work of Minato et al. (2012) develops a monitoring method to extract the variation of subsurface structures as well as seismic velocity, using ambient noise. Since the presented method constructs virtual signals from noise, we can continuously monitor injected CO<sub>2</sub> within the reservoir using only passive seismometer data.

## Selected Publications

Ishitsuka, K., Tsuji, T. and Matsuoka, T. (2012), Detection and mapping of soil liquefaction in the 2011 Tohoku earthquake using SAR interferometry, *Earth, Planets and Space*, 64 (12), 1267-1276

Ito, Y., Hino, R., Kido, M., Fujimoto, M., Osada, Y., Inazu, D., Ohta, Y., Iinuma, T., Ohzono, M., Miura, S., Mishina, M., Suzuki, K., Tsuji, T. and Ashi, J. (2013), Episodic slow slip events in the Japan subduction zone before the 2011 Tohoku-Oki earthquake, *Tectonophysics*, 600, 14-26

Jiang, F. and Hu, C. (2012), Application of Lattice Boltzmann Method for Simulation of Turbulent Diffusion from a CO<sub>2</sub> Lake in Deep Ocean, *Journal of Novel Carbon Resource Sciences*, 5, 10-18

Khakim, M. Y. N., Tsuji, T. and Matsuoka, T. (2012), Geomechanical Modeling for InSAR-derived surface deformation at steam-injection oil sand fields, *Journal of Petroleum Science and Engineering*, 96-97, 152-161

Minato, S., Tsuji, T., Matsuoka, T. and Obana, K. (2012), Crosscorrelation of Earthquake Data Using Stationary Phase Evaluation: Insight into Reflection Structures of Oceanic Crust Surface in the Nankai Trough, *International Journal of Geophysics*, 2012, 101545

Minato, S., Tsuji, T., Ohmi, S. and Matsuoka, T. (2012), Monitoring seismic velocity change caused by the 2011 Tohoku-oki earthquake using ambient noise records, *Geophysical Research Letters*, 39 (9), L09309

Shitashima, K., Maeda, Y. and Ohsumi, T. (2013), Development of detection and monitoring techniques of CO<sub>2</sub> leakage from seafloor in sub-seabed CO<sub>2</sub> storage, *Applied Geochemistry*, 30, 114-124

Tsuji, T., Johansen, T., Ruud, B., Ikeda, T. and Matsuoka, T. (2012), Surface-wave analysis for identifying unfrozen zones in glacial sediments, *Geophysics*, 77(3), EN17-EN27



# ENERGY ANALYSIS

## Executive Summary

The goals of the Energy Analysis Research Division (EAD) are to ensure that IFCNER research is relevant to future low carbon or carbon-neutral energy systems for Japan, to ensure that IFCNER research is informed of all relevant current and future energy options, and to take a lead role in defining an IFCNER Vision and Roadmap for a carbon-neutral energy society for Japan.

In order to help define the vision, the EAD will identify the challenges and technologies that can lead to a carbon-neutral energy society for Japan. The EAD will provide guidance to the IFCNER research divisions to help ensure their efforts are relevant with appropriate objectives and targets. It will also provide guidance as to other technologies not within the IFCNER research portfolio as possible additions to IFCNER research efforts.

In addition to these goals, the EAD will study potential Japan and international energy policy implications. Utilizing a system analysis approach, based on expertise inside and outside the division, the EAD will conduct original research in both natural and social science fields.

EAD analyses will include potential energy use and greenhouse gas (GHG) emissions as well as economic, social, and national security aspects of technologies and energy pathways. Target technologies will be analyzed on a Cradle-to-Grave basis where activities, costs, and energy flows are tracked throughout the life cycles of energy source and technology infrastructure.

The EAD made significant progress this year in three areas:

- Initial study of technology options for a low carbon energy infrastructure for Japan in 2050. This is leading to a Vision for Japan's energy future.
- Improvements and use of the model for energy technology systems for quantification of the potential GHG and energy use reductions in Japan through the use of new low carbon energy technologies.
- An initial roadmap of IFCNER's research projects including timelines with milestones as well as support to the research divisions to help establish clear objectives and targets.

## *Technology Options for a Low Carbon and Carbon-neutral Energy Society in Japan*

The initial study of potential low carbon energy futures for Japan began with examining the current technologies, energy demand and supply, and carbon dioxide emissions associated with each of the major energy consuming sectors. The energy use in 2050 was then projected based on government projections for population and GDP growth. Then each sector was examined relative to the potential use of low carbon emission and more energy efficient technologies. The present perceptions from this initial work can be summarized as follows:

- Energy efficiency improvements on the demand side such as in manufacturing processes, appliances, lighter vehicles, lighting, insulation, a smart grid, and elsewhere can be significant in reducing carbon emissions.
- Electricity generation accounts for 46% of carbon dioxide emissions in Japan and should be a key focus for low carbon emission technologies. The future use of renewable energy resources in Japan (hydroelectric, wind, solar, geothermal, and biomass) and nuclear energy could be significant. The use of fossil fuels in combination with advanced more energy efficient technologies and carbon capture and sequestration (CCS) can also be an important part of the path to low carbon emission power production. Such use of fossil fuels that also permits adjustable power output along with electricity storage would enable use of significant amounts of intermittent wind and solar energy. The I<sup>2</sup>CNER research on organic solar cells, hydrogen production, large-scale solid oxide fuel cells, and CCS can be key enablers for this sector to achieve low carbon emissions.
- The industry sector (excluding electricity use) accounts for 23% of carbon dioxide emissions. It is the need for heat that drives the carbon emissions in this sector. New chemistry technology such as that being researched in the I<sup>2</sup>CNER material transformation division and other process technology developments could reduce the energy requirements. Some of the same advanced, more energy efficient, fossil fuel based energy technology and CCS being developed for electricity production could also enable low carbon emission heat for the industrial sector.
- The transportation sector accounts for 21% of GHG emissions and should also be an important focus for low carbon emissions. There are a number of attractive low carbon technologies being developed and improved for transportation. These are focused on vehicle transportation, which accounts for the vast majority of the carbon emissions. The most promising new vehicle technologies are hybrid electric vehicles (HEV), plug-in hybrid electric vehicles (PHEV), battery electric vehicles (BEV), and fuel cell vehicles (FCV). The HEV could have very low carbon emissions if it used biofuel. PHEV and BEV technology requires an electricity grid with very low carbon emissions to be really attractive. There are some concerns with BEV technology relative to vehicle range, battery performance and cost. The FCV would be an excellent choice as long

as there are sufficient resources for low carbon emission production of hydrogen and refueling infrastructure issues during the transition are addressed. I<sup>2</sup>CNER research on polymer electrolyte fuel cells and low carbon hydrogen production technologies can play important roles for low carbon emission vehicles.

- Biofuels could play a very significant role for a low carbon energy future for Japan. They can replace fossil fuels in both current and advanced more efficient energy technologies. While Japan does not appear to have significant biomass resources, importing biofuels can be a topic to be examined.

There are many possible low carbon emission energy futures for Japan. The exact mix of technologies and fuels will depend greatly on the ultimate cost and performance achieved by the promising technologies being researched, the renewable and CCS resource capacity that can be tapped by Japan, and the social acceptance of technology options.

## *A Model Framework for Assessing Energy Technology Systems*

It is necessary to develop a set of models for energy flows in Japan to evaluate the contributions of potential energy technologies to the realization of a low-carbon or carbon-neutral energy society quantitatively. We therefore adopted as a first step a model framework consisting of the demand-side energy flow model and the centralized power supply system model.

The demand-side energy flow model was developed on the basis of the comprehensive energy statistics of Japan supplemented by other statistical data as necessary. We implemented the model so that it could evaluate the contributions of demand-side technologies through the time horizon of year 2010 to 2050. Examples of demand-side technology impacts are efficiency improvement in energy appliances, residential photovoltaic cell and solar heating, cogeneration systems, insulation efficiency improvement, electrification (kitchen, boiler, and heating), membranes for distillation processes, low-temperature heat recovery, and future vehicles. Note that economic and social scenarios such as population decrease and demand increase associated with economic growth can be set as the model boundary. We can set input scenario parameters related with each technology option (efficiency, penetration ratio, etc.) to obtain the overall change of demand in Japanese society. Estimated power demand data are input to the centralized power supply system model.

The centralized power supply system model is developed on the basis of the traditional power generation dispatch model to optimize power generation from the Japanese centralized grid for the target period. Our model optimizes the centralized grid for minimum cost throughout year 2010 to 2050. The model

incorporates nuclear, thermal combustion (LNG, coal and oil), hydro, pumped hydro, geothermal, photovoltaic, wind, and other potential energy technology options. We collected reference data from literature and published databases.

Preliminary analyses have been conducted to check the validity of the model algorithm using a set of tentative input data. The model is now ready to quantitatively study potential carbon emission and energy reductions scenarios for present and near future technologies.

### Draft Roadmap

In collaboration with all research divisions in I<sup>2</sup>CNER, the EAD has come up with an initial vision and roadmap as illustrated in Fig. 1. Detailed draft timelines with key targets and milestones have also been generated with each I<sup>2</sup>CNER research division.

	Short-Term	2020	Mid-Term	2030	Long-Term	2050	Distant Future
<b>Technology</b>		<ul style="list-style-type: none"> <li>- Commercialization of FCV</li> <li>- Use of Hydrogen Refueling Station</li> <li>- Popularization of Residential PEFC &amp; SOFC</li> <li>- Popularization of Solar Power &amp; On Shore Wind Farm</li> <li>- Energy Efficient Technologies</li> </ul>	<ul style="list-style-type: none"> <li>- Popularization of Low Cost Hydrogen Refueling Station</li> <li>- High Performance Li Battery</li> <li>- Large Scale Battery</li> <li>- Advanced Solar Panel</li> <li>- Popularization of Off Shore Wind Farm</li> <li>- Advanced Residential PEFC &amp; SOFC</li> <li>- Non Incandescent/Fluorescent light</li> <li>- Demonstration of CCS</li> </ul>	<ul style="list-style-type: none"> <li>- Advanced PWR &amp; BWR ??</li> <li>- Commercialization of CCS</li> <li>- Advanced Battery</li> <li>- Popularization of FCV</li> <li>- Next Advanced Solar Panel</li> <li>- Complete Smart Network</li> <li>- Advanced Biomass to Liquid Fuels</li> <li>- Practice of Triple Combined Cycle for Power Plant</li> <li>- Many Geothermal Plants</li> </ul>	<ul style="list-style-type: none"> <li>- Fast Breeder Reactor ??</li> <li>- Solar Hydrogen Production</li> <li>- Popularization of CCS</li> <li>- Introduction of IGFC</li> <li>- Fuels from CO<sub>2</sub></li> </ul>	<ul style="list-style-type: none"> <li>- Nuclear Fusion ???</li> <li>- Carbon Neutral Society</li> </ul>	
<b>Research Area</b>							
Hydrogen Production		- Organic Solar Cell	- OLEDs	- Steam Electrolysis		- Photo Catalytic Water Splitting	
Hydrogen Storage		- High performance MH	- Novel MH (Low Cost)	- Flexible shape MH tank			
Hydrogen Materials Compatibility		- Identification of degradation mechanism(s)	- Low-cost alloys	- High Pressure Registant Materials			
Thermal Science and Engineering		- TP/HMT of CO <sub>2</sub>	- TP/HMT of New Refrigerants	- Waste heat refrigeration	- Non-Freon refrigeration	- Biomimetic use of CO <sub>2</sub> for H <sub>2</sub> and CH <sub>4</sub> production (chlorella algae)	
Fuel Cells		- Meso-porous carbon	- Carbon Free	- High-active cathode electrode (PEFC)			
Catalytic Materials Transformations		- High Temperature / Pressure SOFC	- Metal Oxide Catalyst		- Asymmetric catalysis	- Biomimetics (Artificial photosynthesis)	- CO <sub>2</sub> utilization chemicals
CO <sub>2</sub> Capture & Utilization		- Ceramic Membrane: Post-combustion	- Polymer Membrane: Pre-combustion				
CO <sub>2</sub> Storage		- Reliable and Realistic Monitoring / Modeling	- Decentralized engineering systems				

