

# World Premier International Research Center Initiative (WPI)

## Executive Summary (Interim Evaluation)

Host Institution	Kyushu University	Host Institution Head	Setsuo Arikawa
Research Center	International Institute for Carbon-Neutral Energy Research (I <sup>2</sup> CNER)	Center Director	Petros Sofronis

\*Summarize the Self-Evaluation Report for Interim Evaluation (within 4 pages including this page).

### 1. Summary of State of WPI Center Project Progress

I<sup>2</sup>CNER's energy vision for a carbon-neutral society (CNS) is to enable energy technologies that hold promise for a large reduction of greenhouse gas (GHG) emissions (70-80%) from 1990 levels by 2050. The vision is based on two basic principles: efficiency increase (EI) in energy conversion and use and lowering of carbon intensity (LCI) of fuel and electricity. The I<sup>2</sup>CNER vision includes all EI and LCI technologies, not only those being currently researched within I<sup>2</sup>CNER. There are many possible combinations of new EI and LCI technologies and deployment timing (scenarios) that can lead to the targeted GHG emissions reduction by 2050. I<sup>2</sup>CNER has generated four such scenarios utilizing the more promising new technology options. I<sup>2</sup>CNER's research efforts are intimately tied to these four scenarios because the short-, mid-, and long-term milestones of each of our division roadmaps were established in consideration of the development and deployment timing of the various promising technology options in the scenarios. The scenarios currently under consideration that encompass I<sup>2</sup>CNER research efforts are: a) the Base Scenario, which relies on development of important EI technologies and balanced deployment of renewables and CCS, b) the Renewables Scenario, involving very large penetration of renewables for LCI and development of important EI technologies, c) the CCS Scenario, involving large deployment of CCS for power and industries, especially for coal and development of important EI, and d) the "Some Nuclear" Scenario, involving balanced application of LCI technologies, including nuclear power. These scenarios help ensure the relevance of I<sup>2</sup>CNER's research and roadmaps to CNS.

Fusion of disciplines is fostered by several initiatives, such as "I<sup>2</sup>CNER Competitive Funding," which supports research teams who can pass a rigorous assessment process by providing evidence of fusion work, such as published interdisciplinary papers. I<sup>2</sup>CNER journal publications addressing interdisciplinary subjects cover a wide range of disciplines, e.g. ranging from biology to chemistry and involving theory and experiment. I<sup>2</sup>CNER is achieving recognition as a world class institute. Evidence of this visibility is its increasing number of collaborations worldwide. Papers written by faculty from I<sup>2</sup>CNER and these international partners are being published. For its energy vision and research portfolio, I<sup>2</sup>CNER is exchanging information with the US DOE EERE Fuel Cells Program, co-sponsoring international conferences and symposia, and assisting government agencies both in Japan and the US in the advancement of energy initiatives and technologies. I<sup>2</sup>CNER's advancement of green innovation is demonstrated by the 18 patent applications by I<sup>2</sup>CNER researchers since the inception of the Institute and the large number of industries, such as the automotive (TOYOTA, Nissan, and HONDA), the Kyocera, Mitsubishi Hitachi Power Systems, and the JFE Steel Corporation, benefiting from ongoing joint research projects with I<sup>2</sup>CNER researchers.

I<sup>2</sup>CNER, through its interaction with Kyushu University (KU), is impacting the traditional Japanese research structure and faculty model. I<sup>2</sup>CNER's academic structure and processes of promotion, tenure, and merit-based compensation of its faculty and postdocs are according to the highest standards for international research centers. I<sup>2</sup>CNER is spearheading KU's globalization efforts within the University Reform Revitalization Program and its faculty are instructors in the G30 Engineering Project, which KU plans to expand by establishing an education program that involves energy, the "Global Education Course." At the same time, I<sup>2</sup>CNER is competing and has been granted tenured positions within the KU system. Through these activities, the Institute is becoming an influential and integral component of the university. Further evidence of the impact of I<sup>2</sup>CNER on KU is the establishment of the Intra-University Faculty Transfer System, which aims to improve the standards of education and research conducted at the university. Transforming the research enterprise and system of Kyushu University was an initial goal and significant progress has been achieved, although much remains to be done.

### 2. Center's Research Activities

State-of-the-art research aiming at the short term milestones in the Division roadmaps is attacking the

problem of energy demand through both the source (production of fuels, their storage and transport) and sink (improved fuel cells to produce electricity and lower demand through efficiency) areas. A few selected results are as follows: a) correlated metal oxides coupled to  $\text{TiO}_2$  are shown to produce electrodes for photoelectrochemical cells that are stable and promote rapid and efficient  $\text{H}_2\text{O}$  electrolysis; b) development of polybenzimidazole members for fuel cells; these have delivered high power densities for 400,000 cycles at  $120^\circ\text{C}$ , a dramatic advance; c) discovery that charge localization on reduced cations is the origin of the detrimental chemical expansion in oxides commonly used in SOFCs; d) enhanced performance of light emitting devices through use of molecules incorporating large spin-orbit coupling, which allow for nearly 100% of the excitons in the device being able to generate electroluminescence. This highlight demonstrates how advanced computational models can be used to accelerate the discovery of new molecules and materials, which can then be synthesized. The strategy of using computational methods to explore for new systems will be an emerging theme in the institute; e) discovery of the activation mechanism in TiFe intermetallics by High Pressure Torsion, a promising system for stationary energy storage; f) development of a new model of hydrogen-induced cracking that is hydrogen-accelerated plasticity-mediated failure; g) high speed imaging has been used to demonstrate hydrothermal waves to be bulk waves in heat transfer fluid droplets. This controls evaporation, a key component of multi-phase heat pumps; h) 200 nm-thick epoxy layers with amine residues on porous membranes have been shown to selectively transport  $\text{CO}_2$  relative to  $\text{N}_2$ ; this has implications for capture of  $\text{CO}_2$ . Poly(amidoamine) dendrimers have also shown selectivity relative to  $\text{H}_2$ ; i) simulation studies of  $\text{CO}_2$  trapping demonstrated that pore space reduction due to mineral precipitation has a greater influence on the non-wetting phase than on the wetting phase. Potential research challenges over the next 5 years include I<sup>2</sup>CNER's consideration of the following directions: renewable carbon capture and storage (CCS) through biological reaction, interaction of CCS with earthquakes; biomimetic catalysis for  $\text{H}_2$  and  $\text{CO}_2$  activation; hydrogen production and steam electrolysis using waste heat; and extreme materials and extreme physical and chemical processes. The latter has implications for the potential use of nuclear power in Japan's vision for a carbon neutral future.

Systems and actions needed for better science include: access to graduate research assistants by I<sup>2</sup>CNER young faculty; resources for maintaining/updating existing equipment and purchasing new equipment; strengthening and reinforcing the presence of the Internal Programs Review Committee (IPRC) within the Institute—to make it more enmeshed in the research culture/research planning efforts through sporadic evaluation of programs; incentivize senior faculty and PIs to increase their participation in the Institute Interest Seminar Series so that the series is transformed into a “think tank” for sharing ideas between young and senior researchers; analysis and study of several research projects by the Energy Analysis Division (EAD), which requires strengthening the EAD through new faculty and postdoctoral researchers; expanding the Institute's computational capabilities; and convincing young Japanese scientists to gain exposure to the research enterprise outside Japan.

To advance fusion of its basic science research with energy systems research, I<sup>2</sup>CNER signed an agreement with the National Fuel Cell Research Center (NFCRC) at the University of California, Irvine. I<sup>2</sup>CNER is also interacting strongly with the Sandia National Laboratories at Livermore, CA. Dr. Brian Somerday, a distinguished member of the technical staff, is the Division Lead PI for I<sup>2</sup>CNER's Hydrogen Materials Compatibility Division. I<sup>2</sup>CNER is achieving recognition as a world class institute from Japan's government agencies, who are seeking the services of its PIs in various national projects, and from international government agencies and societies, as indicated by the international awards its members have received.

### 3. Feeding Research Outcomes back into Society

I<sup>2</sup>CNER's basic research, although fundamental in nature, is impacting the transition to a low carbon society by discovery and development of pathways toward low carbon technology solutions and identifying strategies to removing the technology roadblocks to achieving a carbon neutral footprint. Select examples include: Pioneering results for organic light emitting diodes impacting energy efficiency; High performance photocatalysts that can efficiently utilize solar energy to potentially produce clean burning fuels, thereby reducing carbon production at all stages of the process; mitigation processes of the hydrogen-degradation effect on metals and alloys, and development of new materials with unique hydrogen resistance for safety and reliability of application components in a hydrogen economy; Development of novel PEFCs free from acid leaching with a remarkably high durability (single cell test: >400,000 cycling) and a high power density at  $120^\circ\text{C}$  under non-humidified conditions. Such performance opens the door for the next-generation PEFC for the “real world;” Discovery of the origin of detrimental chemical expansion in oxides commonly used in fuel cells. This discovery was achieved through synergistic coupling of atomistic level computational and experimental studies. This lays the groundwork to mitigate chemical expansion and improve fuel cell

mechanical durability and lifetime; TiFe, a potential candidate for hydrogen storage, was demonstrated to absorb and desorb hydrogen without activation when processed by High Pressure Torsion. It is for the first time that such a result has been reported and if scaled, it may lead to technology innovation; fundamental results for the development of Pt-free, non-precious catalysts in fuel cell technology by copying biology's ways to activate hydrogen; development of nanosized CO<sub>2</sub> separation membranes with high selectivity and flux to be used to control release of CO<sub>2</sub> emissions to the atmosphere and re-use the CO<sub>2</sub> as a carbon source for useful products (e.g. hydrocarbons); pioneering monitoring technology for detecting potential CO<sub>2</sub> leakage from sub-seabed storage reservoirs.

In addition, I<sup>2</sup>CNER is advancing green innovation, as demonstrated by the 18 submitted applications for patents and the large number of industries such as the automotive (TOYOTA, Nissan, and HONDA), Kyocera, Mitsubishi Hitachi Power Systems, JX Nippon Oil and Energy, Air Liquide, and the JFE Steel Corporation, that are benefiting from ongoing joint research projects with I<sup>2</sup>CNER researchers. A technology transfer event has already taken place through TOKi engineering on a new type of metal packing for high-pressure hydrogen.

#### 4. Interdisciplinary Research Activities

Fusion of disciplines is fostered by several initiatives, such as "I<sup>2</sup>CNER Competitive Funding," which supports research teams who can pass a rigorous assessment process by providing evidence of fusion work, such as published interdisciplinary papers. Cross-division collaborations in particular by young researchers have been initiated through several venues, such as the Institute Interest Seminar Series and Division retreats, which encourages I<sup>2</sup>CNER researchers to form teams by connecting with colleagues outside their group. The importance of interdisciplinary research is a requirement for promotion and tenure within the Institute, a fact that is clearly stated in the Institute's governing document on Faculty Promotion. By way of example, the Institute's list of interdisciplinary publications features articles that combine: materials synthesis, organic chemistry, nanotechnology, advanced characterization techniques, and electrochemistry for the synthesis of nitrogen-doped graphene as model metal-free non-precious electrocatalyst for PEFCs that shows impressive activity; thermodynamics, mechanical deformation, crystallography, and computational materials science that led to the discovery of the origin of the chemical expansion in SOFCs. Impressively, Prof. Ogo's group alone has produced 22 interdisciplinary publications that fuse several aspects of biology and inorganic chemistry to design catalysts for hydrogen activation and production, CO<sub>2</sub>-conversion and for water-splitting.

#### 5. International Research Environment

The Illinois satellite was established in August 2011 and its linkage with I<sup>2</sup>CNER has reached the level of joint publications between Kyushu and Illinois researchers in all thematic research areas of I<sup>2</sup>CNER's Divisions. Researchers from the two institutions have formed interdisciplinary teams, and mutual visits of graduate students, postdocs, and faculty between KU and the University of Illinois advance the interaction amongst the members. In addition, I<sup>2</sup>CNER's list of joint publications with international researchers features institutions such as MIT, Texas A&M University, the Dalian Institute of Chemical Physics, Tsinghua University, the University of Gottingen, Sandia National Laboratories, and the Plymouth Marine Laboratory. All 8 of our overseas Principal Investigators actively participate in I<sup>2</sup>CNER. They all visit I<sup>2</sup>CNER at least once a year, spending between one and four weeks at Kyushu to carry out collaborative research and participate in events. Recruitment of international postdocs and faculty is administered by the Faculty Recruiting Committee (FRC), which includes key members of the Institute and any other faculty who can provide input for cases of targeted hiring. I<sup>2</sup>CNER's assistant and associate professors are encouraged to develop their own research programs, independent of senior faculty. Young researchers, especially Japanese, are using the "Collaborative Foreign Exchange Program" in order to visit our overseas collaborating institutions. The program requires that interested researchers submit a 2-page proposal for approval. As of March 31, 2014, 7 young researchers (6 Japanese, 1 non-Japanese) had their proposals approved and 6 of them visited the Illinois Satellite through this program. Beginning in April 2014, one of our female assistant professors will start her 6-month stay at Sandia National Laboratories. The Administrative Office is in close communication with the existing International Student and Researchers Support Center of Kyushu University, and offers full-time support to international researchers in all areas including invitation procedures and living arrangements for campus accommodations or fully furnished private apartments with easy-access to Kyushu University.

#### 6. Implementing Organizational Reforms

Individual faculty and researcher salaries in I<sup>2</sup>CNER are based on individual accomplishments and contributions to the interests of the Institute. This is decided by the Director, in consultation with the two Associate Directors. As a follow-up, in order to promote revitalization and secure diverse and competent

personnel within the university, KU introduced a new merit-based annual salary system for faculty members in November 2011. Furthermore, KU went a step ahead of the MEXT "National University Reform Plan," and decided that the renewed system shall start in March 2014. To improve the standards of education and research, KU established rules on the Intra-University Faculty Transfer System, which went into effect December 1, 2012. Utilizing this personnel- system reform, 9 senior-level Kyushu PIs were transferred to the Institute from the Faculty of Engineering as of April 1, 2013, and as a result, their main affiliation is now with I<sup>2</sup>CNER. The same system is now used by the "Institute of Mathematics for Industry" for personnel transfers. I<sup>2</sup>CNER is spearheading KU's globalization efforts within the University Reform Revitalization Program and its faculty are instructors in the G30 Engineering Project. A New Education and Research Field, "Energy International Education," has been introduced in the Graduate School and School of Engineering as a vehicle for I<sup>2</sup>CNER full time faculty to teach and supervise graduate student research. At the same time, I<sup>2</sup>CNER is competing and has been granted tenured positions within the KU system. Through these activities, the Institute is becoming an influential and integral component of KU.

## 7. Future Vistas

I<sup>2</sup>CNER is at the center of KU's mid-term plan, which specifies that "Kyushu University will advance the cutting-edge research in carbon-neutral energy-related areas in collaboration with the University of Illinois." In addition, I<sup>2</sup>CNER is a unique asset for KU's globalization efforts in the context of the University Reform Revitalization Program. Its faculty will be engaged in education within the framework of KU's "Leaping into the World's Top 100" Action Plan (KU Globalization Strategy) and through the establishment of a new international course, "Carbon-Neutral Energy International Education," which is intended to advance undergraduate education taught in English. Within the globalization initiative, KU is planning to negotiate a program with the University of Illinois to send KU researchers from all disciplines to spend time in residence at Illinois for extended periods of time.

To sustain the I<sup>2</sup>CNER as a WPI program after the termination of the WPI funding, KU currently is planning to: a) raise the number of I<sup>2</sup>CNER's faculty to 20 through the Intra-University Faculty Transfer System and I<sup>2</sup>CNER's proposals for tenured positions; and b) explore the case of corporation-supported non-tenured faculty members whose research is impactful to the corporation's operations, securing resources from technology transfer or patent sales through active engagement of the KU office for technology transfer (IMAO), seeking contributions from foundations associated with KU, leveraging of the initiatives of the Government of Japan for globalization due to KU's unique position through its linkage with the University of Illinois.

## 8. Others

In order to promote engagement with leaders of the national and international community, and enhance its visibility, the Institute is running the "I<sup>2</sup>CNER Seminar Series," which features distinguished and internationally-recognized researchers from academia, national laboratories, and industry, as well as policy makers in government agencies. More than 50% of the speakers in this series have been non-Japanese.

## 9. Center's Response to Results of FY2013 Follow-up (including Site Visit Results)

*Director's Physical Presence:* increased from 46% in FY 2012 to 48% in FY 2013. *Recruitment of Permanent-staying Foreign PIs:* The Institute's Faculty Recruiting Committee (FRC) has conducted an extensive recruiting campaign to hire permanent-staying foreign principal investigator(s); *Kyushu-Illinois Researcher Exchange:* In FY 2013, this exchange has intensified. 23 researchers from KU visited UIUC, of which 16 stayed for under 1 week, 5 stayed between 1 week and 1 month, and 2 stayed for a period longer than 1 month. 22 researchers from UIUC visited KU in FY 2013, of which 19 stayed for a period of less than 1 week, and 3 stayed between 1 week and 1 month; *Post-doc Appointments:* Candidates for PI lines are hired after screening by the FRC and approval by the Director; *Division Research Themes/Projects & Research Work by Young Faculty:* In FY2013, close interaction of the EAD with the research divisions resulted in roadmap maturation for all divisions with refocused projects and objectives. Young researcher's efforts now have clear milestones and ultimate targets. This, along with support which the division PIs provide, helps them focus their research activities; *Internal Programs Review Committee (IPRC):* it is now a standing committee that reviews each individual research effort of the Institute; *Success Metrics:* I<sup>2</sup>CNER is a mission-driven (Green Innovation) research center, but is focused on basic science. As such, it can be evaluated on metrics that assess: relevance to enabling the green innovation initiative of the government of Japan, quality of the publications in high impact, discipline-oriented journals, degree of realization of milestones and targets in research roadmaps, number and quality of participating industrial partners, and quality of international collaborations; *Technology transfer:* From the inception of I<sup>2</sup>CNER, there have been 16 applications for patents, one (1) technology transfer event, and one licensing event.

# World Premier International Research Center Initiative (WPI)

## Self-Evaluation Report for Interim Evaluation

Host Institution	Kyushu University	Host Institution Head	Setsuo Arikawa
Research Center	International Institute for Carbon-Neutral Energy Research (I <sup>2</sup> CNER)	Center Director	Petros Sofronis

Common Instructions:

- \* Please prepare this report based on the current (31 March 2014) situation of your WPI center.
- \* As a rule, keep the length of your report within the specified number of pages. (The attached forms are in addition to this page count.)
- \* Use yen (¥) when writing monetary amounts in the report. If an exchange rate is used to calculate the yen amount, give the rate.

### 1. Summary of State of WPI Center Project Progress (write within 2 pages including this page)

*Describe the center's identity and the achievement status of its initially stated goals.*

- *On the sheets in Appendix 1, list the Principle Investigators, and enter the number of center personnel, a chart of the center's management system, a campus map showing the center's locations on the campus, and project funding.*

I<sup>2</sup>CNER will achieve its vision for a carbon-neutral society (CNS) through discovery, development, and deployment of energy technologies capable of reducing greenhouse gas (GHG) emissions by 70-80% from 1990 levels by 2050. Achieving this target is critical to the energy security and economic welfare of Japan because of the nation's dependence on imported fossil fuels; it also is central to the long-term well-being of the world. The vision is based on two basic principles, which guide the strategy behind the research and development of new technologies in I<sup>2</sup>CNER: efficiency increase (EI) in energy conversion and use and lowering of carbon intensity (LCI) of fuel and electricity. EI is pursued in energy transformation systems as well as end use systems, including those in the residential and commercial sectors. This idea will also be pursued in industrial processes. EI can be applied to existing systems, but is also achieved by replacing existing systems with new technology. LCI in electricity and fuel supply-use pathways can be achieved using either renewables, carbon capture and sequestration, or nuclear energy. LCI tends to need new facilities or new infrastructure or both. The I<sup>2</sup>CNER vision includes all EI and LCI technologies, not only those currently being researched within I<sup>2</sup>CNER.

There are many possible combinations of new EI and LCI technologies and deployment timing (scenarios) that can lead to the targeted GHG emissions reduction by 2050. To date, I<sup>2</sup>CNER has generated four such scenarios utilizing the most promising of the new technological options. The degree of success and deployment timing of the selected EI and LCI technologies creates the variability among the scenarios. I<sup>2</sup>CNER's research efforts are intimately tied to these four scenarios because the short-, mid-, and long-term milestones of each of our division roadmaps were established in consideration of the development and deployment timing of the various promising technology options in the scenarios. The scenarios currently under consideration, which include the I<sup>2</sup>CNER research efforts, are: a) the Base Scenario, which relies on development of important EI technologies and balanced deployment of renewables and carbon capture and storage (CCS), b) the Renewables Scenario, involving very large penetration of renewables for LCI and development of important EI technologies, c) the CCS Scenario, involving large deployment of CCS for power and industries, especially for coal and development of important EI, and d) the "Some Nuclear" Scenario, involving balanced application of LCI technologies, including nuclear power. These scenarios, which help ensure the relevance of I<sup>2</sup>CNER's research and roadmaps to CNS, enable assessment and determine future directions, including pursuit of new research strategies such as biological CCS, biomimetic catalysis, and nuclear safety and reliability of materials.

State-of-the-art research aiming at the short term milestones in the Division roadmaps is attacking the problem of energy demand through both the source (production of fuels, their storage and transport) and sink (improved fuel cells to produce electricity and lower demand through efficiency) areas. A few selected results are as follows: a) correlated metal oxides coupled to TiO<sub>2</sub> produce electrodes for photoelectrochemical cells that are stable and promote rapid and efficient H<sub>2</sub>O electrolysis; b) development of polybenzimidazole membranes for fuel cells; these have delivered high power densities for 400,000 cycles at 120°C, a dramatic advance; c) discovery that charge localization on reduced cations is the origin of the detrimental chemical expansion in oxides commonly used in SOFCs; d) enhanced performance of light emitting devices through use of molecules incorporating large spin-orbit coupling, which allows for nearly 100% of the excitons in the device to be able to generate electroluminescence. This highlight demonstrates how advanced computational models can be used to accelerate the discovery

of new molecules and materials, which can then be synthesized. The strategy of using computational methods to explore for new systems will be an emerging theme in the institute; e) discovery of the activation mechanism in TiFe intermetallics by High Pressure Torsion, a promising system for stationary energy storage; f) proposed a new model of hydrogen-induced cracking that is hydrogen-accelerated plasticity-mediated failure; g) high speed imaging has been used to demonstrate hydrothermal waves to be bulk waves in heat transfer fluid droplets. This controls evaporation, a key component of multi-phase heat pumps; h) 200 nm-thick epoxy layers with amine residues on porous membranes have been shown to selectively transport CO<sub>2</sub> relative to N<sub>2</sub>; this has serious implications for capture of CO<sub>2</sub>. Poly(amidoamine) dendrimers have also shown selectivity relative to H<sub>2</sub>; i) simulation studies of CO<sub>2</sub> trapping demonstrated that pore space reduction due to mineral precipitation has a greater influence on the non-wetting phase than on the wetting phase.

Fusion of disciplines is fostered by several initiatives, such as "I<sup>2</sup>CNER Competitive Funding," which supports research teams who can pass a rigorous assessment process by providing evidence of fusion work, such as published interdisciplinary paper. Cross-division collaborations involving young researchers have been initiated through venues such as the Institute Interest Seminar Series and division retreats. These activities enable I<sup>2</sup>CNER researchers to pursue new research directions by forming teams with colleagues outside their traditional group. The fact that Prof. Ogo's group alone has produced 22 publications that are interdisciplinary indicates that interdisciplinary research is part of the Institute's research culture.

I<sup>2</sup>CNER is achieving recognition as a world class institute. Evidence of this visibility is its increasing number of collaborations worldwide. Across the USA, the Institute is engaged with Sandia National Laboratories at Livermore, CA; Pacific Northwest National Laboratory, WA; University of Wisconsin-Madison; MIT; the National Fuel Cell Research Center at the University of California, Irvine; and in Europe, the Norwegian University of Science and Technology (NTNU), Norway; SINTEF, Norway; Imperial College, London, UK; University of Göttingen, Germany; and the University of Oxford, UK. Papers written by faculty from I<sup>2</sup>CNER and these international partners are being published. For its energy vision and research portfolio, I<sup>2</sup>CNER is exchanging information with the US DOE EERE Fuel cells program, co-sponsoring international conferences and symposia with international societies such as the Minerals, Metals, and Materials Society (TMS) and the International Society of Solid State Ionics (ISSI), and assisting government agencies both in Japan and the US in the advancement of initiatives on renewable energy, energy efficiency, and new energy technologies.

I<sup>2</sup>CNER is advancing green innovation through several venues: applications for 18 patents have been submitted by I<sup>2</sup>CNER researchers since the inception of the Institute. A large number of industries such as the automotive (TOYOTA, Nissan, and HONDA), Kyocera, Mitsubishi Hitachi Power Systems, JX Nippon Oil and Energy, Air Liquide, and the JFE Steel Corporation are benefiting from ongoing joint research projects with I<sup>2</sup>CNER researchers.

I<sup>2</sup>CNER, through its interaction with Kyushu University (KU), is impacting the traditional Japanese research structure and faculty model. I<sup>2</sup>CNER's academic structure and processes of promotion, tenure, and merit-based compensation of its faculty and postdocs are according to the highest standards for international research centers. In this capacity, I<sup>2</sup>CNER is enabling the actualization of the mid-term plan of Kyushu University, which specifies that "Kyushu University will advance the cutting-edge research in carbon-neutral energy-related areas in collaboration with the University of Illinois." I<sup>2</sup>CNER is also spearheading KU's globalization efforts within the University Reform Revitalization Program and its faculty are instructors in the G30 Engineering Project. A New Education and Research Field, "Energy International Education," has been introduced in the School and Graduate School of Engineering as a vehicle for I<sup>2</sup>CNER full time faculty to teach and supervise graduate student research. At the same time, I<sup>2</sup>CNER is competing and has been granted tenured positions within the KU system. Through these activities, the Institute is becoming an influential and integral component of the university. Further evidence of the impact of I<sup>2</sup>CNER on Kyushu University is the establishment of the Intra-University Faculty Transfer System, which aims to improve the standards of education and research conducted at the university. Transforming the research enterprise and system of Kyushu University was an initial goal and significant progress has been achieved, although much remains to be done.

In summary, I<sup>2</sup>CNER has achieved many of the initial targets: it is becoming an integral and influential part of Kyushu University, it has established a new model for faculty points, it has introduced a competitive peer-reviewed research methodology, and it continues to build and gain international stature as a leading research institute in creating a carbon neutral energy society.

## 2. Center's Research Activities (within 10 pages)

### 2-1. Research results to date

Provide an overall picture of the Center's research activities and select 10 representative results achieved during the period from 2010 through March 2014. Number the results [1] to [10] and provide a description of each.

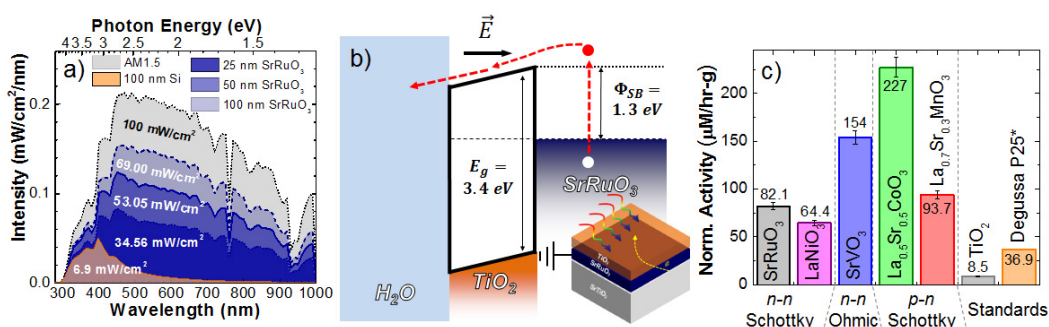
-In Appendix 2-1, list the papers underscoring each research achievement and provide a description of each of their significance.