TP =Thermophysical propaties, HMT=Heat and Mass Transfer, OLED=Organic light emitting diode

Fig. 1. I<sup>2</sup>CNER Draft Vision and Research Timeline



## *Future Directions*

The EAD's future research efforts are summarized as follows:

- Continue to work with the research divisions to help ensure their projects are relevant to a low carbon emission energy infrastructure for Japan's future and that they have appropriate performance and economic targets. This will include system modeling and analysis as appropriate.
- Analyzing and modeling I<sup>2</sup>CNER technologies so as to incorporate them into the present model framework together with competing technologies.
- Quantifying the potential contribution of I<sup>2</sup>CNER technologies to reduce carbon emissions and energy use in Japan by using the energy technologies systems model and other analytical tools that will be developed by the EAD.
- Develop an I<sup>2</sup>CNER Vision for a low carbon emission energy infrastructure for Japan through the use of the technology options study, ETSS model potential scenarios, and other information and tools.
- Define one or more national security metrics and incorporate them into EAD analyses.
- Development of a computer-based database system that will include the data required to quantify the cost, energy use, and GHG emissions for the current energy pathways in use in Japan. Extend this to include I<sup>2</sup>CNER and other energy technologies being researched and developed.
- Analyze and model the potential energy pathways that could utilize the I<sup>2</sup>CNER research efforts, stressing analysis on vehicle system.
- Conduct social science research to assess the social acceptability in Japan of key technologies and pathways that can reduce carbon emissions and characterize social aspects of these technologies. This can help inform the public and increase public awareness of these new technologies.
- Study of the penetration process of energy technologies based on social choice theory.

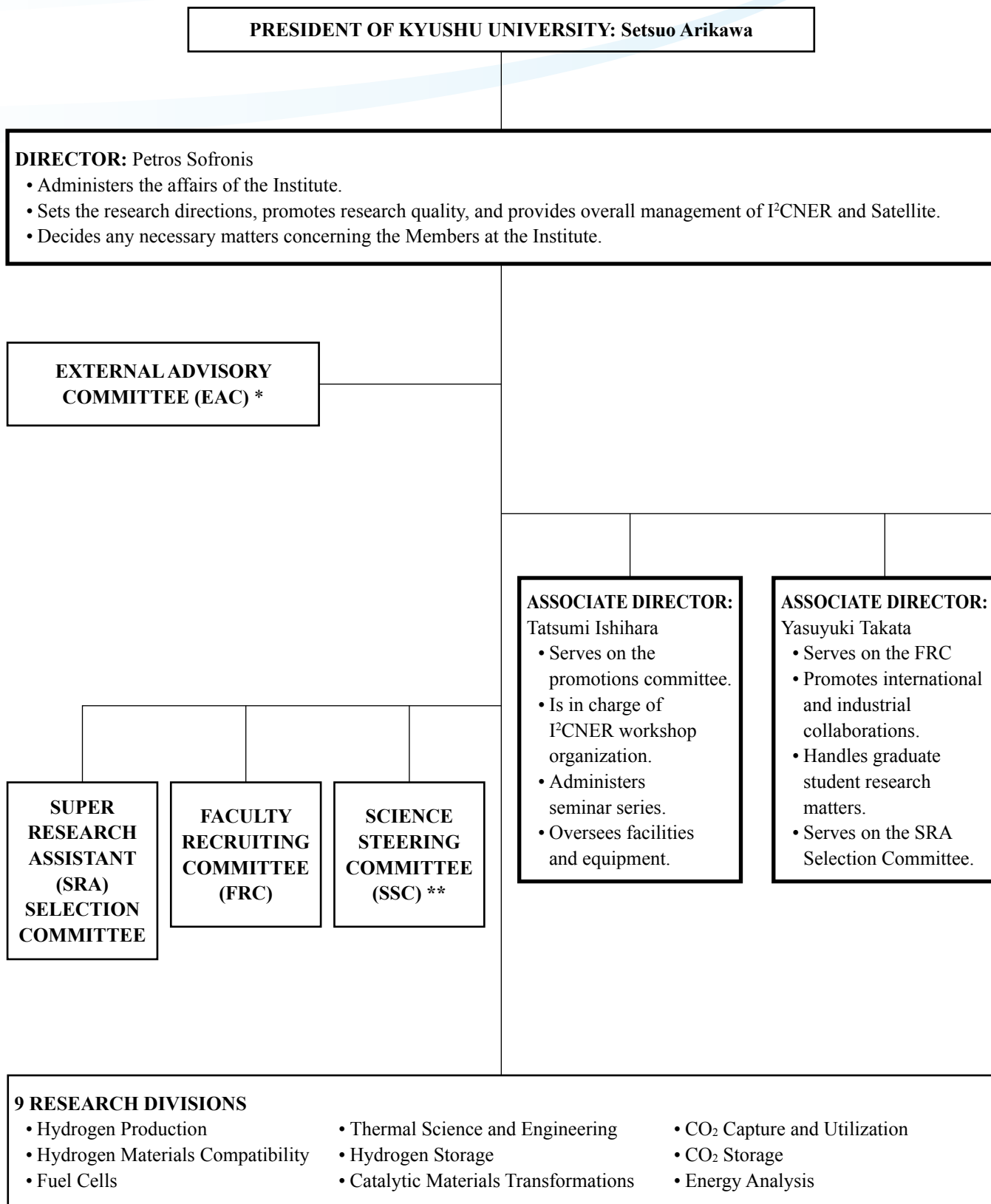
## **Selected Publications**

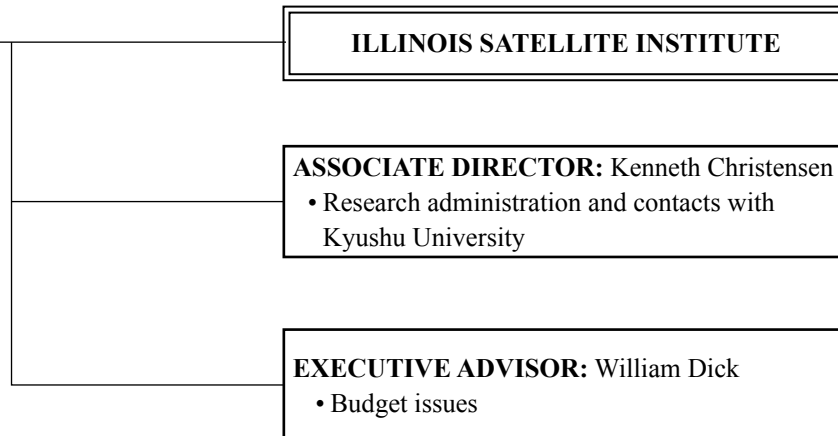
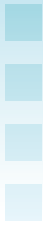
Ishimoto, T. and Koyama, M. (2012), Theoretical Study on Solubility from Pt Electrocatalyst and Reactivity in Electrolyte Environment of Pt Complex in PEFC, *International Journal of Electrochemistry*, 318461

Ishimoto, T. and Koyama, M. (2012), A review of molecular-level mechanism of membrane degradation in the polymer electrolyte fuel cell, *Membranes*, 2 (3), 395-414

# Researchers & Administrative Personnel

## I<sup>2</sup>CNER Organizational Structure





**ADMINISTRATIVE OFFICE**

**ADMINISTRATIVE DIRECTOR:** Kazuo Funaki

- Administers the affairs of the office to facilitate the operations of the Institute.
- Provides administrative support to the research personnel of I<sup>2</sup>CNER.

**\* External Advisory Committee (EAC)**

The External Advisory Committee (EAC) makes recommendations on the current status of the Institute and its future directions, and provides the Director with a written report detailing their findings and recommendations.

The EAC members are national and international leaders who are identified and selected by the Director.

- Prof. Ronald J. Adrian (Chair), Arizona State University, USA
- Dr. Deborah Myers (Vice-Chair), Argonne National Laboratory, USA
- Dr. Robert J. Finley, Illinois State Geological Survey, USA
- Prof. Reiner Kirchheim, University of Göttingen, Germany
- Prof. Robert McMeeking, University of California, USA
- Dr. Kevin Ott, Los Alamos National Laboratory, USA
- Prof. Tetsuo Shoji, Tohoku University, Japan
- Dr. George Thomas, Retired EERE office of US DOE and Sandia National Laboratories, USA (Advisory member)

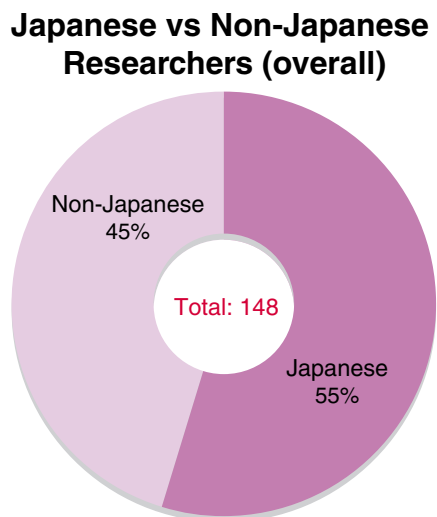
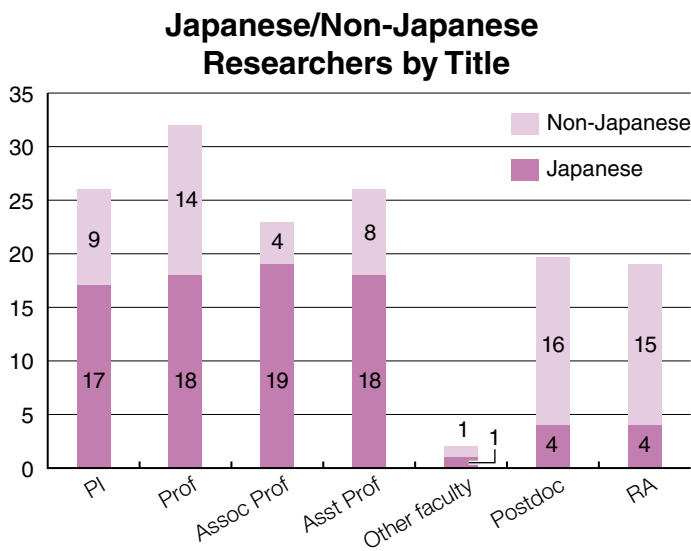
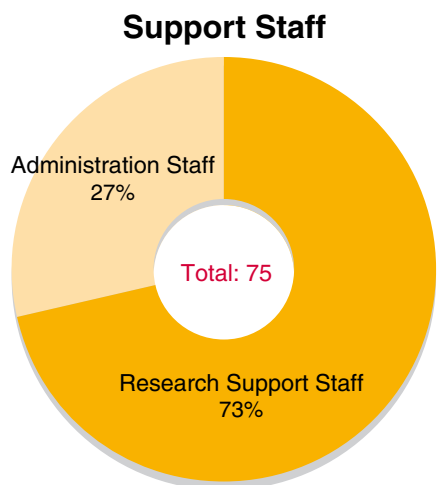
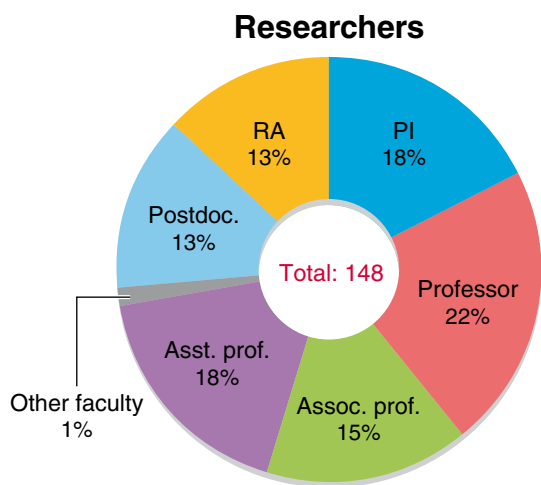
**\*\* Science Steering Committee (SSC)**

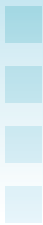
The Science Steering Committee (SSC) is chaired by the Director, and its members are the two Associate Directors and the lead PIs of the thematic research areas (divisions). The SSC is the body that reviews and decides on all matters of the Institute, e.g. planning and operation of research activities, budget implementation, international collaborations, and outreach.

# I<sup>2</sup>CNER Personnel

(as of September 1, 2013)

WPI Title	Total (*Non-Japanese)	Kyushu	Satellite
Principal Investigator (PI)	26 (9)	24	2
Professor	32 (14)	26	6
Associate Professor	23 (4)	22	1
Assistant Professor	26 (8)	24	2
Other faculty	2 (1)	1	1
Postdoctoral researcher (Postdoc.)	20 (16)	18	2
Research Assistant (RA)	19 (15)	6	13
<b>Sub Total</b>	<b>148 (67)</b>	<b>121</b>	<b>27</b>
Research Support Staff	55 (19)	55	0
Administration Staff	20 (2)	18	2
<b>Total</b>	<b>223 (88)</b>	<b>194</b>	<b>29</b>





### *Administration*

#### **Director**

Prof. Petros Sofronis

#### **Associate Directors**

Prof. Tatsumi Ishihara

Prof. Yasuyuki Takata

Prof. Kenneth Christensen

### *WPI Principal Investigators*

#### **Hydrogen Production Research Division**

Prof. Tatsumi Ishihara

Prof. Chihaya Adachi

Prof. Atsushi Takahara

Prof. Ken Sakai

Prof. John Kilner, *Imperial College London*

#### **Hydrogen Materials Compatibility Research Division**

Dr. Brian Somerday, *Sandia National Laboratories*

Prof. Petros Sofronis

Prof. Joichi Sugimura

Prof. Setsuo Takaki

Prof. Reiner Kirchheim, *University of Göttingen*

Prof. Ian Robertson, *University of Wisconsin-Madison*

#### **Fuel Cells Research Division**

Prof. Kazunari Sasaki

Prof. Naotoshi Nakashima

Prof. Harry Tuller, *Massachusetts Institute of Technology (MIT)*

Prof. Andrew Gewirth,

*University of Illinois at Urbana-Champaign*

#### **Thermal Science and Engineering Research Division**

Prof. Yasuyuki Takata

Prof. Xing Zhang, *Tsinghua University*

#### **Hydrogen Storage Research Division**

Prof. Etsuo Akiba

Prof. Zenji Horita

#### **Catalytic Materials Transformations Research Division**

Prof. Seiji Ogo

Prof. Tsutomu Katsuki

Assoc. Prof. Miho Yamauchi

#### **CO<sub>2</sub> Capture and Utilization Research Division**

Assoc. Prof. Shigenori Fujikawa

Prof. Katsuki Kusakabe, *Sojo University*

#### **CO<sub>2</sub> Storage Research Division**

Assoc. Prof. Takeshi Tsuji

Prof. Kenneth Christensen,

*University of Illinois at Urbana-Champaign*

### *PCNER Faculty & Postdoctoral Researchers*

#### **Hydrogen Production Research Division**

Asst. Prof. Aleksandar Staykov

Asst. Prof. Motonori Watanabe

Dr. John Druce

Dr. Limin Guo

Dr. Le Zhang

Dr. Wei Ma

Dr. Myo Minn

Dr. Alexander Parent

#### **Hydrogen Materials Compatibility Research Division**

Dr. Arnaud Macadre

#### **Fuel Cells Research Division**

Asst. Prof. Masamichi Nishihara

Asst. Prof. Stephen Lyth

Asst. Prof. Sean Bishop

Dr. Yuya Tachikawa

Dr. Mohamed Berber

Dr. Nicola Perry

#### **Hydrogen Storage Research Division**

Asst. Prof. Junko Matsuda

Asst. Prof. Huaiyu Shao

Dr. Hoda Sadat Emami Meibody

Dr. Kaveh Edalati

#### **Catalytic Materials Transformations Research Division**

Assoc. Prof. Ki-Seok Yoon

Asst. Prof. Masaaki Sadakiyo

Dr. Kim Chungsik

Dr. Takeshi Matsumoto

Dr. Masaru Konno

#### **CO<sub>2</sub> Capture and Utilization Research Division**

Assoc. Prof. Ikuo Taniguchi

#### **CO<sub>2</sub> Storage Research Division**

Assoc. Prof. Kiminori Shitashima

Asst. Prof. Keigo Kitamura

Dr. Fei Jiang

#### **Energy Analysis Research Division**

Prof. Kuniaki Honda

Prof. Kenshi Itaoka

Dr. Seiichiro Kimura



*Satellite Faculty & Postdoctoral Researchers*

**Hydrogen Production Research Division**

Prof. Angus Rockett  
Asst. Prof. Elif Ertekin  
Asst. Prof. Lane Martin

**Hydrogen Materials Compatibility Research Division**

Dr. Mohsen Dadfarnia

**Thermal Science and Engineering Research Division**

Prof. David Cahill

**Catalytic Materials Transformations Research Division**

Prof. Thomas Rauchfuss

**CO<sub>2</sub> Capture and Utilization Research Division**

Prof. Paul Kenis  
Assoc. Prof. Dimitrios Kyritsis

**CO<sub>2</sub> Storage Research Division**

Prof. Arne Pearlstein  
Dr. Robert Finley

**Energy Analysis Research Division**

Prof. James Stubbins  
Dr. Xuping Li

*WPI Professors & WPI Visiting Professors*

**Hydrogen Materials Compatibility Research Division**

Prof. Nikolaos Aravas, *University of Thessaly*  
Prof. Robert Ritchie, *University of California, Berkeley*  
Dr. Chao-Nan Xu,  
*National Institute of Advanced Industrial Science and  
Technology (AIST)*  
Prof. Kanao Fukuda, *Universiti Teknologi Malaysia*

**Fuel Cells Research Division**

Prof. Ludwig Gauckler,  
*Swiss Federal Institute of Technology Zürich (ETH)*  
Dr. Toyoki Kunitake,  
*Kitakyushu Foundation for the Advancement of Industry  
Science and Technology*

**Hydrogen Storage Research Division**

Prof. Ping Chen, *Dalian Institute of Chemical Physics*  
Prof. Louis Schlapbach,  
*Swiss Federal Institute of Technology Zürich (ETH)*

**CO<sub>2</sub> Storage Research Division**

Dr. Ziqui Xue,  
*Research Institute of Innovative Technology for the Earth  
(RITE)*

**Energy Analysis Research Division**

Dr. Mark Paster,  
*former employee at U.S. Department of Energy*

# I<sup>2</sup>CNER's Network of International Collaborations

One of the cornerstones of the I<sup>2</sup>CNER vision is fusion research—the concept that in order to achieve a carbon-neutral society, numerous scientists, disciplines, and institutions must all come together and work collaboratively. In this spirit, I<sup>2</sup>CNER has developed many significant international relationships in order to bring together the best scientists from around the world who can work together with us to achieve our mission.

- Imperial College London (UK)
- Sandia National Laboratories (USA)
- University of Thessaly (Greece)
- University of California at Berkeley (USA)
- Malaysia-Japan International Institute of Technology, Universiti Teknologi Malaysia (Malaysia)
- University of Göttingen (Germany)
- Massachusetts Institute of Technology (USA)
- Swiss Federal Institute of Technology Zürich (ETH) (Switzerland)
- Tsinghua University (China)
- Dalian Institute of Chemical Physics (China)
- University of Bergen (Norway)
- Bandung Institute of Technology (Indonesia)
- Pacific Northwest National Laboratory (USA)



# International Engagement

## Visitors (I<sup>2</sup>CNER Principal Investigators from Overseas Collaborating Institutions)

### *Hydrogen Production*

Name	Affiliation
Angus Rockett	Prof., University of Illinois at Urbana-Champaign (USA)
Elif Ertekin	Asst. Prof., University of Illinois at Urbana-Champaign (USA)
John Kilner	Prof., Imperial College London (UK)

### *Hydrogen Materials Compatibility*

Name	Affiliation
Ian Robertson	Prof., University of Wisconsin-Madison (USA)
Brian Somerday	Dr., Sandia National Laboratories (USA)
Reiner Kirchheim	Prof., University of Göttingen (Germany)

### *Fuel Cells*

Name	Affiliation
Andrew Gewirth	Prof., University of Illinois at Urbana-Champaign (USA)
Harry Tuller	Prof., Massachusetts Institute of Technology (USA)
Ludwig Gaukler	Prof., Swiss Federal Institute of Technology Zürich (Switzerland)

### *Thermal Science and Engineering*

Name	Affiliation
Xing Zhang	Prof., Tsinghua University (China)
Louis Schlapbach	Prof. Emeritus, Swiss Federal Institute of Technology Zürich (Switzerland)

### *Hydrogen Storage*

Name	Affiliation
Ping Chen	Prof., Dalian Institute of Chemical Physics (China)

### *Catalytic Materials Transformations*

Name	Affiliation
Thomas Rauchfuss	Prof., University of Illinois at Urbana-Champaign (USA)

### *CO<sub>2</sub> Capture and Utilization*

Name	Affiliation
Paul Kenis	Prof., University of Illinois at Urbana-Champaign (USA)
Dimitrios Kyritsis	Assoc. Prof., University of Illinois at Urbana-Champaign (USA)

### *CO<sub>2</sub> Storage*

Name	Affiliation
Kenneth Christensen	Prof., University of Illinois at Urbana-Champaign (USA)
Arne Pearlstein	Prof., University of Illinois at Urbana-Champaign (USA)
Chen-Tung Arthur-Chen	Prof., National Sun Yat-sen University (Taiwan)

### *Energy Analysis*

Name	Affiliation
James Stubbins	Prof., University of Illinois at Urbana-Champaign (USA)



## Visitors (Researchers from Overseas Collaborating Institutions)

### *Hydrogen Production*

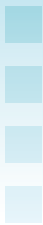
Name	Affiliation
Bruno Ameduri	Dr., National Center of Scientific Research (France)
José Santiso	Dr., Research Centre for Nanoscience and Nanotechnology (Spain)
Richard Glass	Prof., University of Arizona (USA)
Hung Jue Sue	Prof., Texas A&M University (USA)
Hidde Brongersma	Prof., Calipso B.V., the Netherlands (Netherlands)
Licheng Sun	Prof., Dalian University of Technology/KTH (China)
Sumittra Charojrochkul	Dr., National Metal and Materials Technology Center (Thailand)