### Hydrogen Production

The research in the division falls under the themes of energy production, conservation, and storage. Energy production is based on conversion of solar to electric energy. Fuel production is through hydrogen reduction and conservation is through enhanced lighting efficiency based on high efficiency solid state lighting. Research includes use of microstructural characterization techniques for analysis of the interface structure of organic dye and inorganic semiconductors in photocatalysts. Work is also carried out on 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 electrochemical and electrolytic water reduction. In summary, the objective of this division is to develop 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 for high efficiency lighting to contribute to energy consumption. Selected representative results are:

#### [1] Photocatalytic water splitting.

Current solar photocatalysts suffer from two critical problems: 1) those with band gaps that provide for ample light absorption are often not stable in solution and under illumination and 2) those that are stable, often possess band gaps that are too large for the efficient utilization of solar radiation. Our work addresses these challenges directly by applying lessons from condensed matter and semiconductor physics to develop a new class of strongly light-absorbing, stable materials. Our team is pioneering a fresh approach to engineered heterosystems for photocatalytic water splitting illustrated in Fig. 1. The approach is based on a highly-interdisciplinary coupling of 'correlated metal oxides' (a playground material for the condensed matter physics community), with titanium dioxide ( $\text{TiO}_2$ ), the workhorse material for photocatalytic water splitting. A fundamental limitation to the efficiency of  $\text{TiO}_2$  arises from its poor optical absorption ( $< 10\%$ ) of the solar spectrum. By contrast, correlated metal oxides such as  $\text{SrRuO}_3$  are unique because they display semiconductor-like optical absorption together in tandem with metal-like conductivity. The coupling of these two materials together offers a unique integrated functionality: large optical absorption in the correlated metal oxide (Fig. 1a), efficient charge transport of hot carriers from the oxide to the  $\text{TiO}_2$  (Fig. 1b), and the desirable surface chemistry of the  $\text{TiO}_2$  for catalyzing chemical reactions [1]. We have demonstrated the generality and wide-scale applicability of this approach by showing that several correlated metal oxide –  $\text{TiO}_2$  integrated systems ( $\text{SrRuO}_3$ ,  $\text{LiNiO}_3$ ,  $\text{SrVO}_3$ ,  $\text{LaSrMnO}_3$ ,  $\text{LaSrCoO}_3$ ) exhibit similar dramatically enhanced photocatalytic activity [2] (Fig. 1c).

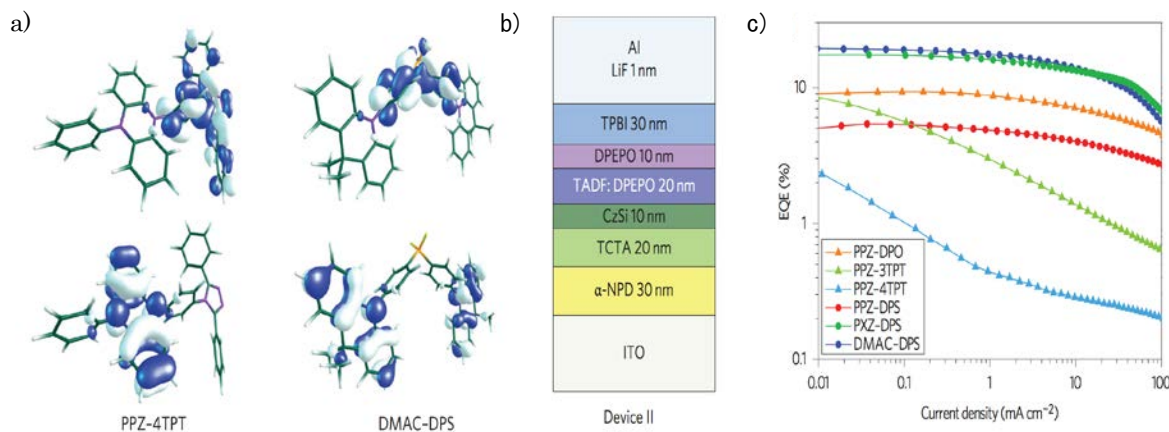


**Fig. 1:** a) Optical absorption from integrated  $\text{SrRuO}_3/\text{TiO}_2$  heterosystem, b) Hot carrier injection enables the photoexcited carriers to quickly transfer from the  $\text{SrRuO}_3$  to the  $\text{TiO}_2$ , c) The relative activity of various correlated metal oxide/ $\text{TiO}_2$  material systems for [1,2].

A parallel notable accomplishment is the creation of nanosheet p-n and n-p junctions [3], (NiO/Ca<sub>2</sub>Nb<sub>3</sub>O<sub>10</sub> and Ca<sub>2</sub>Nb<sub>3</sub>O<sub>10</sub>/NiO, respectively) the latter of which demonstrates substantially enhanced hydrogen evolution in comparison to the former and the isolated nanosheets. We provide a fundamental understanding of the surface chemistry origin of the high activity of the n-p architecture via Kelvin probe microscopy, which shows that the enhanced hydrogen production is accomplished by the introduction of a potential gradient at the surface that spatially separates the oxidation and reduction sites to prevent the recombination reaction.

## [2] Organic light emitting devices (OLEDs)

Organic light-emitting diodes (OLEDs) have been considered for a long time as a promising approach to solid-state, high-efficiency, low power lighting. However, efficiencies remain too low, while costs are sometimes prohibitively high. In the most-commonly used fluorescence-based scheme, light-generating capacity is limited because only 25% of the excited carriers (the singlets) can produce light. This limitation arises from quantum mechanical transition rules that prohibit radiative decay of triplet excitons (which comprise the other 75%). By contrast, in the newer phosphorescence-based schemes, large spin-orbit coupling eliminates this limitation and allows for nearly 100% electroluminescence. However, widespread usage of the phosphorescence schemes is hampered by the need to use expensive and rare noble metals; additionally a reliable blue-emission phosphorescence based scheme had not been demonstrated. In this accomplishment, we have conceived and demonstrated a fundamentally new approach to blue OLEDs that enables light generation from all excited carriers, without the need for noble metals [4]. The approach is based on thermally-activated delayed fluorescence (TADF), a third-generation scheme developed by the Adachi group and subsequently enhanced thereafter [5]. The new approach relies on thermally-activated charge-transfer: a thermally accessible gap between the lowest singlet and the triplet excited states enables the harvesting of both singlet and triplet excitations to achieve high-efficiency. Quantum mechanical computational modeling and simulation was used to design and assess several candidate molecular systems and identify those that exhibit the desired low energy difference between the singlet-triplet charge-transfer state (Fig 2a). The newly conceived system, with device structure shown in Fig 2b, exhibits an external quantum efficiency of 19.5% (Fig 2c), comparable to the best phosphorescent OLEDs that are commonly used today.



**Fig. 2:** a) Molecular complexes considered using first-principles modeling for thermally-activated delayed fluorescence, b) Device structure of the ~20% external quantum efficiency blue OLED, c) Measured external quantum efficiency of several systems, including the ~20% external QE blue OLED [4].

## Hydrogen Storage

The research in the division aims at developing new carrier materials for hydrogen mobile and stationary storage as well as for hydrogen delivery. For mobile hydrogen storage the material based storage system must meet the needs of hydrogen fuel cell vehicles in terms of volume, weight percent hydrogen, cost, fast charging and discharging, and durability with high well-to-wheel energy efficiency. Hydrogen delivery systems based on hydrogen-absorbing materials are focused on cost effective truck transport of large amounts of hydrogen. Material based stationary hydrogen storage applications must be more cost effective and energy efficient than conventional pressurized gaseous hydrogen storage or uniquely meet particular requirements of specific stationary applications.

The uniquely-important accomplishments of this division are: demonstration of the microscopic degradation



mechanisms in certain hydrogen storage materials [6]; development of advanced materials synthesis methods to advance the performance of other hydrogen storage materials [7]; and a method has been discovered that greatly enhances the performance of a third hydrogen storage material and opens an entirely new range of materials and approaches to hydrogen storage [8, 9]. Selected representative results are:

### [3] Hydrogen storage materials for fuel cell vehicles and stationary storage, and a new pathway for development of hydrogen storage materials using High Pressure Torsion (HPT)

V-Ti-based BCC structure alloys are one of the most promising candidates for on board applications. The research in the division focuses on removing the two major roadblocks: low gravimetric capacity and short cycle life. The gravimetric capacity roadblock derives from microstructure evolution and lattice defect generation with hydrogenation cycles. With the use of transmission electron microscopy (TEM) the division's work elucidated the effects of Ti/V ratio on the microstructure and hydrogenation/dehydrogenation properties of Ti-V binary BCC [6]. It was found that the effective hydrogen capacity decreases and the density of twin boundaries increases with increasing Ti content. This indicates that twin boundaries formed upon hydrogenation act as hydrogen traps, thus increasing the desorption resistance of these alloys which was also found to correlate with the increased enthalpy for hydride formation with increasing V content. Metal borohydrides, e.g.  $M(BH_4)_n$ , have hydrogen capacity of over 10 wt %, but reaction speed and hydrogen release temperature are serious roadblocks at present. To study and improve the thermodynamic and kinetic properties of this system, the division developed a novel solvent-free synthesis process [7] that can be applied to the synthesis of various kinds of dehydrogenation intermediates (e.g.  $[B_3H_8]^-$ ,  $[B_5H_9]^{2-}$ ), which are extremely important to the clarification of the de- and re-hydrogenation mechanisms of metal borohydrides.

TiFe is a low price ideal hydrogen storage material for stationary storage. It absorbs and desorbs hydrogen at room temperature under ambient hydrogen pressure in a more compact form than liquefied hydrogen. Although it has been reported as a storage system in late 1970s, it was abandoned for decades because activation (hydrogen absorption/desorption) requires heating at temperatures higher than 400°C under 30 bar (or higher) of hydrogen. In an ongoing collaboration, PIs Akiba and Horita targeted this issue of activation based on their complementary background, ideas, and techniques. Using high-pressure torsion (HPT) techniques, PI Horita and his co-workers introduced enormously large strains in TiFe samples and measured their hydrogen storage and cycle life properties. Surprisingly, TiFe after the HPT treatment readily absorbs hydrogen without activation at high temperature and high pressure as was required before (Fig. 3) [8]. In addition, even though Ti and Fe are easily oxidized, TiFe exposed to air for a few months after several cycles of hydrogenation/dehydrogenation still readily reacts with hydrogen without activation. Fe-rich islands forming by HPT are suggested to act as catalysts for hydrogen dissociation, the microcracks and nanograin boundaries act as pathways for hydrogen transport, and probably dislocations for the sites of hydride formation [9].

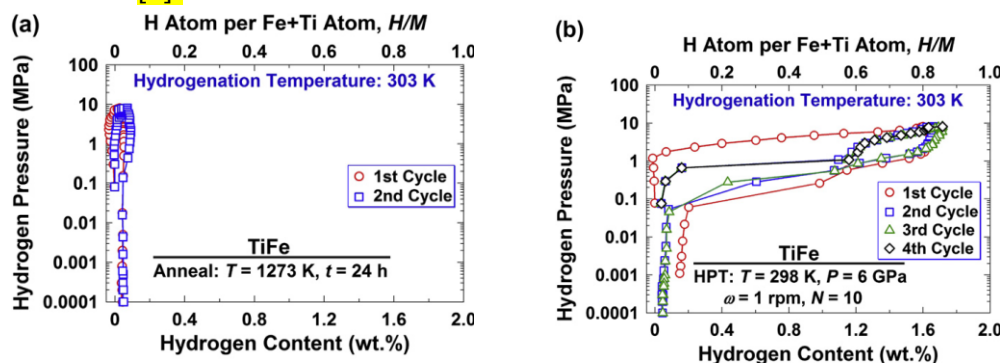


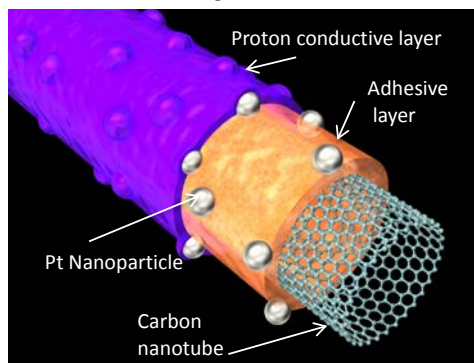
Fig. 3: Pressure-composition isotherms for (a) annealed samples and (b) HPT-processed sample

### Fuel Cells

The objective of this division is to develop more durable and efficient lower cost fuel cells (polymer electrolyte fuel cells (PEFC) and solid oxide fuel cell (SOFC)) to significantly reduce CO<sub>2</sub> emissions in the production of electricity and heat. In PEFCs efforts are directed at a) the development of a higher temperature (> 100°C) hydrogen PEM fuel cell with durable catalyst support (e.g. graphene, carbon nanotube, mesoporous carbon, SnO<sub>2</sub>), b) finding and evaluating high temperature electrolytes with

emphasis on a polybenzimidazole (PBI)-based ionomer in combination with carbon nanotubes, but other materials such as graphene and charge-transfer complexes (CT-complex hybrid films) are also examined. In SOFCs efforts are directed at exploring degradation mechanisms of pressurized SOFCs and understanding fundamental surface/interfacial catalytic processes on metal oxides for fuel-flexible stationary and power-plant applications, especially Integrated Gasification Fuel Cell Combined Cycle (IGFC) and Natural Gas Triple Combined Cycle. Selected representative results are:

#### [4] Alternative Electrocatalysts



**Fig. 4:** Carbon nanotube-based fuel cell electrocatalyst without any defect sites that shows ~100 times higher durability than a conventional carbon black fuel cell catalyst [10]. The catalyst was fabricated by a bottom-up nano-assembly method.

A novel polymer electrolyte fuel cell (PEFC) exhibiting remarkably high durability (single cell test: >400,000 cycles) along with high power density operating at 120 °C under non-humidified conditions has been developed (Fig.4). It should be noted that since the current state-of-the-art PEFC for high-temperature operation only shows durability much below 80,000 cycles, the results can be deemed outstanding. The dramatic improvement in durability was achieved by the use of a (polybenzimidazole)PBI membrane developed by the group of PI Nakashima and which is free from acid leaching together with a carbon nanotube catalyst support [10-16]. Such a highly durable PEFC for high-temperature operation will accelerate the technological shift from Nafion-based low-temperature PEFC to e.g. PBI-based high-temperature PEFC. By realizing the high-temperature PEFC, PEFC will achieve a higher efficiency and lower Pt poisoning than Nafion-based PEFC. In addition, since high purity of H<sub>2</sub> is not necessary for high-temperature PEFC, large cost reduction can be expected.

In the area of Pt-free/non-precious catalysts for the oxygen reduction reaction at PEFC cathodes, the conventional approach utilizes pyrolyzed Fe/N/C-based catalysts; nitrogen-doped, iron-containing catalysts. However these catalysts have complicated chemical structures and therefore the reaction mechanisms are poorly understood. Our approach is to synthesize a simplified Fe-free model catalyst system in order to clarify the role of nitrogen in these catalysts; specifically if 4-electron oxygen reduction to water is possible in the absence of Fe in order to engineer better, non-precious catalysts. A nitrogen-doped graphene foam has been developed with large surface area (> 700m<sup>2</sup>/g) and optimized over several years for high electrochemical activity, in fact the highest ever reported for such Fe-free catalysts in acid [17]. Because of the higher current density, we have been able to reveal new insights; specifically that majority 4-electron oxygen reduction is possible in the absence of Fe. For the first time a double-Tafel slope has been recorded which indicates a Pt-like oxygen reduction mechanism.