### *Hydrogen Materials Compatibility*

Name	Affiliation
Darrell Socie	Prof., University of Illinois at Urbana-Champaign (USA)
Kelly Nygren	Satellite Ph.D Student, University of Illinois at Urbana-Champaign (USA)
Megan Emigh	Satellite Ph.D Student, University of Illinois at Urbana-Champaign (USA)
Kanao Fukuda	Prof., Universiti Teknologi Malaysia (Malaysia)
Antti Vaajoki	Research Scientist, VTT (Finland)
Paulo Ferreira	Asst. Prof., The University of Texas at Austin (USA)
Tsutomu Mori	Prof., University of Manchester (USA)
Monterey Gardiner	Dr., U.S. Department of Energy (USA)
Laurent Briottet	Dr., CEA/Grenoble, LITEN/DTBH/LCTA (France)
George Crabtree	Dr., Argonne National Laboratory (USA)
Jussi Solin	Principal Scientist, VTT (Finland)
Hannu Hännien	Prof., Aalto University School of Engineering (Finland)
Paolo Bortot	Dr., Tenaris-Dalmine (Italy)
Stefano Beretta	Prof., Politecnico di Milano (Italy)
Dilson S dos Santos	Prof., COPPE/UFRJ (Brazil)
Vigdis Olden	Dr., SINTEF (Norway)
Jesús Torbio	Prof., University of Salamanca (Spain)
Viktor Kharin	Prof., University of Salamanca (Spain)

### *Fuel Cells*

Name	Affiliation
Huei-Ru Jhong	Satellite Ph.D Student, University of Illinois at Urbana-Champaign (USA)
Edmund Tse	Satellite Ph.D Student, University of Illinois at Urbana-Champaign (USA)
Masaru Tsuchiya	Dr., SiEnergy Systems, LLC (USA)
Subhash Singhal	Dr., Pacific Northwest National Laboratory (USA)
Nigel Brandon	Prof., Imperial College London (UK)
Calvert Barclay	M. Phil. Student, University of the West Indies (Jamaica)



### *Thermal Science and Engineering*

Name	Affiliation
Weigang Ma	WPI Visiting Researcher, Tsinghua University (China)
Jiung Cho	Satellite Postdoc., University of Illinois at Urbana-Champaign (USA)
Jungho Kim	Prof., University of Maryland (USA)
Sang Yong Lee	Prof., Korea Advanced Institute of Science and Technology (Korea)
Sushanta Mitra	Prof., University of Alberta (Canada)
Srinivas Garimella	Prof., Georgia Institute of Technology (USA)

### *Hydrogen Storage*

Name	Affiliation
Tom Autrey	Dr., Pacific Northwest National Laboratory (USA)
Martin Dornheim	Prof., Nanotechnology, Helmholtz-Zentrum Geesthacht (Germany)

### *Catalytic Materials Transformations*

Name	Affiliation
Bruce Garrett	Dr., Pacific Northwest National Laboratory (USA)
Richard Tuenge	Prof., Portland Community College (USA)

### *CO<sub>2</sub> Capture and Utilization*

Name	Affiliation
Huei-Ru Jhong	Satellite Ph.D Student, University of Illinois at Urbana-Champaign (USA)
Peter McGrail	Dr., Pacific Northwest National Laboratory (USA)

### *CO<sub>2</sub> Storage*

Name	Affiliation
Rajat Saksena	Satellite Ph.D Student, University of Illinois at Urbana-Champaign (USA)
Jeremy Blackford	Dr., Plymouth Marine Laboratory (UK)
Jonathan Bull	Prof., NOC, University of Southampton (UK)
Henrik Stahl	Dr., Scottish Association for Marine Science (UK)

### *Energy Analysis*

Name	Affiliation
Mark Paster	WPI Visiting Prof.
Xuping Li	Satellite Postdoc., University of Illinois at Urbana-Champaign (USA)

# Selected Awards

Awardee	Award
Tatsumi Ishihara, John Kilner and Harry Tuller	Somiya Award 2012
Junji Hyodo	MRS oral presentation award
John Kilner	Institute of Materials, Minerals and Mining Platinum Award for “Outstanding contributions to materials science”
Chihaya Adachi	Outstanding achievement award from Japan Society of Organic Electroluminescence
Atsushi Takahara	The Society of Rheology, Japan Award
Yasuhiko Hirana, Yasuro Niidome, and Naotoshi Nakashima	The Bulletin of the Chemical Society of Japan Award Article
Harry Tuller	Helmholtz International Fellow Award from the Helmholtz Association of German Research Centers
Sean Bishop	Young Scientist Gold Award for an oral presentation at the International Union of Materials Research Societies - International Conference on Electronic Materials, Yokohama, Japan
Zenji Horita	The Japan Institute of Metals Distinguished Contribution Award
Seiji Ogo	The 30 <sup>th</sup> Chemical Society of Japan Award



Somiya Award 2012 awardees



Prizes shine at the entrance of the ICNER building

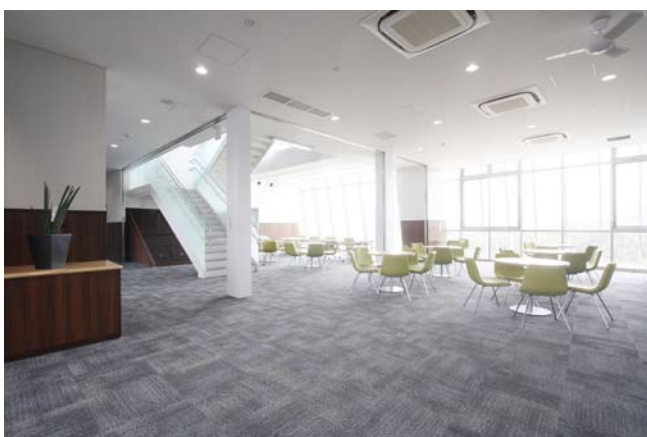
# The New I<sup>2</sup>CNER Building

Construction of the new building of the International Institute for Carbon-Neutral Energy Research (I<sup>2</sup>CNER) of Kyushu University was completed at the Ito campus in December 2012. This new I<sup>2</sup>CNER building, which is shared by I<sup>2</sup>CNER on the left-hand side and the Next-Generation Fuel Cell Research Center, Kyushu University on the right-hand side, provides an attractive research environment for top researchers from Japan and overseas to work together in pursuit of multi-disciplinary (fusion) research.

The overhead view of the new I<sup>2</sup>CNER building portrays the Keeling Curve\*, which rises over time. This curve was embedded in the structure of the building itself in order to intimate I<sup>2</sup>CNER's eventual contributions to the downward turn of this curves.



Left: I<sup>2</sup>CNER, Right: NEXT-FC



Lounge



Foyer

*\* In 1958, Charles David Keeling began taking daily measurements of the concentration of atmospheric carbon dioxide (CO<sub>2</sub>) at the Mauna Loa Observatory on the Big Island of Hawaii. Keeling's measurements were the first significant evidence of rapidly increasing carbon dioxide in the atmosphere.*



Left: NEXT-FC, Right: I<sup>2</sup>CNER

# Outreach Activities

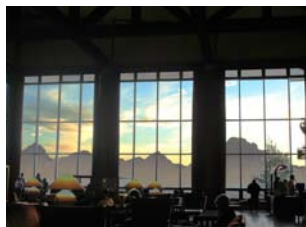
## Symposia and Workshops

*The 2012 International Hydrogen Conference  
September 9-12, 2012*



The 2012 International Hydrogen Conference was held at Jackson Lake Lodge in Moran, Wyoming, September 9-12, which was organized by Dr. Brian Somerday (Lead Principal Investigator of Hydrogen Materials Compatibility Research Division) and Director Petros Sofronis. Jackson Lake Lodge is located in the majestic Grand Teton National Park, overlooking the Grand Teton mountain range, and has been the venue for the last six conferences in the series. Previous conferences in this series were held in 1973, 1975, 1980, 1989, 1994, 2002, and 2008.

The conferences in this series have been the premier topical meetings on hydrogen effects in materials, as demonstrated by past attendance and extensive citations of the conference proceedings in technical literature. Since interest in developing hydrogen as a fuel is casting more attention on hydrogen-materials interactions, the continuation of this conference series was very timely.



The View from Jackson Lake Lodge

The 2012 Conference attracted the most prominent researchers on hydrogen and materials interactions from around the world for a four-day event in which they exchanged and debated ideas, presented new research, and formulated future research projects on hydrogen. On Sunday, September 9, the conference officially began with brief opening remarks from Dr. Brian Somerday. The technical program for Sunday evening included invited presentations from two of the most renowned researchers in the field, Professor Bill Gerberich, University of Minnesota, and Professor Reiner Kirchheim, University of Göttingen.



Asst. Prof. J. Matsuda and Prof. R. Kirchheim

Professor Gerberich provided a historical review of hydrogen interactions as well as proposed future opportunities. Professor Kirchheim discussed generally hydrogen-induced defect generation and enhanced mobility of defects by hydrogen, based on his recently developed novel

thermodynamic analysis called defactant concept. The program concluded with an invited presentation on materials issues in implementing a hydrogen infrastructure from Katie Randolph, project officer for the U.S. Department of Energy's Fuel Cell Technologies Program.

Each technical session of the conference featured invited presentations from an impressive group of scientists, including Jader Furtado (Air Liquide), Richard Gangloff (University of Virginia), Valentin Gavriljuk (G.V. Kurdyumov Institute for Metal Physics), Phil Irving (Cranfield University), Jorg Neugebauer (Max-Planck-Institut für Eisenforschung), Joichi Sugimura (Kyushu University), Neeraj Thirumalai (ExxonMobil), Kaneaki Tsuzaki (National Institute for Materials Research), and Kim Verbeke (Ghent University).



Opening Session

The Conference was attended by over 160 researchers, and included 55 oral presentations and 100 poster presentations. The presenters covered a wide area of subjects, including effects of hydrogen on deformation, wear, fatigue, and fracture, fracture mechanisms

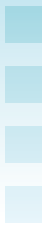


Japanese Participants



Poster Presentations

in hydrogen environments, hydrogen-deformation interactions, hydrogen dissolution, diffusion, and trapping in materials, hydrogen-induced phase transformations, life predictions of structures in hydrogen environments, hydrogen effects on polymers, hydrogen effects on tribo-interfaces, effects of hydrogen isotopes and helium on materials, and modeling of hydrogen-materials interactions, including finite element, atomistics, and first principles.



This year, the conference was co-organized by Dr. Brian Somerday, Division Lead Principal Investigator of the International Institute for Carbon-Neutral Energy Research (I<sup>2</sup>CNER) Hydrogen Structural Materials Division and materials scientist at Sandia National Laboratories, and Professor Petros Sofronis, Director of I<sup>2</sup>CNER and professor at the University of Illinois at Urbana-Champaign.



Director P. Sofronis and Dr. B. Somerday offer opening remarks

This year's conference was sponsored by: Air Liquide, the American Society of Mechanical Engineers (ASME), ExxonMobil, and I<sup>2</sup>CNER.

### *WPI Joint Symposium 2012 November 24, 2012*

On Saturday, November 24<sup>th</sup> 2012, the second All-WPI Research Center Joint Symposium titled "Inspiring Insights into Pioneering Scientific Research" was held at the Tsukuba International Congress Center. The response was overwhelmingly positive, with 663 participants, many of whom were high school students.



Tsukuba International Congress Center Auditorium

Last year, Kyushu University's International Institute for Carbon-Neutral Energy (I<sup>2</sup>CNER) hosted the first symposium. This year's symposium was organized by the International Center for Materials Nanoarchitectonics (MANA).

The day officially began with remarks from Mr. Kenichi Ichihara, Mayor of Tsukuba, and a keynote lecture presented by Toshio Kuroki, WPI Program Director, who sent a message to the young audience. This was followed by five WPI research center presenters who each introduced their center's research. They also expressed hopes and dreams for the young peoples' future.

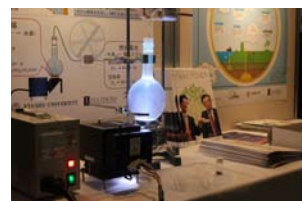


Prof. Tatsumi Ishihara

In addition, young participants had a chance to try challenging science quizzes while learning about science in a fun and humorous way.

I<sup>2</sup>CNER's Associate Director, Prof. Tatsumi Ishihara, gave a lecture with the theme of "Dream Artificial Photosynthesis; challenge to the creature." After reporting on the current energy situation of the world, he presented the latest research on the method of extracting hydrogen by water splitting with a photocatalyst.

The day concluded with an opportunity for the participants to view the booths that each center developed, and for the high school students to personally meet and engage with the WPI speakers and staff.

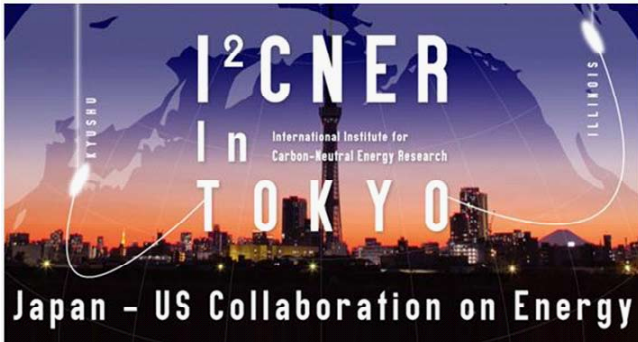


I<sup>2</sup>CNER's booth



Students visiting the I<sup>2</sup>CNER booth

*I<sup>2</sup>CNER in Tokyo Symposium  
December 7, 2012*



The symposium was attended by approximately 150 guests, including several international participants, as well as special guests Mr. Daisuke Yoshida, Director-General, Research Promotion Bureau, Ministry of Education, Culture, Sports, Science and Technology (MEXT), Dr. Toshio Kuroki, WPI Program Director, Ambassador John V. Roos, U.S. Embassy in Japan, and Setsuo Arikawa, Kyushu University President, who each gave opening remarks. Mr. Yoshida outlined how the WPI Program reflects and promotes the MEXT vision for education and research. Dr. Kuroki presented a general overview of the WPI Program from its inception in 2007 through current day, emphasizing that the WPI Program is a new initiative designed to cultivate the fusion of scientific disciplines as a new approach to discovery and to promote conversation amongst young researchers. Ambassador Roos stressed the importance of leveraging resources and scientific talent between the US and Japan to find 21<sup>st</sup> century energy solutions. In particular, the Ambassador suggested that educational exchange of young scientists between the two countries would make future scientific collaborations more productive.



Daisuke Yoshida  
Director-General, Research  
Promotion Bureau, MEXT



John V. Roos  
Ambassador Extraordinary and Plenipotentiary, the U.S. Embassy in Japan

During the keynote speech, I<sup>2</sup>CNER Director Petros Sofronis emphasized that I<sup>2</sup>CNER is an international collaboration between Japan and the U.S., based at Kyushu University with a satellite at the University of Illinois at Urbana-Champaign. I<sup>2</sup>CNER's mission is to contribute to the creation of a sustainable and



Director Petros Sofronis

environmentally-friendly society by conducting fundamental research for the advancement of low carbon emission and cost effective energy systems, and improvement of energy efficiency.

Session 1 featured three topical lectures, the first of which was given by Dr. Katsuhiko Hirose, Project General Manager, R&D Management Division, TOYOTA Motor Corporation. Dr. Hirose advised attendees that since the future of energy is unpredictable, innovation is the key to finding the solutions to energy problems. In fact, Dr. Hirose drew a comparison between the present day and the Stone Age, pointing out that the Stone Age didn't end because we ran out of stone, but because we found materials that were superior to stone. Lead Principal Investigator Kazunari Sasaki, Fuel Cells Research Division, I<sup>2</sup>CNER, Kyushu University, outlined the current status and the future research directions of I<sup>2</sup>CNER in the field of Fuel Cells. Specifically, Professor Sasaki explained how Kyushu University advances next generation fuel cell concepts such as durability, efficiency, cost reduction, and new materials. Satellite Associate Director Kenneth Christensen, I<sup>2</sup>CNER, University of Illinois at Urbana-Champaign, presented the ways in which I<sup>2</sup>CNER tackles the fundamental science that is needed to develop safe CO<sub>2</sub> storage technologies and monitor and predict the long-term behavior of safely stored CO<sub>2</sub>.

Session 2 featured an invited lecture given by Dr. Monterey Gardiner, Technology Development Manager, Office of Hydrogen, Fuel Cells and Infrastructure Technologies, U.S. Department of Energy. Dr. Gardiner spoke about the technology, economics, and infrastructure requirements underlying the introduction of fuel cell and hydrogen vehicles, and the commercialization of stationary fuel cells. He issued a grand challenge to the energy stakeholders in attendance to support and conduct research to enable technology for a carbon-neutral society, such as efficient energy storage, harmonization of safety codes and standards, and materials issues.

Following Sessions 1 and 2, a panel discussion was held, which involved open scientific debate between the lecturers and the audience. The panel discussion was moderated by WPI Visiting Professor Mark Paster, Energy Analysis Research Division, I<sup>2</sup>CNER, Kyushu University. Topics

covered in the panel discussion included the role of society/ individuals in energy conservation, infrastructure vs. commercialization of fuel cell vehicles (the chicken or the egg problem), safety of fuel cell technologies, dissemination of information to the public, and international regulation of emerging technologies in consideration of differing interests in developing countries.

In his closing remarks, Professor Nobuhide Kasagi, WPI Program Officer, stated that although the future of energy is uncertain and predictions are very difficult to make, we need to develop a scenario on how we can establish optimum energy solution pathways. Professor Kasagi also prompted the scientific community and I<sup>2</sup>CNER researchers in particular to try to challenge the unyielding problems involved in the realization of a carbon-neutral energy society. Professor Kasagi stressed the importance of fostering the US-Japan collaboration on research and development for energy and sustainability, suggesting that not only both countries, but also our “human-dominated planet” stand to gain from this relationship.

*I<sup>2</sup>CNER New Building Completion Ceremony & Annual Symposium 2013*  
January 29, 2013

*HYDROGENIUS & I<sup>2</sup>CNER Joint Research Symposium*  
January 28, 2013

*I<sup>2</sup>CNER International Workshop 2013, HYDROGENIUS & I<sup>2</sup>CNER Joint Research Symposium*  
January 31, 2013



On January 29, 2013, the I<sup>2</sup>CNER New Building Completion Ceremony was held at Kyushu University’s Ito Campus. The ceremony was attended by more than 200 people, including many international guests.



New I<sup>2</sup>CNER building inauguration

Welcome addresses were given by Setsuo Arikawa, President of Kyushu University, and Professor Petros Sofronis, Director of I<sup>2</sup>CNER. In his remarks, Director Sofronis warmly welcomed all the participants to the I<sup>2</sup>CNER New Building Completion Ceremony and expressed his sincere gratitude for their support of the Institute. Congratulatory addresses were given by special guests Dr. Hiroo Imura, Chairperson of WPI Program Committee, Mr. Koichi Morimoto, Deputy Director-General of the Research Promotion Bureau, Ministry of Education, Culture, Sports, Science and Technology (MEXT), Mr. Hiroshi Ogawa, Governor of Fukuoka Prefecture, Dr. Toshio Kuroki, WPI Program Director, Dr. Monterey R. Gardiner, Technology Development Manager, Office of Hydrogen, Fuel Cells and Infrastructure Technologies, U.S. Department of Energy, and Dr. Peter Schiffer, Vice Chancellor for Research at the University of Illinois at Urbana-Champaign.

After the congratulatory remarks, a ribbon-cutting ceremony was performed at the entrance of the I<sup>2</sup>CNER building.



Ribbon-cutting ceremony

Following the ribbon-cutting ceremony, all participants were led in a facility tour which was conducted by faculty and staff.

That afternoon, I<sup>2</sup>CNER hosted the Annual Symposium 2013 in I<sup>2</sup>CNER Hall. During his overview of I<sup>2</sup>CNER, Director Sofronis emphasized that the Institute is an international collaboration between Japan and the US, and that its mission is to contribute to the creation of a sustainable and environmentally-friendly society by conducting fundamental research for the advancement of low carbon emission and cost effective energy systems, and improvement of energy efficiency. He also stressed the high level of intellectual talent and rich resources that exist within I<sup>2</sup>CNER.



Director Petros Sofronis



The first session of the Annual Symposium 2013 featured two keynote lectures, the first of which was given by Dr. Eiichi Harada, Associate Officer and Deputy General Manager of the Corporate Technology Planning Center of Kawasaki Heavy Industries, LTD. Dr. Harada pointed out the need to promote renewables and fossil fuels with efficient CCS (Carbon Capture and Storage) in order to create an energy system with zero emissions. He acknowledged that hydrogen can be produced not only by renewable energy, via electrolysis, but also from fossil fuel. He also stated that hydrogen has considerable potential as a zero emission energy source. Dr. George Crabtree, Director of the Joint Center for Energy Storage Research (JCESR), Argonne



Keynote lecturer, Dr. George Crabtree



Keynote lecturer, Dr. Eiichi Harada

National Laboratory, and recent winner of a US Department of Energy (DOE) Energy Innovation Hub, emphasized the roles of electricity, chemical fuels, and photons as sustainable and fungible energy carriers. He proposed that energy is undergoing a historic transition, and thus the agendas for scientific discovery and technology innovation needed to achieve a vibrant, interactive, and rapidly advancing global society over the next fifty years will be examined from the perspectives of societal needs, international relationships, and relevant research directions.

The second session included four topical lectures by I<sup>2</sup>CNER researchers. Dr. Tatsumi Ishihara, Associate Director of I<sup>2</sup>CNER, introduced recent progress in his approach to solar hydrogen production. He explained that solar power is by far the most abundant source. However, energy density from solar power is low. Therefore, from accumulating and leveling, production of hydrogen using solar energy is highly important and effective for achieving a carbon-neutral energy society. Dr. Brian Somerday, Lead Principal Investigator of I<sup>2</sup>CNER and Materials Scientist at Sandia National Laboratories, showed that the I<sup>2</sup>CNER Structural Materials Division focuses on providing cost-effective, science-based solutions to hydrogen embrittlement by improving measurement methods, developing next-generation materials, and establishing predictive models. He also explained a recent discovery whereby small concentrations of oxygen, a potential impurity, dramatically affect hydrogen-enhanced fatigue crack growth, and that two fundamental characteristics of oxygen were identified that could contribute to the observed fatigue behavior. Dr. Naotoshi Nakashima, Principal Investigator of I<sup>2</sup>CNER,

gave a talk with a theme of “Nanocarbon-based Novel Fuel Cell Catalysts with Very High Performance.” Dr. Nakashima demonstrated that the polymer electrolyte fuel cell (PEFC) is one of the most promising power sources for transportation and houses due to its high-energy conversion efficiency. Increasing effort has been made to find a higher temperature operation of PEFCs in order to enhance cell performance, accompanied by high durability. Dr. Kenneth Christensen, I<sup>2</sup>CNER Satellite Associate Director and professor at the University of Illinois at Urbana-Champaign, highlighted the significant carbon dioxide sequestration research which is presently being carried out in I<sup>2</sup>CNER. He asserted that achieving safe, long-term sequestration of carbon dioxide (CCS) in the geosphere is a crucial aspect of I<sup>2</sup>CNER’s overall research mission.