These results provide considerable hope that a low-cost, highly durable fuel cell operating at temperatures between 100 and 200 °C with attendant increase in kinetics and decrease in sensitivity toward poisons, especially CO, might be possible.

#### [5] Understanding the origin of chemical expansion in SOFCs and developing new materials with reduced chemical expansion.

In many advanced electrodes for low temperature SOFCs, non-stoichiometry induced dilation, known as chemical expansion, can lead to large strains with consequent stresses during operation, ultimately resulting in mechanical failure. The group of PI Tuller, Bishop, and Perry undertook an empirical and computational study of the origins of chemical expansion in fluorite structured SOFC materials in FY2011 resulting in a publication in *Advanced Functional Materials* showing the critical role of both cations and oxygen vacancies [18]. Building upon this study, the group found with the help of PI Kilner's insight in FY2013 that lattice relaxation around oxygen vacancies was a potential key method to manipulate, by cation substitution, the chemical expansion coefficient [19]. The group then undertook an experimental/computational study to identify the role of isovalent Zr substitution in cerium oxide on

chemical expansion. With the aid of K. Ameszawa (Tohoku University) chemical expansion was derived experimentally using HTXRD, dilatometry, and TGA measurements on  $\text{Pr}_{0.1}\text{Zr}_{0.4}\text{Ce}_{0.5}\text{O}_{1.95-\delta}$  and computationally with density functional theory (DFT) calculations on  $\text{Zr}_{0.5}\text{Ce}_{0.5}\text{O}_{2-\delta}$  [20]. Though Zr was found to increase the reducibility and the corresponding chemical expansion of ceria (in the studied range), the relationship between chemical expansion and non-stoichiometry (the chemical expansion coefficient) was significantly smaller (54% less) than that observed in ceria, and consistent with predictions from the previous work. The origin of the reduced chemical expansion coefficient, associated with a larger contraction of the lattice around oxygen vacancies, was explained using DFT calculations and corroborated with prior investigations of enhanced reducibility of ceria-zirconia and published by the group in FY2013

The team is now extending this work to perovskite structured oxides, which are more commonly found in energy related applications such as SOFCs, though due to their more complicated structure, are inherently more challenging to study. Recent work by the group has demonstrated that charge localization on reduced cations can play a significant role in chemical expansion, as published in FY2012-2013. Lastly, this intensive research on chemical expansion has culminated in the publication of the first comprehensive review of chemical expansion in energy-related materials available online [21].

This discovery has strong implications for reducing chemical expansion in SOFCs, thus increasing their durability, and the studied material has potential for use in SOFC electrode functional layers as is currently being investigated.

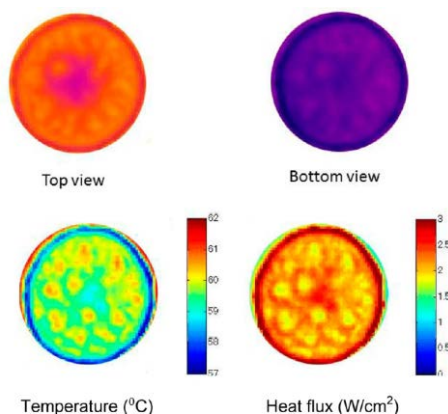
### Thermal Science and Engineering

The objective of this division is to enable the most effective use of materials in carbon-neutral energy technologies and to improve the energy efficiency of thermal processes by expanding our knowledge of material thermophysical properties and thermal science and engineering. More specifically research in the division aims at: expanding our knowledge-base of thermophysical properties of hydrogen and alternative refrigerants to enable their most efficient use to reduce  $\text{CO}_2$  emissions; improving our understanding of the basic science of heat and mass transfer to enable the development of more efficient energy systems; and researching new thermal energy heat pump and refrigeration systems focused on the use of waste heat and new refrigerants for improved overall energy efficiencies and reduced  $\text{CO}_2$  emissions.

Selected representative results are:

#### [6] Interaction between evaporation and dynamic wetting

The evaporation and interaction of liquids with solid materials [22, 23] have direct consequences on technologies such as power generation, heat pump, refrigeration systems, and thermal control. Two important types of liquid heat transfer can be highlighted: evaporation in which a phase change occurs leading to motion of the vapor until it recondenses elsewhere and dynamic wetting in which the triple line corresponding to the meeting of the three phases moves over a solid are fundamental heat-transfer phenomena that although have been studied separately, it is only recently that their interaction effects have been explored. Using infrared (IR) thermography, PI Takata and coworkers [24] were the first who reported experimental measurements of temperature and heat flux at the liquid-wall interface during the evaporation of sessile FC-72 (a working fluid for thermal transport devices). Simultaneous high-speed imaging of the evaporating drop was also carried out to monitor the drop profile (Fig. 5).



**Fig. 5.** Evaporation of a 2.5- $\mu\text{L}$  FC-72 droplet on a substrate at 66 °C as represented by a snapshot at  $t = 0.167$  s of its lifetime. Upper panels show raw IR data from the top and bottom surfaces. Lower panels show the extracted temperature and heat-flux distributions on the bottom surface [24]

The study demonstrates that recently evidenced hydrothermal waves are actually bulk waves that extend across the entire droplet volume. More importantly, thermal patterns occurring in the bulk of

the drop affect the temperature and heat-flux distributions on the solid substrate and ultimately influence the droplet evaporation rate. These effects were found to be increasingly pronounced as the substrate temperature was raised.

### Catalytic Materials Transformations

The objective of this division is to contribute to the creation of innovative carbon-neutral technologies by developing novel catalysts, underlining both aspects of basic science and engineering. These activities are focused on investigating catalysis-related "Solar Energy and Energy Conservation," all of which have the potential to significantly increase energy efficiency and reduce CO<sub>2</sub> emissions in energy, power or industrial production processes. Projects in the division address the development of: novel biomimetic catalysts for H<sub>2</sub>, CO<sub>2</sub>, and H<sub>2</sub>O activation based on naturally occurring enzymes; new less energy-requiring and green material transformation systems using ubiquitous and abundant air as oxidant; and catalysis for fuel oxidation and regeneration and production of novel materials for carbon neutral power generation cycles. Selected representative results are:

#### [7] Biology's ways with hydrogen: The first synthetic analog of the active site of the [NiFe] hydrogenase that oxidizes hydrogen

Chemists have long sought to mimic enzymatic hydrogen activation with structurally simpler compounds. The group of PI Ogo reported a functional [NiFe]-based model of [NiFe]hydrogenase enzymes (Fig. 6). This complex heterolytically activates hydrogen to form a hydride complex that is capable of reducing substrates by an electron transfer or a reaction with a hydride. Structural investigations were performed by a range of techniques, including x-ray diffraction and neutron scattering, resulting in crystal structures. It was found that the hydrido ligand is predominantly associated with the Fe center. The ligand's hydridic character is manifested by the liberation of H(2) via reactions with strong acids. This successful synthesis of the [NiFe]hydrogenase mimic heterolytically activates hydrogen to form a hydride complex that is capable of reducing substrates by an electron transfer or a reaction with a hydride [25-27]. These results will help accelerate hydrogen fuel cell technology, and emphasize the dramatic progress of hydrogen activation using a non-precious metal catalyst, leading the way toward a low-cost hydrogen fuel cell [28].

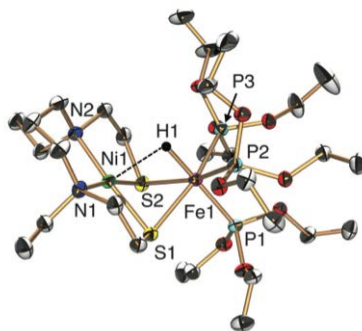


Fig. 6: Electron extraction from hydrogen gas with the nickel-iron catalyst [25].

### Hydrogen Materials Compatibility

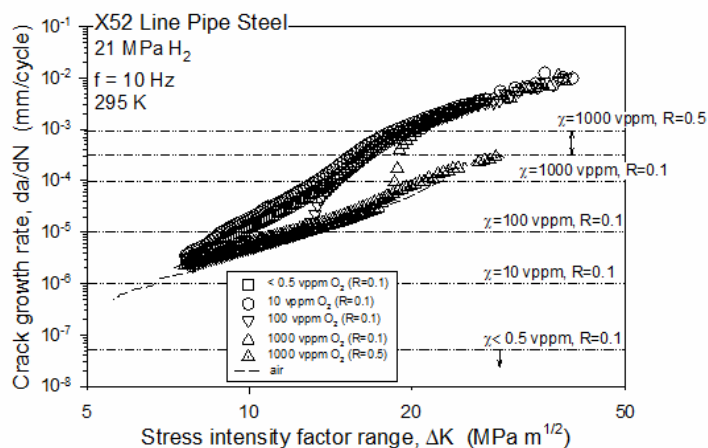
The goal of this division is to provide the basic science that enables optimization of the cost, performance, and safety of pressurized hydrogen containment systems. In particular the objectives include: development and use of advanced methods for experimentally characterizing the effects of hydrogen on the fatigue, fracture, and tribological properties of materials; development of models of hydrogen-affected fatigue, fracture, and tribo-interfaces; and development of next-generation monolithic and functionally graded materials having lower cost and improved performance (e.g., higher strength) while retaining resistance to hydrogen-induced degradation. Selected representative results are:

#### [8] Elucidating the variables affecting accelerated fatigue crack growth in hydrogen gas with low oxygen concentrations.

Hydrogen gas can dramatically accelerate fatigue crack growth rates in low strength ferritic steels that are technologically favored for hydrogen production, storage, and distribution components. Evidence indicates that such accelerated crack growth can be inhibited by trace concentrations of oxygen in the hydrogen gas. However, this inhibition has never been quantified as a function of the environmental

and mechanical variables that govern cracking.

In FY2011 and FY2012, fatigue crack growth rate experiments were performed on the pipeline steel X52 in hydrogen gas with controlled oxygen concentrations. The approach in these experiments represented a radical departure from previous studies, since key variables, e.g., oxygen concentration, load-cycle frequency, and mean stress, were identified and systematically varied. As a result, unequivocal trends for the effects of oxygen on hydrogen-accelerated crack growth were revealed for the first time. The quality of these data enabled postulation of the physics governing oxygen inhibition of hydrogen-accelerated crack growth [29]. Based on these proposed physics, in FY2012 and FY2013 an analytical model was developed to predict inhibition as a function of inert-environment crack growth rate, oxygen concentration, load-cycle frequency, and mean stress. The model accurately quantifies how these variables affect the onset of accelerated crack growth for X52 steel in hydrogen gas containing trace oxygen concentrations (Fig. 7). In summary, this model is the only predictive capability for quantifying the effects of oxygen on hydrogen-accelerated fatigue crack growth.



**Fig. 7:** The measured onset of hydrogen-accelerated crack growth (symbols) is reliably predicted (dashed lines) as a function of oxygen concentration ( $\chi$ ) and mean stress (R) [29].

In parallel with development of the predictive analytical model, a first-principles study was conducted to define the basic mechanisms for oxygen inhibition of hydrogen uptake into steel [30]. By applying density functional theory (DFT) modeling, several characteristics of hydrogen-oxygen competitive co-adsorption on iron surfaces were discovered, i.e.: 1) oxygen can out-compete hydrogen for surface adsorption sites since the gas molecule-iron surface attractive force is stronger for oxygen compared to hydrogen, and 2) adsorbed oxygen on iron surfaces increases the activation barrier for molecular hydrogen dissociation on this surface, since the highly electronegative oxygen concentrates electron density in its vicinity. Although the poisoning effect of oxygen on hydrogen dissociation has been recognized for catalysts, the association of this phenomenon with oxygen inhibition of hydrogen uptake into steels was not previously demonstrated.

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

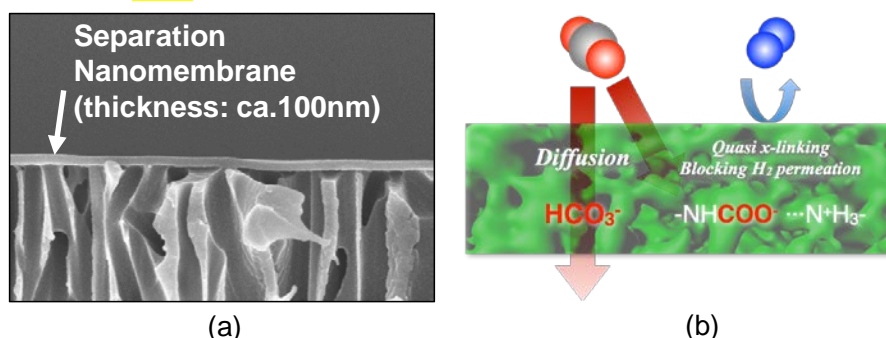
The objective of this division is to develop: highly efficient materials for CO<sub>2</sub> separation in power generation and industrial processes; and electrochemical systems to convert CO<sub>2</sub> into value-added chemicals, such as a liquid fuel or their intermediates, by an energy efficient and cost effective way. More specifically in the area of CO<sub>2</sub> separation the objective is to develop novel membrane technology to separate CO<sub>2</sub> in the process of pre-combustion for Integrated Coal Gasification Combined Cycle (IGCC), post-combustion at power plants and other industries, and gas purification at natural gas wells. In the area of electrochemical conversion to develop novel catalysts and electrodes. It is emphasized that membrane separation presents serious scientific challenges. Conventional membrane technologies are currently suffering from small gas permeability, though their CO<sub>2</sub> selectivity is now reaching levels which are practically acceptable. In order to solve this problem, membrane thinning is a most promising approach. However, the thickness of current membranes is still in the order of a few micron scale. Thus, the material design and development of thinner membranes for selective gas separation are central research issues in the division. Selected representative results are:

### [9] Free-standing and nanometer-thick membrane for gas separation and elucidation of the mechanism of preferential CO<sub>2</sub> permeation

The group of PI Fujikawa succeeded in preparing a nanometer-thick membrane by a conventional spincoating process (patent submitted). It was demonstrated that the membrane of an epoxy resin

with less than 200 nm can be transferred and fixed on to a porous support stably (Fig. 8a) and CO<sub>2</sub> gas passes through preferentially in comparison to nitrogen gas under humid conditions. This result was a first example of preferential CO<sub>2</sub> separation by a nanometer-thick membrane. In this membrane, amine residues of epoxy resin are necessary not only for making a membrane hydrophilic but also for good affinity with CO<sub>2</sub>.