Following these sessions, Dr. Nobuhide Kasagi, WPI Program Officer, gave concluding remarks.

### AAAS Annual Meeting 2013 February 14-18, 2013



The Ministry of Education, Culture, Sports, Science and Technology in Japan (MEXT) and several WPI Institutes, including the International Institute for Carbon-Neutral Energy



At the Venue

Research (I<sup>2</sup>CNER), represented the World Premier International Research Center Initiative (WPI) at the 2013 American Association for the Advancement of Science (AAAS) Annual Meeting in Boston, Massachusetts, USA from February 14-18.

Founded in Philadelphia in 1848, AAAS is the world’s largest general scientific society and is the publisher of the journal *Science*, as well as *Science Translational Medicine* and *Science Signaling*. AAAS is open to all and currently serves around 10 million people throughout its 261 affiliated societies and academies of science. AAAS is a non-profit organization that fulfills its mission to “advance science and serve society” through initiatives in science policy, international programs, science education, and more.



Asst. Prof. Sean Bishop exchanges ideas over coffee

Each year, the AAAS Annual Meeting brings together a diverse group of attendees, including scientists, parents and children, and national and international media. The meeting, which hosts as many as 11,000 participants, promotes effective communication among policymakers, researchers, and the public. The 2013 AAAS Annual Meeting offered a blend of more than 160 symposia, lectures, and specialized seminars, as well as poster presentations and an exhibition hall. Although AAAS is in its 165<sup>th</sup> year, the 2013 meeting is actually the 179<sup>th</sup> AAAS Annual Meeting. This year's meeting theme was "The Beauty and Benefits of Science."



The Japan Pavilion

The WPI Institutes and MEXT hosted the WPI booth as part of the Japan pavilion, which was organized by the Japan Science and Technology Agency (JST). Over the course of the three day exhibition during the meeting, participants ranging from scientists to administrators to lawmakers visited the Japan pavilion.



WPI is well-represented in the Japan Pavilion

On February 15, the WPI program, RIKEN, and the University of Tsukuba held a workshop with the theme; "Japan: Your next career destination." In the workshop, Mr. Mitsuyuki Ueda, Director, WPI / Office for Promotion of Basic Research, Basic Research Promotion Division, Research Promotion Bureau, MEXT, outlined the WPI program and described exciting career opportunities in Japan for foreign researchers.



Mr. Mitsuyuki Ueda, Director, Office for Promotion of Basic Research, MEXT

### *Science and Technology Festa in Kyoto 2013 March 16-17, 2013*

The World Premier International Research Center Initiative (WPI) Institutes, including the International Institute for Carbon-Neutral Energy Research (I<sup>2</sup>CNER), ran booths at "Science and Technology Festa in Kyoto 2013," which was held at Kyoto Pulse Plaza on March 16<sup>th</sup> and 17<sup>th</sup>. This science event was organized by the Cabinet Office, the Ministry of Education, Culture, Sports, Science and Technology in Japan

(MEXT), and several other ministries and agencies targeting mainly at high school students.



Mini-lecture for future scientists    Demonstration of photocatalysis

This year, I<sup>2</sup>CNER shared a booth with Osaka University Immunology Frontier Research Center (IFReC), and held several seminars with the theme: "Let's take a look at Cutting-Edge Science." Associate Professor Ikuo Taniguchi, CO<sub>2</sub> Capture and Utilization Research Division, presented I<sup>2</sup>CNER's cutting-edge technology in CO<sub>2</sub> Capture & Storage. Assistant Professor Aleksandar Staykov, Hydrogen Production Research Division, introduced Theoretical Chemistry. Assistant Professor Stephen Lyth, Fuel Cells Division, described Graphene and Fuel Cells. There were also demonstrations of how to produce Hydrogen gas and how a fuel cell works.

About 500 participants, including politicians and government officials, visited the I<sup>2</sup>CNER booth during the event.



"I<sup>2</sup>CNER's cutting-edge technology in CO<sub>2</sub> Capture & Storage"  
Assoc. Prof. Ikuo Taniguchi



"Graphene and Fuel Cells: Green Technology for Today and Tomorrow!"  
Asst. Prof. Stephen Lyth



"Theoretical Chemistry: Our Eyes into the Quantum World"  
Asst. Prof. Aleksandar Staykov

## Press Releases

In an effort to familiarize Japanese society with the research activities of I<sup>2</sup>CNER, we issued several press releases throughout FY 2012 through various media outlets (primarily newspapers).

Date	Topics
October 12, 2012	Thermodynamics on Soluble Carbon Nanotubes: How Do DNA Molecules Replace Surfactants on Carbon Nanotubes? <b>Prof. Naotoshi Nakashima, Assoc. Prof. Yasuro Niidome, Fuel Cells Research Division</b>
October 19, 2012	Role of Ga <sup>3+</sup> and Cu <sup>2+</sup> in the High Interstitial Oxide-Ion Diffusivity of Pr <sub>2</sub> NiO <sub>4</sub> -based Oxides: Design Concept of Interstitial Ion Conductors through the Higher-Valence d <sup>10</sup> Dopant and Jahn-Teller Effect <b>Prof. Tatsumi Ishihara, Hydrogen Production Research Division</b>
December 5, 2012	Highly efficient organic light-emitting diodes from delayed fluorescence <b>Prof. Chihaya Adachi, Hydrogen Production Research Division</b>
February 6, 2013	A Functional [NiFe]Hydrogenase Mimic That Catalyzes Electron and Hydride Transfer from H <sub>2</sub> <b>Prof. Seiji Ogo, Catalytic Materials Transformations Research Division</b>
February 21, 2013	Fuel Cell Electrocatalyst Using Polybenzimidazole-Modified Carbon Nanotubes As Support Materials <b>Prof. Naotoshi Nakashima, Assoc. Prof. Tsuyohiko Fujigaya, Fuel Cells Research Division</b>
February 22, 2013	Extension of continental crust by anelastic deformation during the 2011 Tohoku-oki earthquake: The role of extensional faulting in the generation of a great tsunami <b>Assoc. Prof. Takeshi Tsuji, CO<sub>2</sub> Storage Research Division</b>
February 25, 2013	High-pressure torsion of TiFe intermetallics for activation of hydrogen storage at room temperature with heterogeneous nanostructure <b>Prof. Zenji Horita, Prof. Etsuo Akiba, Hydrogen Storage Research Division</b>



Prof. Seiji Ogo



Prof. Chihaya Adachi



Members of the press film Prof. Ogo's presentation



Prof. Zenji Horita, Prof. Etsuo Akiba

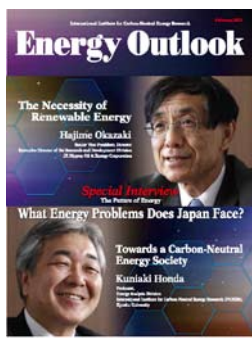
## Publications

### Hello! I<sup>2</sup>CNER and Energy Outlook



As part of our efforts to publicize the research activities of I<sup>2</sup>CNER, we publish a newsletter entitled “Hello! I<sup>2</sup>CNER.” The newsletter is published three times a year, and each publication highlights the research activities of a given research division. We sincerely hope that many of our readers gain an increased interest in I<sup>2</sup>CNER through these outreach efforts.

In FY 2012, Hello! I<sup>2</sup>CNER was merged with a brand new Institute publication, Energy Outlook. The object of Energy Outlook is to give I<sup>2</sup>CNER a medium through which to communicate industry and government perspectives on energy to the general public. In order to accomplish this goal, each issue of Energy Outlook features an interview of an industry or government official by an I<sup>2</sup>CNER researcher, as well as related research highlights and awards. This regular interaction with industry and government officials not only allows I<sup>2</sup>CNER to facilitate public understanding of new technologies, which is a vital part of outreach for the Institute, but it also provides I<sup>2</sup>CNER researchers with opportunities to check the relevance of their ongoing basic research projects against industry and government perspectives. Hello! I<sup>2</sup>CNER and Energy Outlook are published simultaneously in the same volume; each publication has its own front cover—the reader must simply flip over Hello! I<sup>2</sup>CNER in order to read Energy Outlook.



### I<sup>2</sup>CNER Fuse News

In an effort to further fuse and promote collaboration between Japanese and overseas researchers, we initiated an internal newsletter, called “I<sup>2</sup>CNER Fuse News.” The goal

of this internal newsletter is to enhance information-sharing amongst our members. The initial purpose of I<sup>2</sup>CNER Fuse News is to help introduce the researchers of I<sup>2</sup>CNER to one another by including short descriptions of the researchers’ scientific and personal interests along with their photos. The newsletter also provides a platform for communicating institutional policy, events and news. As collaborations are established and discoveries are made, the newsletter will evolve into a medium for reporting research findings, a springboard for new collaborative relationships, and a resource for new research paths.



### I<sup>2</sup>CNER P.I.peline

Beginning in December 2012, I<sup>2</sup>CNER Director Petros Sofronis began issuing an internal newsletter entitled “I<sup>2</sup>CNER P.I.peline.” As the name suggests, the newsletter is designed to be a source of information, or a “pipeline” for I<sup>2</sup>CNER Principal Investigators (PIs), as well as all other researchers. More specifically, the purpose of the P.I.peline is to allow the Director to share information directly with all members of the Institute. Subjects covered in the P.I.peline include latest news, funding opportunities, collaborations, policy changes, “kudos,” and reports on special topics. One advantage of this publication is that the Director appears more accessible to younger members of the Institute, who may not otherwise have frequent personal contact with him. For example, in the newsletter, I<sup>2</sup>CNER members are invited to suggest matters for discussion/items for inclusion in the next issue, and the Director’s email address is listed. Another benefit of the P.I.peline is that it slashes the traditional hierarchy which would be used to relay information and thus further reinforces the “transformative” nature of the I<sup>2</sup>CNER research culture. Finally, it ensures that all I<sup>2</sup>CNER researchers have the same basic information about what is happening at the Institute. While only one issue was published in FY 2012, several issues are planned for FY 2013.



## I<sup>2</sup>CNER Seminar Series

The I<sup>2</sup>CNER Seminar Series, now a customary event which is symbolic of the Institute's "global visibility," has hosted a total of 43 distinguished, internationally-recognized researchers from Japan, North America, Europe, and Asia since it was launched back in March 2011, including 23 in FY 2012. The invited speakers discuss a variety of topics, including hydrogen production, fuel cells, heat transfer mechanisms, nanomaterials, and renewable energy policy, among others. A total of 1,714 people from both inside and outside I<sup>2</sup>CNER attended the 23 seminars this year. This seminar series can be characterized by the robust and enthusiastic audience participation in the Q&A sessions, which are often very lengthy, and spill over into the welcome reception that is hosted after each seminar. I<sup>2</sup>CNER is very optimistic about this opportunity to impact the audiences of this seminar series and the way they think about a "carbon-neutral future."