The group of Dr. Taniguchi applied photopolymerization of poly(ethylene glycol) (PEG) dimethacrylate in the presence of dendrimers to fabricate dendrimer-containing polymeric membranes. The group found that Poly(amidoamine) (PAMAM) dendrimers exhibit excellent affinity to CO<sub>2</sub> [31]. The resulting membranes show excellent CO<sub>2</sub> separation performance over H<sub>2</sub>. It was identified that the parameters controlling the CO<sub>2</sub> separation membrane properties are PAMAM dendrimer fractions, generation, phase-separated structures (PEG length), and humidity. The mechanism of preferential CO<sub>2</sub> separation of PAMAM dendrimers was elucidated (Fig. 8b) and can be summarized by the term "Molecular Gate:" CO<sub>2</sub> turns to bicarbonate and carbamate, and the former is the major migrating species through the polymeric membrane while the latter suppresses H<sub>2</sub> permeation by the formation of quasi-crosslinking with PAMAM dendrimers [32].



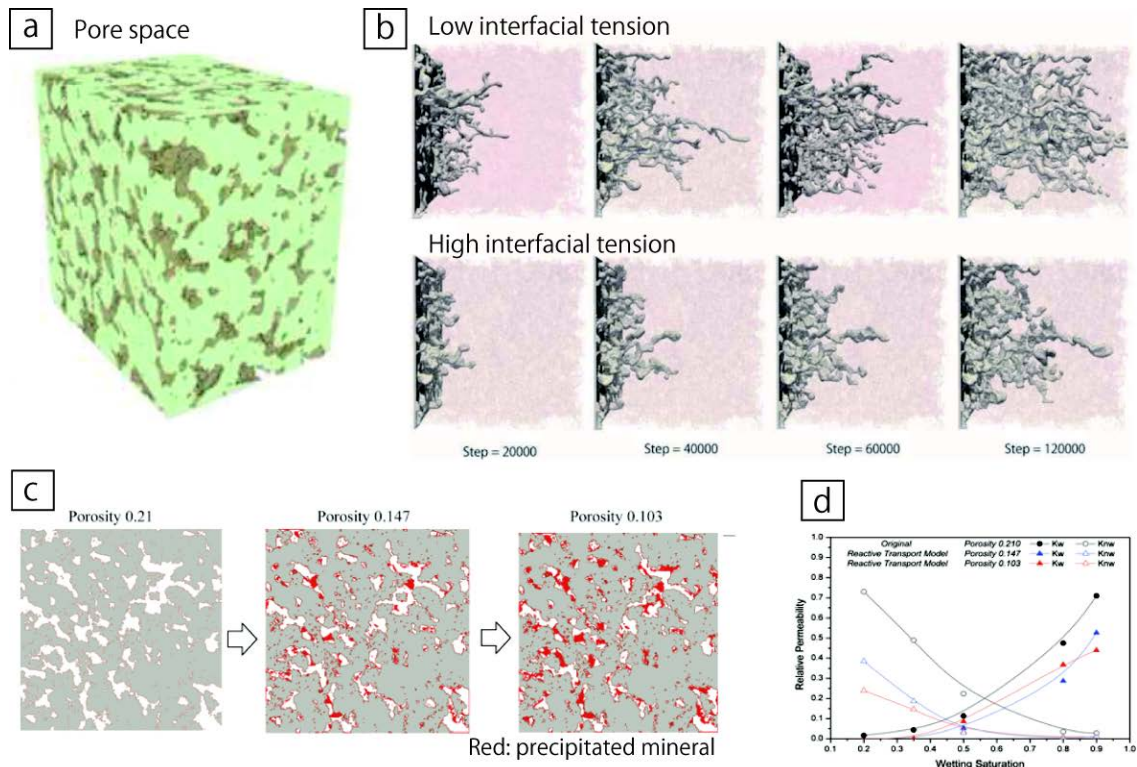
**Fig. 8.** a) A uniquely thin membrane (<100nm) for high flux CO<sub>2</sub> separation, b) Mechanism for preferential CO<sub>2</sub> permeation of the in-house developed PAMAM dendrimer-containing membranes: quasi-crosslinking of dendrimers through carbamate forms that prevent H<sub>2</sub> permeation.

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

The objective of this division is to: develop methods of reservoir characterization and modeling, and new effective monitoring of injected/leaked CO<sub>2</sub> to help ensure safe and permanent CO<sub>2</sub> sequestration in sub-seabed geologic formations; and propose and realize new carbon storage concepts suitable for geological formations and rock types typical in Japan. The research projects and efforts have been established in such a way that they take into consideration the heterogeneity of the geological formations in Japan, the limited availability of geological data for CO<sub>2</sub> injection in aquifer formations and the requirement for long term monitoring of pressure variations near seismogenic faults. Selected representative results are:

### [10] Simulation of injected and trapping of CO<sub>2</sub> and estimation of CO<sub>2</sub> stored volume from seismic velocity.

Accurate a priori evaluation of potential storage site fidelity and prediction of CO<sub>2</sub> fate following injection, both via reservoir-scale simulations, requires a fundamental understanding of the physical and chemical processes responsible for residual trapping of CO<sub>2</sub> at the pore scale. To this end, the group of PI Tsuji accomplished ground-breaking modeling and simulation of multiphase reactive flow in rocks. This work is part of the broader division effort to eventually model the large-scale CO<sub>2</sub> fate in geological formations and to assess the viability of the pore-space trapping mechanisms. Using a digital rock model that was reconstructed from the micro-CT scanned images of reservoir rocks (Fig. 9a), the group simulated and studied CO<sub>2</sub> residual trapping mechanisms in heterogeneous geologic formations and calculated relative permeability by the lattice Boltzmann method (LBM; Fig. 9b). The study revealed a strong interfacial effect on the relative permeability which is one of the most important parameters in reservoir monitoring and characterization [33]. The influence of mineralization on the hydrological properties was studied by integrating a mineralization model into the LBM fluid simulation (Fig. 9c). The simulation study demonstrated that, for the relative permeability, pore space reduction due to mineral precipitation (Fig. 9d) has a greater influence on the non-wetting phase than on the wetting phase [34]. These LBM simulations are, to our knowledge, the largest of their kind for studies of CO<sub>2</sub> trapping mechanism in heterogeneous geologic formations.



**Fig. 9.** a) Pore geometry of the Berea sandstone extracted from micro-X CT images, b) Supercritical CO<sub>2</sub> behavior within pore space parameterized by interfacial tension [33], c) Mineral precipitation calculated from the CO<sub>2</sub> flow within rock pore [34], d) Relative permeability calculated from the precipitated rock models.

Dr. Kitamura and WPI visiting professor Xue demonstrated the importance of the S-wave velocity in the estimation of the volume of stored CO<sub>2</sub> in future sub-seabed reservoirs—a critical issue in the arena of CO<sub>2</sub> reservoir monitoring that remains unresolved [35]. In the injected CO<sub>2</sub> monitoring, CO<sub>2</sub> saturation is typically estimated from the P-wave velocity. However, Dr. Kitamura and WPI visiting professor Xue demonstrated the existence of hysteresis in the relationship between the P-wave velocity and CO<sub>2</sub> saturation during drainage and imbibition processes. This hysteresis indicates that supercritical CO<sub>2</sub> and water have different flow patterns and displacement mechanisms within the pore space. It is therefore concluded from the presence of this hysteresis that CO<sub>2</sub> saturation cannot be accurately estimated solely from the P-wave velocity, as is presently done in conventional monitoring. Thus, a more reliable monitoring method must be developed to ensure accurate tracking of CO<sub>2</sub> fate post-injection in geologic formations. From laboratory experiments, Drs. Kitamura and Xue demonstrated the importance of the S-wave velocity in the reliable estimation of the volume of stored CO<sub>2</sub>. By using both P- and S-wave velocities, CO<sub>2</sub> saturation can be accurately estimated in both drainage and imbibition processes. An accurate method to estimate the S-wave velocity for deep subsurface reservoirs is currently under development [36].

## 2-2. New Challenges

*Describe the new challenges befitting a WPI center that have been undertaken.*

### Systems and Actions for better Science

#### *Supervision of graduate students by I<sup>2</sup>CNER Faculty*

In order for I<sup>2</sup>CNER faculty to be able to expand their research programs, they must be given access to graduate research assistants. In the US academic system, direct supervision by young faculty of graduate thesis work is a typical practice. I<sup>2</sup>CNER is working with Kyushu University to enable specifically our young faculty to engage in this practice in the future. Some I<sup>2</sup>CNER faculty members are able to directly supervise MS/PhD students through cooperating Departments of Kyushu University, such as Prof. H. Matsumoto in the Department of Hydrogen Energy Systems and Prof. M. Kubota in the Department of Mechanical Engineering. These faculty members are selected to supervise students in these departments based upon the needs of the department (e.g. on an individual basis), but I<sup>2</sup>CNER aims to expand its list of individuals

who are approved to supervise students in these departments. In addition, many I<sup>2</sup>CNER faculty members participate in MS/PhD student supervision either directly or indirectly through partnerships with professors in the Graduate School of Engineering.

### *Equipment*

Obtaining resources for maintaining/updating existing equipment and purchasing new equipment is always a pressing issue. I<sup>2</sup>CNER must find a way to continuously add new equipment and maintain/upgrade existing items. By way of example:

- The Hydrogen Storage Division would benefit from the purchase of PCT (pressure-composition-temperature) isotherm measurement equipment. Once the PCT isotherm is available, almost all storage properties of hydrogen storage materials are identified. This division would also benefit from the purchase of an In-situ X-ray diffractometer, which is an ideal piece of equipment that can help us understand structural change even under high pressure of hydrogen and elevated temperatures.
- In the Hydrogen Materials Compatibility Division, the realization of several milestones depends upon performance of mechanical property testing of materials in high pressure hydrogen gas. Currently, such testing capabilities are primarily accessible through coordination with the HYDROGENIUS project at Kyushu University. However, the HYDROGENIUS project relies heavily on these capabilities for satisfying their ambitious objectives, so accommodating I<sup>2</sup>CNER is not a high priority. Establishing a system for such testing would be highly beneficial. Acquisition of an atom probe tomography (APT) instrument would facilitate the possibility of significant research breakthroughs through 3D imaging and chemical composition measurements at the atomic scale. (Approximate cost: 1 million USD)

### *Internal Programs Review Committee (IPRC)*

In response to prior recommendations by the WPI Working Group, the ad-hoc Internal Programs Review Committee (IPRC) was called by the Director in FY 2012 to “provide information to the Director on the entire spectrum of the Institute’s research activities in anticipation of the upcoming mid-term review of I<sup>2</sup>CNER.” As a result of this review, several of the “Start-up funding for interdisciplinary research” projects initiated in FY 2011 were halted and the total budget for that program was reduced by more than 50%. In addition, programs of 2 Satellite faculty have been terminated. The IPRC was made into a standing committee as of November 1, 2013 in response to the recommendation by the WPI Working Group at the FY 2013 Site Visit Review. Subsequently, the Director called the IPRC to do a “deep dive” review of all research projects of the Institute in order to determine their relevance in relation to their Division’s specific research objectives. The IPRC turned in their reviews on January 31, 2014. The Director is working with the IPRC to review all results. Action will be initiated after the Site Visit Review. The Director will use the report as a tool when making decisions about the reallocation of man power and resources in order to best-serve the I<sup>2</sup>CNER roadmap. In addition, each of I<sup>2</sup>CNER’s researchers will be given his or her individual project review. Moving forward, the challenge will be to strengthen and reinforce the presence of the IPRC within the Institute—to make it more enmeshed in the research culture/ research planning efforts through sporadic evaluation of programs, etc.

### *WPI Faculty Fellows Program*

We established a WPI Faculty Fellows Program in order to encourage promising or eminent scientists from preeminent international universities and institutes to conduct short-term, onsite, interdisciplinary, institute-related research at Kyushu University/I<sup>2</sup>CNER for periods of three to six months. The program is intended to help recruit foreign researchers who may consider accepting permanent positions at I<sup>2</sup>CNER. In the future, our goal is to integrate this program with Kyushu University’s newest initiatives, the Progress 100 Program and the Top Global University Project, in order to achieve synergy through sharing of resources.

### *Institute Interest Seminar Series (IISS)*

In order to foster a climate of collaboration and interdisciplinary research that cross-cuts division boundaries, the Institute regularly hosts the “Institute Interest Seminar Series (IISS).” This series serves as a forum to help our young researchers (graduate students, post-docs, and assistant and associate professors) further develop their abilities to present and argue for their viewpoints, scientific methods, and approach before an audience of experts. Moving forward, the Administration would like to transform the series into a “think tank” that can be shared equally by young and senior faculty in order to explore new



ideas for fusion research. The long-term vision for the series is to maintain the “open attitude” of young faculty even as senior faculty participation increases so that the IISS atmosphere is similar to that of typical meetings of research teams in the US, wherein the young people freely express their ideas and research progress, and the senior faculty listen and suggest strategies for improvement, etc. To achieve this, the Administration will need to incentivize senior faculty and Lead PIs to increase their participation. A total of 52 seminars have been held since the series' inception: 16 in FY 2011, 16 in FY 2012, and 20 in FY 2013.

#### *Energy Analysis/Assessment and Coordination of Research Efforts*

The Energy Analysis division was established to continuously review and revise the Institute's vision and roadmap toward a carbon-neutral society over time scales of short, middle, and long ranges. The idea is that the Institute addresses the roadblocks for a carbon-neutral energy society which are caused by the constraint of primary energy resources and availability on the basis of CO<sub>2</sub> emissions, efficiency, cost, national security, and resilience. The division's goals are to: i) assess the relevance of the Institute's research activities vis-à-vis I<sup>2</sup>CNER's roadmap for a carbon-neutral society and ii) ensure that I<sup>2</sup>CNER's research is informed of all relevant current and future energy options of Japan. Moving forward, one of the challenges for I<sup>2</sup>CNER is to further strengthen the EAD to promote the coordination of the Institute's research efforts. One strategy for strengthening the division is to hire two additional professors and three postdoctoral researchers who will conduct process and system analyses. An open international call for two EAD positions has already been initiated. Once these additional positions have been filled, the following projects will be analyzed, in accordance with I<sup>2</sup>CNER's commitment to conducting state of the art research:

- Techno-economic analysis on CO<sub>2</sub> utilization
- Energy/exergy analysis on the carbon neutral cycle
- Techno-economic analysis on new heat pump (new low GHG refrigerant, adsorption material, and desiccant materials)
- Techno-economic analysis on organic PV plus HT electrolysis comparing to advanced multi-crystal PV plus room temperature electrolysis
- Techno-economic analysis on PEFC / SOFC combined heat and power operation for residential or other distributed co-generation energy pathways comparing to conventional heat power supply (grid and boiler) and grid electricity with a heat pump
- Storage efficiency and economic analysis of Ti-based alloys based on broad storage system
- Energy analysis on FCV, EV, and hybrid with latest parameters
- Energy saving analysis on molecular brush applications
- Techno-economic analysis on energy storage system using H<sub>2</sub> adjusting intermittent renewables
- Applicability analysis of tribology research to energy conversion systems
- Applicability analysis of new battery (dual carbon)
- Exploration of applicable energy production system for water splitting with organic and inorganic composite
- Exploration of applicable energy production system for novel biomimetic catalysis for H<sub>2</sub>, CO<sub>2</sub>

Another challenge for the Institute is to develop our bottom-up model of energy systems based on our current analytical tool. Further, the GIS (geographic information system) should be utilized as a part of the model. To accelerate data collection and improve reliability of our analyses, we will need to use large databases of energy facilities and market movement created by outside entities (e.g. Bloomberg New Energy Finance). Bloomberg New Energy Finance provides data and information not only to government organizations such as METI or US-DOE, but also to several universities.

An additional potential challenge is the extension of the future directions of our research to include analysis of the contribution of Japanese technologies or I<sup>2</sup>CNER's enabling technologies to international CO<sub>2</sub> emission reduction. It does not make sense for us to try to achieve a large-scale reduction of CO<sub>2</sub> emissions only in Japan if we intend to impact global climate mitigation/international emission reduction. To conduct this kind of international research, the collaboration with NCFRC and contacts with the above-mentioned database organizations will be highly beneficial.

### *Expanding our Computational Capabilities*

As the EAC has suggested, we need to expand our computational science and engineering capabilities, in particular, through technical staff to maintain our computational facilities. Consideration will also be given for the establishment of a new division on Computational Science and Engineering.

### *Convincing Young Japanese to spend time overseas*

We need to further increase our efforts to convince young Japanese scientists to spend longer periods of time at the University of Illinois and our other international partner institutions.

### *Director's expansion of International Collaborations*

The Director further consolidates and initiates collaborations with HEmS of the University of Oxford. In addition, the Director will work to establish new partnerships with the Helmholtz Institute in Germany.

### *General Personnel Goals*

In order to reach our research goals for the next 5 years, we plan to have the following personnel by the end of FY 2016:

- Increase the number of postdocs to ~35
- Increase the number of foreign PIs, including 2 permanent-staying positions
- Increase the overall percentage of female researchers (12%) as much as possible, while always remaining above the KU average (11%)

These levels warrant smooth operations for our current research agenda. Additional personnel will be needed if we are to expand in directions listed below.

## **Potential research challenges over the next 5 years**

### *Steam Electrolysis*

We will continue studying the surface composition and structure, in conjunction with studies of the transport (oxygen ionic and electronic) properties and electrochemical performance, of the materials targeted for application as air electrodes, in order to understand the factors which contribute to high performance as electrodes under electrolysis conditions. Through this combination, we will realize the short-term milestone of increasing the energy efficiency above 90%, while also decreasing the operating temperature to 773 K and increasing system durability. Once this characterization has identified promising candidates, and a fundamental understanding of the oxygen transport properties at elevated oxygen activities has been developed, we will work to optimize the composition and structure of electrodes to maximize the rates of hydrogen production, working towards our midterm goal of achieving the performance of a unit capable of producing more than 10 NM<sup>3</sup>/h of hydrogen while again maintaining high durability.

### *Renewable CCS through Leveraging Biological Reaction*

In renewable Carbon Capture and Storage (CCS), injected CO<sub>2</sub> is converted into CH<sub>4</sub> (fuel) through remediation reactions driven by the local microbial environment of the injection reservoir. Although this reaction may not be fast in the subsurface reservoir, the amount of CO<sub>2</sub> for transformation can be significant. However, the potential of this CCS is unknown and depends on (i) the conversion rate from CO<sub>2</sub> to CH<sub>4</sub> and (ii) the available coalbed sequence (i.e., advantageous environment for microbe activity). To enhance this biological transformation of CO<sub>2</sub> into fuel, I<sup>2</sup>CNER will bring microbiologists into the fold for collaborations within the CO<sub>2</sub> Storage Division. We will collaboratively explore the development of targeted microbial environments that can maximize this conversion process. Doing so will leverage existing expertise at Illinois in the BP Energy Biosciences Institute and the Institute for Genomic Biology within which researchers are pursuing complementary studies for microbially-enhanced oil recovery. Furthermore, the coalbed sequence in this scenario could be used as a seal layer because CO<sub>2</sub> absorption would seal cracks within the coalbed and thus decrease its effective permeability. This coalbed-sealing concept would be revolutionary if successful.

### *CCS and Earthquakes*

Pressure modifications of the pore fluid by injected CO<sub>2</sub> may interact with seismogenic faults. Understanding this interaction is of great societal interest and I<sup>2</sup>CNER may elect to develop an effort in this area, of course, if manpower is available.

### *Biomimetic Catalysis for H<sub>2</sub> and CO<sub>2</sub> Activation*

In nature, biological CO<sub>2</sub> conversion is extremely important; however, many key aspects of the biochemistry and molecular control of this process are not well understood. We have found the very important CO<sub>2</sub> fixing enzymes of new formate dehydrogenase, new formate hydrogen lyase, and new pyruvate ferredoxin oxidoreductase from the our isolated strain S-77. These research efforts are aimed at providing new information for "the mechanism of biological CO<sub>2</sub> conversion", how enzymes effectively reduce CO<sub>2</sub> to valuable energy carriers.

On the other hand, the Synthetic Chemistry for carboxylation must be carried out under the expensive energy carrier of "CO," which is the most significant roadblock in the reaction process. The Ogo group has a great challenge to synthesize all valuable hydrocarbons from "CO<sub>2</sub>" instead of CO i.e., new hydroformylation, new Monsanto process, new water-gas shift reaction, and new Fischer-Tropsch process. These novel approaches will be applied to many areas for reducing environmental CO<sub>2</sub> and for generating new sustainable clean energy.

PI S. Ogo (Kyushu) and Prof. T. Rauchfuss (Illinois) will work collaboratively to evolve and optimize synthetic hydrogenases at an accelerated pace. In light of the Ogo group's breakthroughs, the pace of this work is entirely on course. Between the efforts of these two research groups, I<sup>2</sup>CNER is in a position to lead the world in the elucidation of mechanisms for biomimetic hydrogen activation. These research efforts based on biological and chemical studies in our group are very important toward for understanding catalytic mechanisms for H<sub>2</sub>-activation, CO<sub>2</sub>-conversion, and artificial photosynthetic water-oxidation. All of these processes are crucial to exploring novel catalysts for Carbon-Neutral Energy Technology.

### *Nuclear Future for Japan*

Following the widespread development of nuclear power, Japan made a critical energy policy decision to provide a substantial portion of its electric power need using nuclear fission energy. This policy led to the 30% of the electricity production by nuclear power in early 2011 with plans for 41% by 2017 and 50% by 2030. In order to meet these goals, Japan became the world leader in the development of current light water reactor (LWR) technologies. Japanese nuclear industry set the international standard for nuclear plant construction with world records for plant completion times and within target costs. The leading Japanese nuclear firms are now partners with other global nuclear firms. In particular, Toshiba and GE-Hitachi both have a substantial international market in nuclear power. In addition, Mitsubishi Heavy Industries is the world leader in the fabrication of nuclear pressure vessels.

Building on Japan's international leadership in the Light Water Reactor technology, Japan has made major investments in advanced nuclear power technologies. These include, "Fast" Reactor technology, High Temperature Reactor technology as well as a major leadership role in the development of nuclear fusion technology. (Nuclear fusion will likely not influence power supply in the period up to 2050 in any major way.) The Fast Reactor technology is important for both "breeding" new nuclear fuel and can be deployed to "burn" the long-lasting isotopes that would otherwise cause problems with nuclear waste storage. These systems also offer an enhanced level of safety in accident conditions.

More importantly for Japan's energy supply is the development of High Temperature Reactor technologies where Japan is also the world leader with the operation of the gas-cooled High Temperature Test Reactor (HTTR) which has set a world record for reactor outlet temperature of 950C. At this temperature, energy conversion efficiencies (the Carnot efficiency) are very high, usually around 60% compared to 33 to 38% in conventional nuclear and coal powered energy systems. However, this very high operation temperature can also be employed to produce hydrogen through one of many thermo-chemical cycles. The thermo-chemical cycle which has received the most attention so far is the S-I, sulfur-iodine, cycle which has already been deployed on the HTTR but not tested due to the 3-11 secession of nuclear power operation in Japan. Alternately, the very high temperature reactor output could be used for high-temperature electrolysis in the case where both cogeneration of both electricity and hydrogen were of interest.

I<sup>2</sup>CNER could provide use input about the impact, re-start, and future deployment of nuclear technologies for Japan's carbon neutral future by taking on challenges that are related to extreme materials and extreme physical and chemical processes.

## 2-3. Joint Research Advanced

*Describe the joint research that the Center has undertaken with research organizations in and outside Japan.*

*-In Appendix 2-3, list and describe the cooperative research agreements that the Center has with other organizations.*

### **National Fuel Cell Research Center (NFCRC)**

In order to advance the fusion of I<sup>2</sup>CNER's fundamental research with the energy systems research that is being carried out at the National Fuel Cell Research Center (NFCRC) at the University of California, Irvine, an agreement with University of California Irvine (NFCRC) was signed on December 31, 2013. So far, 3 research areas of overlapping interests have been identified: (1) systems' approach to a sustainable society, (2) SOFC/SOEC cathodes using proton conducting oxides, and (3) challenges related to implementation of SOFCs operating in low and high pressure applications from both a systems and materials level.

### **Air Resources Board of the State of California (CARB)**

The purpose of this collaboration is to reinforce the idea of Green Innovation, with 1) I<sup>2</sup>CNER becoming familiar with the types of policy and regulation that California is implementing as a world leader on advanced energy technology efficiency and conservation, and 2) CARB becoming familiar with the investment on mission-driven science for carbon-neutral energy technologies. In order to promote future interactions, a letter of understanding is currently being negotiated.

### **Norwegian University of Science and Technology (NTNU) and SINTEF**

In order to begin exploring potential collaborations between I<sup>2</sup>CNER, NTNU, and SINTEF, a joint workshop was held November 15-16, 2012. After over 1 year of mutual effort, an MOU was signed on March 17, 2014. As part of I<sup>2</sup>CNER's collaborative research with NTNU, a joint research proposal on understanding the fundamentals of materials degradation in hydrogen-containing environments has been awarded. The project is funded by the Norway Research Council.

### **Sandia National Laboratories at Livermore, CA**

I<sup>2</sup>CNER is interacting strongly with the Sandia National Laboratories at Livermore, CA. Dr. Brian Somerday, a distinguished member of the technical staff, is the Division Lead PI for I<sup>2</sup>CNER's Hydrogen Materials Compatibility Division. In particular, this relationship with Sandia National Laboratories allows I<sup>2</sup>CNER to stay informed about hydrogen-related technologies in the US and development of codes and standards for hydrogen materials compatibility.

### **Pacific Northwest National Laboratory (PNNL)**

Following the participation of Dr. Bruce Garrett in the 2012 I<sup>2</sup>CNER Annual Symposium, I<sup>2</sup>CNER began exploring potential collaborations with PNNL. Though this collaboration is still at an early stage, we have already identified topics of mutual interest, including the enhancement of computational capabilities in the areas of captured CO<sub>2</sub> and catalysis.

### **University of Oxford**

The Director is serving on the Strategic Advisory Panel of HEmS (Hydrogen in Metals—From Fundamentals to the Design of New Steels) at the University of Oxford, which is a multi-million dollar program funded by the British government. The Director of HEmS, Prof. Alan Cocks, already visited I<sup>2</sup>CNER for a day of discussions for a plan for future collaboration.

## **2-4. Appraisal by Society and Scientific Organizations**

*Describe how society and/or scientific organizations in and outside Japan have recognized the Center's research achievements.*

*-In Appendix 2-4, list the awards received and invitational lectures given by the Center's researchers.*

### **US Energy Secretary Moniz in Tokyo on Oct. 31, 2013**

Identified I<sup>2</sup>CNER as a prime example of successful cooperation between DOE and Japanese researchers.

## **Interactions with National and International Organizations**

### *PI Akiba*

Prof. Etsuo Akiba is playing an important role in an international network for research and development of hydrogen storage materials as an expert adviser of Tasks 22 and 32 for Hydrogen Implementing Agreement in the International Energy Agency. Within Japan, he is acting as the project leader for basic research on compact and energy efficient hydrogen storage systems, such as NEDO projects "Advanced Hydrogen Storage Materials" (FY2007-FY2012). For the NEDO project "Survey and Study of Hydrogen Storage Materials for Fuel Cell Vehicles" (FY2012), he was the chairman of the committee for roadmap development for hydrogen storage materials. The committee was composed of members from academia,

government and industries, including Japanese big-three motor companies. The Japan roadmap constitutes the basis of the roadmap for I<sup>2</sup>CNER's Hydrogen Storage Division.

#### *PI Sasaki*

Prof. Kazunari Sasaki is a member of the Strategic Council of Hydrogen and Fuel Cell which was established in December 2013 by the Agency of Natural Resources and Energy. The aims of the council are (i) to hold their understandings among Industry, government and academia on significance of hydrogen energy and perspective of hydrogen demand in future, and (ii) to define role-sharing among industries and government and a roadmap to complete the sharing roles up to 2030 when global commercialization is estimated. Prof. Sasaki is one of three participating members from academia.

#### *PI Tsuji*

Prof. Takeshi Tsuji is a member of the committee of the Japan CCS Corporation which will decide the next CO<sub>2</sub> storage site around the Japanese Islands.

### **Interactions with US DOE**

Dr. Somerday, the Division Lead PI of the Hydrogen Materials Compatibility Division, leads several research projects at Sandia National Laboratories that require interaction with Technology Development Managers (TDMs) at the US Department of Energy (DOE) Fuel Cell Technologies Office. In this capacity, Dr. Somerday is responsible for establishing and managing expectations for project objectives, milestones, and work progress through direct communication with the TDMs. Since some of these projects involve collaborative activities with I<sup>2</sup>CNER, Dr. Somerday references and promotes I<sup>2</sup>CNER during these communications. As a result of his recognized technical expertise and ability to productively manage projects, the DOE recently approved Dr. Somerday to assume another leadership role in a high-profile project titled H2FIRST (Hydrogen Fueling Infrastructure Research and Station Technology), which emphasizes public-private cooperative R&D to stimulate the development of hydrogen fueling stations in the U.S.

Former US DOE Energy Analyst Mark Paster is a key member and contributor to the Energy Analysis Division.