### 1<sup>st</sup> I<sup>2</sup>CNER Seminar

**Date:** April 13, 2012

**Speaker:** Dr. Bruno Ameduri, National Center of Scientific Research, FRANCE

**Title:** Recent Advances on Fluoromembranes for Fuel Cell



### 5<sup>th</sup> I<sup>2</sup>CNER Seminar

**Date:** June 1, 2012

**Speaker:** Dr. Monterey R. Gardiner, U.S. Department of Energy, USA

**Title:** Renewable Energy Policy (Barriers and Motivation): Perspectives on Progress in Japan, Germany/EU, and the U.S.



### 2<sup>nd</sup> I<sup>2</sup>CNER Seminar

**Date:** April 27, 2012

**Speaker:** Dr. Tom Autrey, Pacific Northwest National Laboratory, USA

**Title:** Hydrogen activation in molecular complexes: Chemical approaches to catalysis and energy



### 6<sup>th</sup> I<sup>2</sup>CNER Seminar

**Date:** June 8, 2012

**Speaker:** Dr. Kazunari Domen, The University of Tokyo

**Title:** Hydrogen production from water on heterogeneous photocatalysts



### 3<sup>rd</sup> I<sup>2</sup>CNER Seminar

**Date:** May 18, 2012

**Speaker:** Dr. Richard Glass, University of Arizona, USA

**Title:** Biomimetic Diiron Catalysts for Hydrogen Production



### 7<sup>th</sup> I<sup>2</sup>CNER Seminar

**Date:** June 29, 2012

**Speaker:** Dr. Sang Yong Lee, Korea Advanced Institute of Science and Technology (KAIST), KOREA

**Title:** Two-phase Flow Distribution in Heat Exchangers



### 4<sup>th</sup> I<sup>2</sup>CNER Seminar

**Date:** May 18, 2012

**Speaker:** Dr. Jungho Kim, University of Maryland, USA

**Title:** Flow Boiling Heat Transfer Mechanisms Using IR Thermography



### 8<sup>th</sup> I<sup>2</sup>CNER Seminar

**Date:** July 13, 2012

**Speaker:** Prof. Hung-Jue Sue, Texas A&M University, USA

**Title:** Nanomaterials and Polymer Nanocomposites for Energy



### 9<sup>th</sup> I<sup>2</sup>CNER Seminar

**Date:** July 27, 2012

**Speaker:** Dr. Koji Tanaka, Institute for Integrated Cell-Material Sciences, Kyoto University

**Title:** Synthesis of metal complexes aimed at reversible conversion between chemical energy and electrical one



### 13<sup>th</sup> I<sup>2</sup>CNER Seminar

**Date:** September 28, 2012

**Speaker:** Dr. Makoto Akai, National Institute of Advanced Industrial Science and Technology (AIST)

**Title:** Discussion on Energy Portfolio of Japan under a New Myth



### 10<sup>th</sup> I<sup>2</sup>CNER Seminar

**Date:** August 10, 2012

**Speaker:** Dr. Kazuhito Hashimoto, The University of Tokyo

**Title:** Photocatalysis and Artificial Photosynthesis



### 14<sup>th</sup> I<sup>2</sup>CNER Seminar

**Date:** October 19, 2012

**Speaker:** Dr. Noritaka Mizuno, The University of Tokyo

**Title:** Design of Highly Functionalized Polyoxometalate-based Nano-structured Catalysts



### 11<sup>th</sup> I<sup>2</sup>CNER Seminar

**Date:** September 7, 2012

**Speaker:** Prof. Sushanta Mitra, University of Alberta, CANADA

**Title:** Micro and Nano-scale Transport Processes for Energy Applications



### 15<sup>th</sup> I<sup>2</sup>CNER Seminar

**Date:** October 26, 2012

**Speaker:** Prof. Hidde Brongersma, Calipso B.V., The Netherlands, Imperial College, U. K.

**Title:** High-Sensitivity LEIS: A new tool in the understanding of the performance of catalysts and other (sub-) nanometer



### 12<sup>th</sup> I<sup>2</sup>CNER Seminar

**Date:** September 21, 2012

**Speaker:** Dr. José Santiso, Research Center for Nanoscience and Nanotechnology, SPAIN

**Title:** Oxygen Surface exchange kinetics for intermediate temperature SOFC applications



### 16<sup>th</sup> I<sup>2</sup>CNER Seminar

**Date:** October 26, 2012

**Speaker:** Dr. Masahiro Watanabe, University of Yamanashi

**Title:** Development of Pt and Pt-Alloy Electrocatalysts for the Next Generation Polymer Membrane Fuel



**17<sup>th</sup> I<sup>2</sup>CNER Seminar**

**Date:** November 2, 2012  
**Speaker:** Prof. Hiroshi Kitagawa, Kyoto University  
**Title:** Solid-State Protonics for Clean Energy



**21<sup>st</sup> I<sup>2</sup>CNER Seminar**

**Date:** March 1, 2013  
**Speaker:** Prof. Peter Stephan, Technical University Darmstadt, GERMANY  
**Title:** Local heat transfer near moving 3-phase contact lines and its influence on nucleate boiling and drop evaporation



**18<sup>th</sup> I<sup>2</sup>CNER Seminar**

**Date:** December 14, 2012  
**Speaker:** Dr. Masakazu Iwamoto, Tokyo Institute of Technology  
**Title:** Synthesis of Propene from Ethene or Bio-ethanol



**22<sup>nd</sup> I<sup>2</sup>CNER Seminar**

**Date:** March 9, 2013  
**Speaker:** Dr. Ming Zheng, National Institute of Standards and Technology, USA  
**Title:** Probing Redox and Photochemistry of Single-wall Carbon Nanotubes for Energy Conversion



**19<sup>th</sup> I<sup>2</sup>CNER Seminar**

**Date:** December 21, 2012  
**Speaker:** Prof. Srinivas Garimella, Georgia Institute of Technology, USA  
**Title:** Reducing the Carbon Footprint of Energy Utilization through Advances in Microscale Heat and Mass Transfer



**23<sup>rd</sup> I<sup>2</sup>CNER Seminar**

**Date:** March 15, 2013  
**Speaker:** Prof. Teruo Kishi, Tsukuba Innovation Arena, the University of Tokyo, NIMS  
**Title:** Nano Technology Research Strategy and Current Activity in Japan



**20<sup>th</sup> I<sup>2</sup>CNER Seminar**

**Date:** February 8, 2013  
**Speaker:** Prof. Toshiharu Teranishi, Kyoto University  
**Title:** Inorganic Nanoparticles as Innovative Energy Materials



Q&A session

## Institute Interest Seminar Series

In its second year, the “Institute Interest Seminar Series (IISS)” continued to play an important role in terms of facilitating interaction and advancement of interdisciplinary (fusion) research both inside and beyond ICNER. This regular seminar was held on 16 occasions in FY 2012, which gave 32 young researchers and students the opportunity to give talks on their research and actively engage in thought-provoking Q&A sessions. One attractive feature of this series is the open and relaxed “coffee shop” atmosphere for discussion and exchange of ideas.

### 18<sup>th</sup> IISS Seminar, April 18, 2012

**Speaker:** Assoc. Prof. Miho Yamauchi

**Title:** Structural control and catalytic application of alloy nanoparticles

**Speaker:** Assoc. Prof. Shintaro Ida

**Title:** Two-dimensional semiconducting nanocrystals for photocatalytic hydrogen production from water

### 19<sup>th</sup> IISS Seminar, April 26, 2012

**Speaker:** Dr. Yanqion Zheng

**Title:** Highly efficient bulk heterojunction photovoltaic cells based on small molecule donor and C70,

**Speaker:** Takahiro Fukumaru, Ph.D student

**Title:** Development of porous polybenzoxazole for low dielectric constant materials

### 20<sup>th</sup> IISS Seminar, May 23, 2012

**Speaker:** Assoc. Prof. Toshihiko Tsuchiyama

**Title:** Prevention of hydrogen permeation by surface-layer microstructure control in type 304 stainless steel

**Speaker:** Dr. Zaki N. A. Zahran

**Title:** Efficient water oxidation with manganese and cobalt porphyrin dimers assembled on metal oxide surfaces

### 21<sup>st</sup> IISS Seminar, June 7, 2012

**Speaker:** May Martin, Ph.D Student, University of Illinois

**Title:** Discovering the Fundamental Mechanisms of Environmental Fracture

**Speaker:** Dr. Weigang Ma, Tsinghua University

**Title:** Pulsed laser pump-probe thermoreflectance method for thermophysical properties measurement

### 22<sup>nd</sup> IISS Seminar, June 20, 2012

**Speaker:** Assoc. Prof. Takeshi Tsuji

**Title:** Monitoring of dynamic subsurface activities: My past and present researches

**Speaker:** Dr. John Druce

**Title:** Characterisation of  $(\text{Pr},\text{La})_2\text{NiO}_4$  as an oxygen electrodes for reversible SOEC/SOFCs

### 23<sup>rd</sup> IISS Seminar, July 5, 2012

**Speaker:** Yuki Fukatani, Ph.D Student

**Title:** Study on evaporation and heat transfer of a small droplet

**Speaker:** Akihiro Orita, Ph.D Student

**Title:** Tensile and fatigue crack growth properties of high strength stainless steel with high resistance to hydrogen embrittlement in 100 MPa hydrogen gas

### 24<sup>th</sup> IISS Seminar, July 25, 2012

**Speaker:** Assoc. Prof. Teppei Ogura

**Title:** Computational Study of Reaction Mechanisms on Solid Oxide Fuel Cell Anodes

**Speaker:** Asst. Prof. Takahiro Matsumoto

**Title:** Molecular Fuel Cell

### 25<sup>th</sup> IISS Seminar, October 17, 2012

**Speaker:** Asst. Prof. Huaiyu Shao

**Title:** A new challenge -nano processing and properties of Mg based materials for energy storage

**Speaker:** Tafiq Bin Nur, Ph.D Student

**Title:** Greenhouse gas (GHG) emissions reduction potentials by SOFC: case for distributed and centralized electricity generations



Assoc. Prof. Miho Yamauchi



Hwei-Ru "Molly" Jhong



Dr. John Druce



**26<sup>th</sup> IISS Seminar, November 8, 2012**

**Speaker:** Koichi Tsuboi, Ph.D Student

**Title:** Application of Solution Nitriding to Metastable Austenitic Stainless Steel for Improving Hydrogen Embrittlement Resistance

**Speaker:** Tran Quang Tuyen, Ph.D Student

**Title:** Biodiesel fuel conversion to renewable electricity with a new SOFC concept

**27<sup>th</sup> IISS Seminar, November 21, 2012**

**Speaker:** Asst. Prof. Masaaki Sadakiyo

**Title:** Creation of Novel Ionic Conductors with Metal-Organic Frameworks

**Speaker:** Dr. Chungsik Kim

**Title:** An Efficient Asymmetric Olefin Aziridination Using a Newly Designed Ru(CO)(salen) Complex as Catalyst

**28<sup>th</sup> IISS Seminar, December 5, 2012**

**Speaker:** Takamichi Shinohara, Ph.D Student

**Title:** Structure Control and Precise Characterization of Nanostructured Organic Heterojunction Photovoltaics by Synchrotron X-ray Structure Analyses