### **I<sup>2</sup>CNER in Tokyo**

The I<sup>2</sup>CNER in Tokyo symposium was an event sponsored by the US Embassy which was opened by the then-US Ambassador to Japan, Dr. John V. Roos. For full details, please refer to Section 3-2 of this report.

### **Sample of Prestigious Recognition from National and International Organizations**

#### *The 2012 Somiya Award*

The Somiya Award is given biennially to scientists who have collaborated across two continents. The 2012 Somiya Award was given to PIs Kilner, Tuller, Ishihara, Prof. Yildiz, and Dr. Santiso.

#### *2012-2013 Hydrogen Student Design Contest*

Students from Kyushu University, including team members from I<sup>2</sup>CNER, won the 2012-2013 Hydrogen Student Design Contest, which was sponsored by the US DOE, the National Renewable Energy Laboratory, Mercedes-Benz, and Toyota. Their grand-prize winning project was focused on the "Development of a Hydrogen Production and Fueling Infrastructure in the Northeastern United States."

#### *JST Breakthrough Report 2013*

Prof. Ogo's research was featured in this important publication of Japan Science & Technology Agency (JST).

#### *International Society of Solid State Ionics Officers*

During the International Society of Solid State Ionics (ISSI) officer elections, which were held at the 19<sup>th</sup> International Meeting on Solid State Ionics in Kyoto, Japan, PI Tuller was elected as Vice President/President Elect and PI Tatsumi Ishihara was elected as Treasurer.

#### *US Department of Energy Hydrogen and Fuel Cells Program Research and Development Award*

In 2011, PIs Ian Robertson and Petros Sofronis won the US Department of Energy Hydrogen and Fuel Cells Program Research and Development Award "in recognition of outstanding contributions to the understanding of hydrogen embrittlement."

### *Joint Japan-Switzerland Workshop on Energy Technology Research*

On March 9-12, 2014, three I<sup>2</sup>CNER PIs (Sofronis, Ishihara, and Akiba) were invited by the organization committee to participate in the Joint Japan-Switzerland Workshop on Energy Technology Research, which was hosted to celebrate the 150<sup>th</sup> anniversary of diplomatic relations between Switzerland and Japan. Director Sofronis was a member of the international organizing and program committee for this event.

## 2-5. Center's Research Environment including Facilities and Equipment

*Describe the Center's research environment including facilities and equipment and the state of its utilization.*

### **I<sup>2</sup>CNER Building 1**

In order to continue developing a research environment befitting a top world-level research institute, and to promote collaboration and fusion research, I<sup>2</sup>CNER building 1 (approximately 4,873 m<sup>2</sup>) was completed at the end of November 2012. All the Institute's members moved "under one roof" into I<sup>2</sup>CNER building 1 in January 2013. In fact, the building itself was designed in this spirit—it is home to several common laboratories which are available for use by any I<sup>2</sup>CNER researcher. The first floor lobby features a spacious lounge with a high ceiling and electronic black boards in order to encourage impromptu meetings and exchange of scientific views among I<sup>2</sup>CNER members. Facility equipment such as fume hoods and pneumatic piping has been installed in I<sup>2</sup>CNER Building 1. I<sup>2</sup>CNER Building 2 has been designed similarly.

### **Space Sharing with Next-Generation Fuel Cell Research Center**

In January 2013, an additional 7 labs, 15 researcher offices, and a server room were secured for I<sup>2</sup>CNER's Fuel Cell researchers out of the space allocated to the Next-Generation Fuel Cell Research Center within the I<sup>2</sup>CNER building. We have also secured labs for researchers of MIT and Imperial College London in order to promote exchange of researchers between KU and these renowned foreign institutions.

### **I<sup>2</sup>CNER Building 2**

A second I<sup>2</sup>CNER building which has 4 stories and a total floor space of 5,000 m<sup>2</sup> is currently being built. Floor plans for the building include 8 large-scale labs, 2 open offices, and 1 administrative office, with the majority of rooms being designed as open, common experimental spaces in order to promote interdisciplinary research. This building is funded by the FY 2012 supplementary budget from the Japanese government. Completion of I<sup>2</sup>CNER building 2 is planned for the end of February 2015.

### **Five main apparatus in I<sup>2</sup>CNER**

#### *Small Complex Fatigue Testing System*

The small complex fatigue testing system is capable of monitoring slip bands, micro cracks, and others on the specimen surface while the fatigue test is in operation. The system is designed for combined use with the scanning electron microscope.

#### *RF Plasma Sputtering Apparatus (Thin Film Deposition Methods)*

Sputter deposition is a physical vapor deposition (PVD) method of depositing thin films by sputtering (ejecting) material from a "target" (source) which then deposits onto a "substrate," such as a silicon wafer. This equipment can deposit multi composition film using simultaneous sputtering of three targets.

#### *Secondary Ion Mass Spectrometry*

Time-of-Flight secondary ion mass spectrometry (TOF-SIMS) is a very sensitive surface analytical technique. It provides detailed elemental and molecular information about the surface, thin layers, and interfaces of the sample, and gives a full three-dimensional analysis. The use is widespread, including semiconductors, polymers, glass, paper, metals, ceramics, biomaterials, and organic tissue.

#### *Ar Cluster Ion Beam XPS*

X-Ray Photoelectron Spectroscopy (XPS) is the technique for elemental analysis of the sample surface. Mono-energetic x-rays irradiate the sample surface causing photoelectrons. An analyzer determines the binding energy and intensity of the photoelectrons, which are correlated with the elemental identity, chemical state, and quantity of a surface element. The Ar cluster beam attached to this XPS system can etch the sample surface to obtain the depth profile of the sample elements.

### *Nuclear Magnetic Resonance Spectroscopy System*

Nuclear Magnetic Resonance (NMR) spectroscopy is used to study the structure of molecules, the interaction of various molecules, the kinetics or dynamics of molecules, and the composition of mixtures of solutions or composites. The advantage is the unique ability of a nuclear spectrometer to allow both the non-destructive and the quantitative study of molecules in a solution and in a solid state.

## **I<sup>2</sup>CNER Satellite Laboratory Facilities**

### *Cahill Laboratory*

The Cahill laboratory employs three pump-probe metrology systems for studies of elastic constants and thermal transport properties by pump-probe picosecond acoustics and time-domain thermoreflectance. The further development of these techniques and applications to novel materials systems has been the point of collaboration between Cahill's laboratory and I<sup>2</sup>CNER researchers. Laboratory equipment purchased by I<sup>2</sup>CNER in the Cahill laboratory includes a preamp, a programmable signal generator, and a pulsed laser diode. The preamp and signal generator are parts of one of the new pump-probe systems. The pulsed laser diode was used in experiments on heat transport at solid/liquid interfaces. The signal-to-noise proved to be insufficient and we are instead using plasmonic structures for this work.

### *Christensen Laboratory*

Prof. Christensen's laboratory at Illinois houses a range of microfluidics capabilities germane to his I<sup>2</sup>CNER research, and his group also leverages micro fabrication facilities on the Illinois campus. In his lab, Prof. Christensen has a fluorescent microscopy arrangement that allows for dual-camera imaging for either two-fluid micro-PIV investigations, dual-fluorescence microscopy/thermometry or a combination of velocity and scalar measurements. A truly unique aspect of his microfluidics capabilities is the ability to reach realistic reservoir conditions of high pressure (80-100 bar) in microfluidic systems to study realistic transport (particularly, attaining liquid and supercritical CO<sub>2</sub> conditions in microfluidic systems). His group utilizes extensive micro fabrication facilities on campus that allow the realization of micro models with sub-micron accuracy via etching of silicon.

### *Ertekin Laboratory*

Due to the computational nature of her work, Prof. Ertekin's group does not have a formal laboratory, but utilizes a wide range of on-campus computing resources. Professor Ertekin's research group has access to high-performance computing resources through the University of Illinois Shared Computing Cluster. Our resources include 52 compute nodes and 624 compute cores (for which we have priority and usage privileges). These are high memory (24 and 48 GB) nodes interconnected with high-speed infiniband for high-performance scalability. The shared computing cluster at Illinois is already equipped with a variety of compilers and math libraries. Other software, including electronic structure codes (Vesta, VMD, Quantum Espresso, SIESTA, QWalk, etc), is freely available for download through public licensing agreements. These computational resources will be supplemented by the computing facilities available through other supercomputing user centers such as the XSEDE and NERSC, all of which will be leveraged to the greatest possible extent. Additionally, we have 20 TB of storage facilities also provided through the University of Illinois Shared Computing Cluster.

**Blue Waters Petascale Computing Project.** The National Center for Supercomputing Applications (NCSA) houses Blue Waters, a petascale computing facility that has recently come online. We intend to make extensive use of this system to carry out the work proposed here, for which 7% of the computing time is dedicated for UIUC faculty use.

### *Gewirth Laboratory*

Laboratory equipment purchased by I<sup>2</sup>CNER in the Gewirth laboratory includes a Raman spectrometer, a high pressure solvothermal synthesis cell (autoclave), and various potentiostats. The solvothermal apparatus was used to make advanced photoelectrochemical materials, the status of which was reported in a recent joint publication between UIUC and Kyushu. The Raman spectrometer was used to interrogate silver electrode surfaces decorated with nitrogen-containing molecules, the presence of which enhances the carbon dioxide reduction reaction (we just submitted a paper describing the origin of this effect). The potentiostats were used, among other things, to aid in the development of our pH sensitive proton coupled electron transfer switch, the description of which is just now being published in Nature Materials.

### *Kenis Laboratory*

The Kenis group has a state-of-the-art facility for the testing of electrochemical processes, using either a standard 3-electrode electrochemical cell or a continuous flow electrolysis cell. The different cells and setups are operated with 3 potentiostats (Autolab PGSTAT 30/302N, one of these purchased with I<sup>2</sup>CNER funds). Syringe pumps (Harvard Apparatus) and mass flow controllers (MKS, different models, one purchased with funds from I<sup>2</sup>CNER) are used to regulate the reactants feeds. Product streams from the electrolyzer are analyzed using Gas Chromatography (GC), either using an Agilent GC-MS or a Thermo Trace GC (purchased with funds from I<sup>2</sup>CNER).

### *Li Laboratory*

Prof. Li has direct access to 8000 square feet of class 1000 crystal growth cleanroom space equipped with all of the equipment necessary for epitaxial growth of III-V semiconductor nanowires and 8000 square feet of class 100 device processing for nanowire device fabrications. Included are MOCVD, PECVD, LPCVD reactors, conventional contact lithography, ebeam lithography, nanoimprint lithography, stepper, e-beam and thermal evaporators, plasma and sputter thin-film deposition systems, ALD, and ICP reactive ion etching, diffusion and oxidation furnace, scanning electron microscopes. Additional facilities are available in the general characterization lab for optical and electrical characterization; and the Materials Research Laboratory for structural, optical, and electrical characterization of materials and devices at the nanoscale.

### *Martin Laboratory*

LCR Meter (Agilent E4980A Precision LCR Meter) – The purpose of this device for the I<sup>2</sup>CNER program is to characterize the electronic and dielectric properties of photocatalytic/photovoltaic materials. In particular we use this system to measure capacitance-voltage characteristics of materials in light and dark to get information about dielectric constant, losses in materials, work-functions, to characterize the nature of contacts between metals and light-absorbing materials, to probe carrier concentrations in semiconductors and heterojunctions, and much more. Recently we have used this system to extract the carrier densities from I<sup>2</sup>CNER supported TiO<sub>2</sub>/SrRuO<sub>3</sub> heterostructures, but it is regularly used to support the program. Overall it provides us with information on the nature of our new photocatalyst materials and how to optimize charge separation and device structures for efficient photocatalysis.

Nanovoltmeter and Nano AC/DC Current Source (Keithley 6221/2182A) – The purpose of these electronics is to enable use to probe low signal electronic response in oxide photocatalysts. In particular we use these devices to measure the electronic properties of large-band gap, co-catalyst materials connected to highly light-absorbing systems to understand charge transport in the more insulating materials. It is currently in use to probe materials such as TiO<sub>2</sub> and others.

Photocatalytic reaction vessel and Gamry Reference 600 Potentiostat – Leveraging existing infrastructure in my labs (including electronics, solar simulator, computers DAQ systems, etc.) we used I<sup>2</sup>CNER funds to design and produce a photocatalytic reaction vessel for study of model thin-film-based oxide and hybrid material photocatalysis systems. We produced a vacuum and water compatible reaction vessel to probe hydrogen and oxygen production from low-volume, low-mass photocatalysis systems and photoelectrochemistry. This can be used in conjunction with the potentiostat which provides advanced photoelectrochemical information of photocatalysis devices in operation - including insight into reaction rates, reaction potentials, decomposition rates, electrical properties, and cyclic voltametry. These are currently being used to probe the photoelectrochemistry of systems produced for the I<sup>2</sup>CNER program including TiO<sub>2</sub>/SrRuO<sub>3</sub> and other heterostructures.

### *Rauchfuss Laboratory*

The Rauchfuss laboratory is equipped with 13 full fume hoods each with a Schlenkline and pump. Air sensitive compounds are handled in 4 glove boxes; three of these with freezer compartments, and two are plumbed to solvent purification systems, each with a freezer and two with deoxygenated solvent supplied directly. Gases are handled on a home-designed vacuum line with a diffusion pump. Reactions are monitored by an Agilent 7820A gas chromatograph equipped with a thermal conductivity detector, and molecular sieve column as well as capillary columns and a Mettler-Toledo Autochem React-IR 15 with a fiber optic probe with a silicon tip. Compounds are analyzed by in-house Perkin Elmer Spectrum 100 FT-IR spectrometer and two CH-Instruments electrochemical analyzers (CHI600D for CV and CHI630D for DPV/CV), and a Cary 50 Bio Varian UV-vis spectrometer for obtaining electronic spectra.



### *Robertson-Sofronis Laboratory*

The Robertson-Sofronis laboratory combines modeling and experimental methodologies to study the effects and determine the mechanisms of hydrogen embrittlement of structural metals. The applications of these methodologies to materials relevant to the I<sup>2</sup>CNER mission is the point of collaboration between the Robertson-Sofronis laboratory and I<sup>2</sup>CNER researchers. Laboratory equipment purchased by I<sup>2</sup>CNER in the Robertson-Sofronis laboratory includes an Instron E10000 fatigue machine. This machine is central to the effort to explore the concept introduced in our previous work in which we proposed that the presence of hydrogen has two important effects on the evolution of the dislocation microstructure. It accelerates the microstructure evolution driving it into configurations unattainable in the absence of hydrogen and hydrogen stabilizes it in these configurations. If substantiated, the concept will have a profound impact on the fundamental understanding of hydrogen embrittlement of structural metals under fatigue loading, as it would show that all previous assumptions about microstructure evolution are too simple. Success of the effort will put the Institute at the forefront of development of physically-based models to predict hydrogen-induced failure of structural components.