**Speaker:** Huei-Ru “Molly” Jhong, Ph.D Student, University of Illinois

**Title:** Catalysts and Electrodes for the Electrochemical Reduction of CO<sub>2</sub> to CO

**29<sup>th</sup> IISS Seminar, December 13, 2012**

**Speaker:** Asst. Prof. Hidehisa Hagiwara

**Title:** Dye-Modified Photocatalyst for Solar Water Splitting

**Speaker:** Antti Vaajoki, Visiting Scholar, VTT Technical Research Centre of Finland

**Title:** Tribological Behaviour of Diamond-like Carbon Coatings in Hydrogen

**30<sup>th</sup> IISS Seminar, January 16, 2013**

**Speaker:** Kotaro Sugi, Ph.D Student

**Title:** Experimental study of CO<sub>2</sub> absorption method

**Speaker:** Kazuhide Shibata, Ph.D Student

**Title:** CNTs Synthesis in Gas Flow with Size Selected Metal Particles under Low Pressure

**31<sup>st</sup> IISS Seminar, February 14, 2013**

**Speaker:** Asst. Prof. Yuji Higaki

**Title:** In-situ Elastomer Structure Analysis on the Deformation Process by Synchrotron Radiation X-ray Scattering

**Speaker:** Dr. Wei Ma

**Title:** Surface Wettability Control for Energy Saving and Restoration

**32<sup>nd</sup> IISS Seminar, March 6, 2013**

**Speaker:** Assoc. Prof. Ikuo Taniguchi

**Title:** CO<sub>2</sub> Separation with Polymeric Membrane

**Speaker:** Nicola H. Perry

**Title:** Developing fundamental understanding of oxygen exchange and associated expansion in solid oxide fuel cell cathodes

**33<sup>rd</sup> IISS Seminar, March 14, 2013**

**Speaker:** Ayanobu Horinouchi, Ph.D Student

**Title:** Aggregation States of Nafion<sup>®</sup> at Interfaces

**Speaker:** Takahiro Kikunaga, Ph.D Student

**Title:** Monooxidation Ability of a Metal Acylperoxo Complex



Q&A Session



Dr. Nicola Perry



Open discussion

# Finances

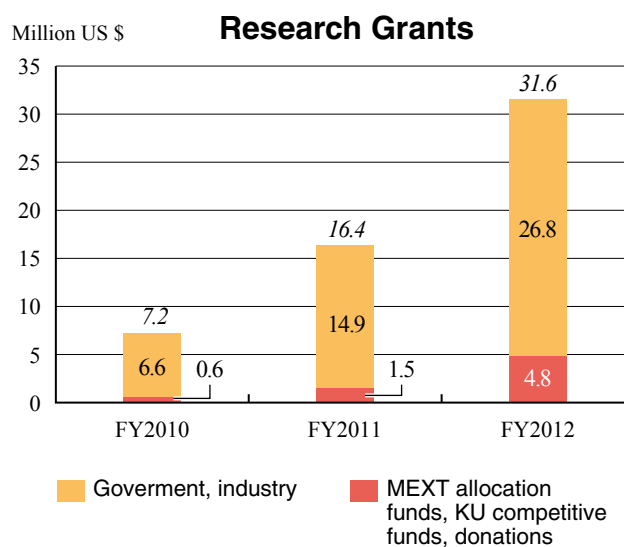
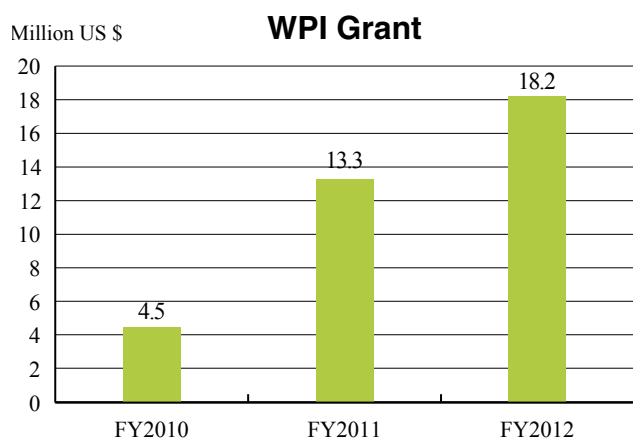
WPI Grant	Millions of USD
<i>FY2010</i>	4.5
<i>FY2011</i>	13.3
<i>*FY2012</i>	18.2
Research Grants	
<i>FY2010</i>	7.2
**MEXT allocation funds, ***KU competitive funds, Donations	0.6
Government, Industry	6.6
<i>FY2011</i>	16.4
**MEXT allocation funds, ***KU competitive funds, Donations	1.5
Government, Industry	14.9
<i>FY2012</i>	31.6
**MEXT allocation funds, ***KU competitive funds, Donations	4.8
Government, Industry	26.8

1USD = 100JPY

\* WPI Grant of FY2012 includes the supplementary budget worth 5 million USD.

\*\* MEXT is an acronym for Ministry of Education, Culture, Sports, Science and Technology

\*\*\* KU is an acronym for Kyushu University



## FY2013 Events Schedule

Date	Events
June 2-7, 2013	19 <sup>th</sup> International Conference on Solid State Ionics (SSI-19) (Kyoto, Japan)
June 6-9, 2013	1 <sup>st</sup> WPI Workshop on Materials Science (Kyoto, Japan)
June 12-13, 2013	The 1 <sup>st</sup> International Symposium on Chemical Energy Conversion Processes (ISCECP-1) (Fukuoka, Japan)
August 7-8, 2013	Super Science Highschool (SSH) National Conference (Yokohama, Japan)
September 4-6, 2013	International Symposium on Innovation Materials for Processes in Energy Systems 2013 (Fukuoka, Japan)
September 13, 2013	Catalytic Concepts for Energy Symposium (Illinois, USA)
October 18-19, 2013	Society of Computer Chemistry, Japan (Fukuoka, Japan)
November 9-10, 2013	Science Agora (Tokyo, Japan)
November 19-20, 2013	International Partnership for Hydrogen and Fuel Cells in the Economy (IPHE) – 20 <sup>th</sup> Steering Committee Meeting (Fukuoka, Japan)
December 14, 2013	WPI Joint Symposium 2013 (Sendai, Japan)
January 30, 2014	I <sup>2</sup> CNER Annual Symposium 2014 (Fukuoka, Japan)
January 31, 2014	HYDROGENIUS & I <sup>2</sup> CNER Joint Research Symposium and I <sup>2</sup> CNER International Workshop (Fukuoka, Japan)
February 2-5, 2014	International Conference on Hydrogen Production 2014 (Fukuoka, Japan)
February 13-17, 2014	AAAS Annual Meeting (Chicago, USA)
February 16-20, 2014	TMS 2014 143 <sup>rd</sup> Annual Meeting & Exhibition (San Diego, USA)

# Access Map



## International Institute for Carbon-Neutral Energy Research (I<sup>2</sup>CNER), Kyushu University

744 Motooka, Nishi-ku, Fukuoka 819-0395 JAPAN Phone: +81(0)92 802 6932 Fax: +81(0)92 802 6939

URL: <http://i2cner.kyushu-u.ac.jp> Facebook: <https://www.facebook.com/I2CNER.news> Twitter: <https://twitter.com/I2CNER>

**From Fukuoka Airport** (30 minutes)

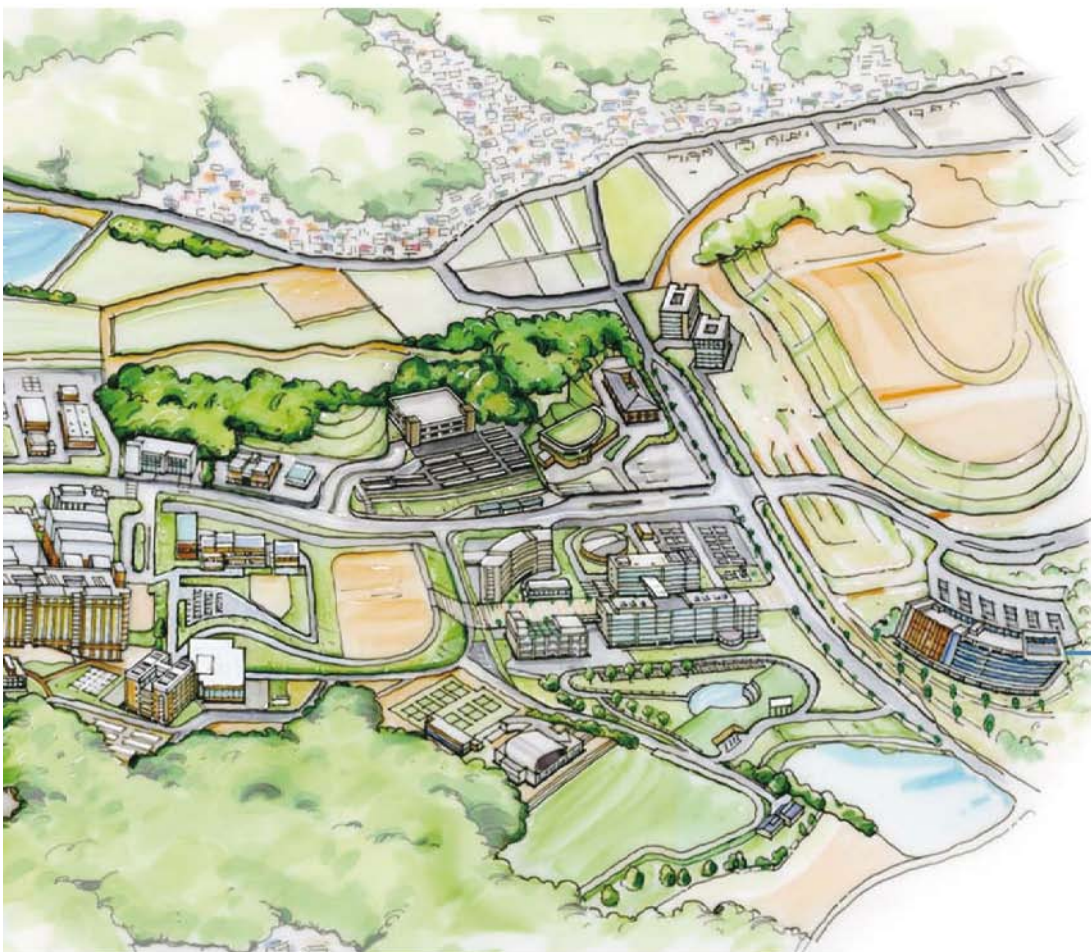
Take the Fukuoka City Subway going to “Meinohama” or “Karatsu” at Fukuoka Airport Station. Meinohama: Take the JR Chikuhi Line going to “Karatsu” at Meinohama Station. Get off at Kyudaigakkentoshi Station. Karatsu: Get off at Kyudaigakkentoshi Station.

**From Hakata Station** (20 minutes)

Take the Fukuoka City Subway going to “Meinohama” or “Karatsu” at Hakata Station. Meinohama: Take the JR Chikuhi Line going to “Karatsu” at Meinohama Station. Get off at Kyudaigakkentoshi Station. Karatsu: Get off at Kyudaigakkentoshi Station.

**From Kyudaigakkentoshi Station** (15minutes)

Take the Showa Bus going to “Kyudaikougakubumae”.









**International Institute for Carbon-Neutral Energy Research  
(I<sup>2</sup>CNER), Kyushu University**

744 Motooka, Nishi-ku, Fukuoka 819-0395 JAPAN

Phone +81-(0)92-802-6932

Fax +81-(0)92-802-6939

<http://i2cner.kyushu-u.ac.jp>