### *Rockett Laboratory*

The Rockett laboratory is equipped with a high performance photodetector, which is used for current electroluminescence and photoluminescence measurements. Prof. Rockett's lab also contains a solar simulator lamp, which is used for device and material characterizations.

## 2-6. Non-WPI Project Funding

*Describe the results in securing non- WPI project funding.*

*-In Appendix 2-6, draw of graph showing the Center's transition in securing non-WPI project funding and list external funding warranting special mention.*

### **FY2011**

The non-WPI research funding included the funding for the Institute for Hydrogen Industrial Use and Storage at Kyushu University (HYDROGENIUS). If the HYDROGENIUS funding is excluded, the annual research funding average of KU PIs who work for I<sup>2</sup>CNER was 9.5 million dollars for the period FY2006-FY2009. The corresponding total amount for FY 2011 was 16.36 million US dollars (Exchange rate: JPY/USD = 100), which amounts to a 30% increase.

### **FY2012**

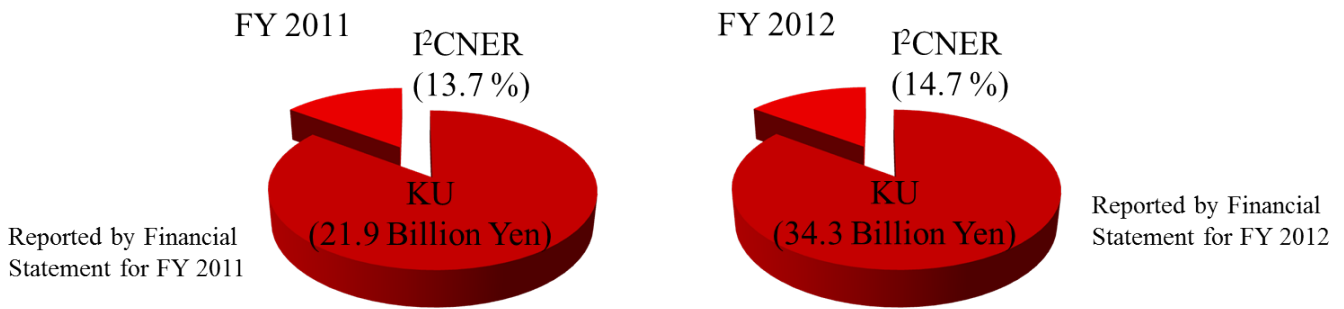
In FY 2012, KU-I<sup>2</sup>CNER researchers acquired a total amount of 31.56 million US dollars (3.16 billion yen), which amounts to a 93% increase compared to FY 2011. This research funding also includes the funding for Installation Project for Base as a Mediator of Technology from the Ministry of Economy, Trade, and Industry (METI) (7 million US dollars, 0.7 billion yen). This funding was allocated only in FY 2012.

6 of the Illinois Satellite Researchers won a total of 15 external funding projects by leveraging their I<sup>2</sup>CNER research, which resulted in the total amount of 4,643,514 US dollars of extra award grants at Illinois (only projects whose period/duration included FY 2012 were counted).

### **FY2013**

In FY 2013, KU-I<sup>2</sup>CNER researchers acquired a total amount of 28.77 million US dollars (2.88 billion yen). If we exclude the funding for Installation Project for Base as a Mediator of Technology from FY 2012, the corresponding total amount in FY 2012 is 24.56 million US dollars (2.46 billion yen), which amounts to a 17% increase. The research funding overall has been increasing steadily from FY 2010 to FY 2013.

10 of the Illinois Satellite Researchers won a total of 48 externally-funded projects by leveraging their I<sup>2</sup>CNER research, which resulted in the total amount of \$4,374,345 US dollars of extra grants at Illinois (only projects whose period/duration included FY 2013 were counted).



**Figure 10:** Comparison of external research funding won by I<sup>2</sup>CNER researchers against total external research funding won by all Kyushu University Faculty.

3. Feeding Research Outcomes back into Society (within 5 pages)

3-1. Contributions to Green Innovation

3-1-1. Center’s Vision and Scenario of Transition to a Low-Carbon Society

*Describe center’s vision and scenario of transition to a low-carbon society that contributes to forming national policy and societal consensus.*

**Vision**

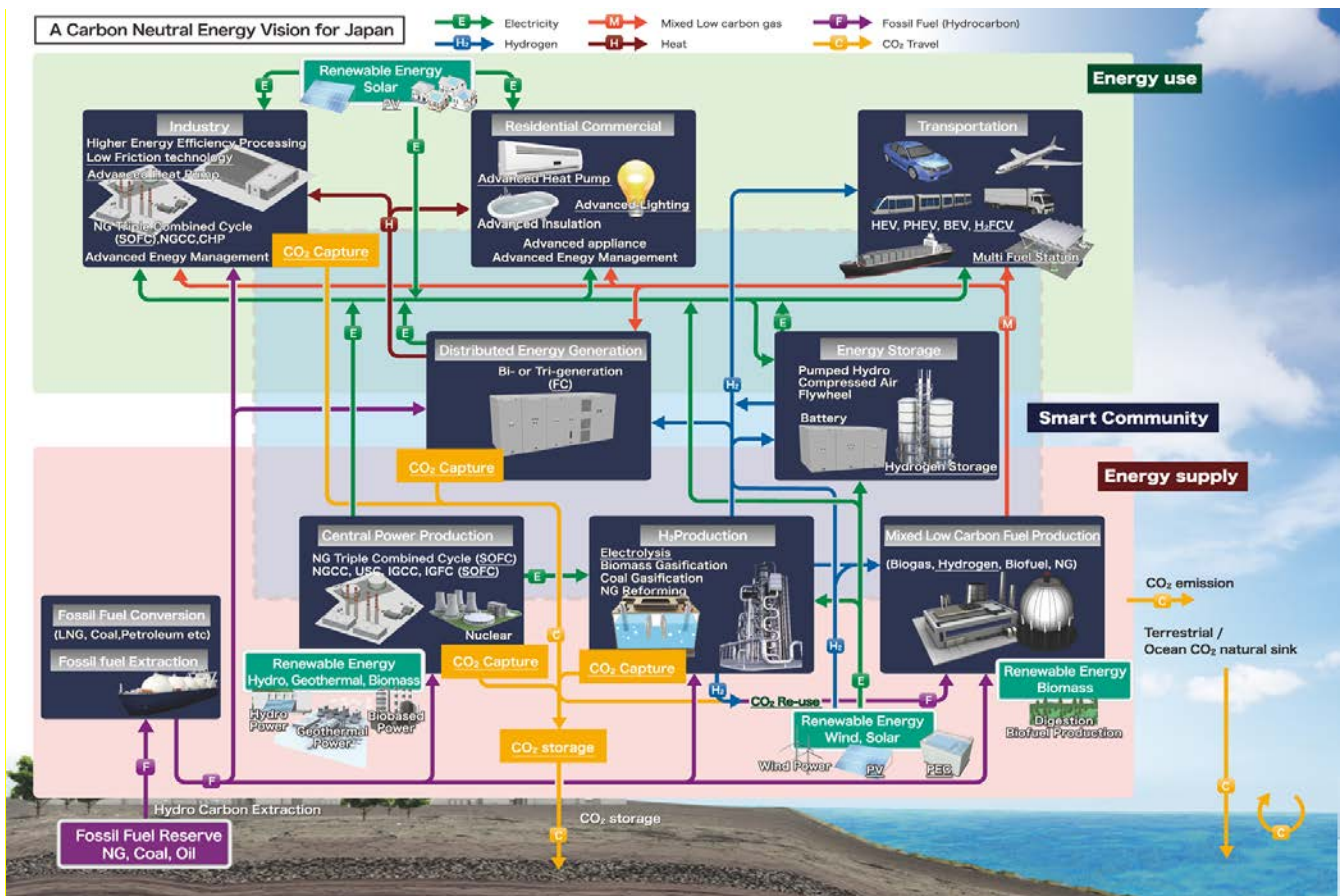


Figure 11: I<sup>2</sup>CNER’s Energy Vision, Carbon-Neutral Society (CNS)

The objective in creating a vision of a carbon-neutral energy society is to help locate the future technology options for a carbon-neutral society (CNS) by sharing a common image of a future for Japan with people in I<sup>2</sup>CNER and outside of I<sup>2</sup>CNER. Researchers in I<sup>2</sup>CNER can then understand the big energy picture and how I<sup>2</sup>CNER’s research will help enable a CNS. In 2009 the G8 announced the commitment of an 80% GHG reduction in 2050 relative to the 1990 level. The I<sup>2</sup>CNER Vision for a low carbon society for Japan is based on setting a long term target of a large reduction (70-80%) of greenhouse gas emissions by 2050. This target is primarily relevant to environmental concerns (climate mitigation) but is also relevant to energy security concerns caused by Japan needing to currently rely heavily on imported fossil

fuels which are depletable and scarce resources. To achieve the target by developing new technology, we also consider economic efficiency and safety issues. As a whole, we consider 3E+S (Environment, Energy Security, Economy and Safety) as basic view points for the vision.

It is expected that the critical point for GHG emission reductions will come before the middle of this century in order to realize stabilization of GHG concentrations in the atmosphere after 2100 at the levels recommended by the IPCC. Therefore, in this energy vision, we first envision the society in 2050. Since we are aiming at a drastic emission reduction, we need revolutionary concepts for new technology which are not significantly bound by the present paradigm. We thus use the back-casting approach, where we start by creating an energy vision of an idealistic future low carbon energy society examining necessary technologies in 2050 to meet the drastic emissions reduction target.

In drawing our vision, we consider two major principles, efficiency increase (we call it "EI" hereafter) in energy conversion and energy use and lowering of carbon intensity (we call it "LCI" hereafter) of fuel and electricity to adopt and develop future technologies. EI should be pursued in energy transformation systems as well as end use systems including home appliances. This idea will also be pursued in industrial processes. EI can be applied to exiting systems but is also achieved by replacing existing system with new technology. LCI in electricity and fuel supply-use pathways is achieved using either renewables, nuclear or CCS. LCI tends to need new facilities or new infrastructure or both.

The figure above shows the image and relation of energy conversion sectors and energy use sectors which are connected by energy pathways represented by secondary energy (electricity, hydrogen and mixed low carbon fuels using bio fuel) in a low carbon society. Some fossil fuel extracted from underground will still be provided to energy conversion sectors and industry with CO<sub>2</sub> capture and sequestration (CCS). Some captured CO<sub>2</sub> can be re-used as an energy carrier.

In the power sector, in addition to efficiency improvements of current technologies, adoption of Natural Gas Triple Combined Cycle using SOFC, IGCC (Integrated coal Gasification Combined Cycle) and IGFC (Integrated coal Gasification Fuel Cell Combined cycle) bring about further advancement in EI. Large deployments of PV and wind power produce low carbon electricity. In the transportation sector, renewable based (wind, solar) electrolysis and natural gas reforming plus CCS produce low carbon hydrogen which is used FCV. Battery electric vehicles (BEV) also have the benefit of low carbon electricity. Residential & commercial sectors use advanced heat pumps for air conditioning and hot water supply and various EI home appliance technology including advanced lighting (e.g. organic LED. Fuel cell cogeneration is used in all end use sectors to improve total efficiency to provide electricity and heat. Industrial sectors adopt various EI technologies including friction loss reduction and utilization of low temperature heat. Finally mixed low carbon fuels including hydrogen or renewable methane (from landfills) mixed with town gas and biofuels produced or imported, can be used by any of the sectors. Biofuels could be used in hybrid electric vehicles (HEV).

### Scenarios

There can be many possible scenarios to achieve a deep cut of GHG emissions. EI technology developments are important. Therefore they are included across the scenarios. LCI technologies can have the greatest impact on GHG emissions and thus enable achieving the challenging GHG emission reduction target.

We developed multiple scenarios by prioritizing different LCI technologies, renewables and CCS. Nuclear is not prioritized in making scenarios at this point because of public concern about safety. The

Table 1: Technologies and their level of development in Scenarios

				Scenarios			
Type	Technology	Application	Metric	A	B	C	D
EI	Thermal power	Combined cycle	Efficiency increase	H	H	H	H
LCI	PV		Deployment	M	H	L	M
LCI	Wind	on-shore, off-shore	Deployment	M	H	L	M
LCI	CCS	off-shore, deep seabed	Deployment	M	L	H	H
LCI	Nuclear		Ratio of restart	NA	NA	NA	L
LCI	Electricity storage	Battery, Flywheel	Deployment	M	H	L	M
EI	High efficiency vehicle	HV, FCV, BEV	Efficiency increase	H	H	H	H
LCI	Low carbon fuel	H2, Biofuel, Electricity	Deployment	M	H	L	M
EI	High efficiency appliance	Heat pump, Co-gene	Efficiency increase	H	H	H	H
LCI	Low carbon fuel	Low-carbon mixed gas	Deployment	M	H	L	M
EI	High efficiency process		Efficiency increase	H	H	H	H
LCI	Low carbon fuel	H2, NG	Deployment	M	H	L	M
LCI	CCS		Deployment	M	L	H	M
Note: EI: Efficiency increase LCI: Lowering carbon intensity				H	:Highly advanced & deployed		
				M	:Moderately advanced & deployed		
				L	:Less advanced & deployed		

table below shows development and deployment timing of EI and LCI technologies across the scenarios. The extent of development and deployment of these technologies makes the differences among the scenarios. The following figures show results of four possible low carbon society scenarios and the contribution of I<sup>2</sup>CNER's research on enabling technologies to GHG emission reduction in these scenarios.

Table 2: Timeline of technology development and deployment  
(Blue fonts are relevant to I<sup>2</sup>CNERs enabling technologies.)

Sector	Type	SHORT TERM - 2020	MID TERM 2020 - 2030	LONG-TERM 2030 - 2050	VERY LONG TERM
Power and energy transformation	EI	Efficiency increase in PC and NGCC IGCC deployment Smart community	Large scale SOFC	SOFC triple combined cycle, IGFC	
	LCI	NGCC replacement for PC Large deployment of PV and wind power Demonstration of CCS	Large deployment of PV and wind power Demonstration of CCS Medium scale of CCS	Next generation PV Full scale CCS deployment SOFC+CCS	Photo water splitting Artificial photosynthesis
Transportation	EI	Large penetration of Hybrid car Introduction of FCV and EV Hydrogen infrastructure introduction	Early penetration of FCV and EV Hydrogen infrastructure development	Large penetration of FCV and EV	
	LCI			Low carbon hydrogen from renewable electrolysis Low carbon hydrogen from NG reforming + CCS	
Residential & commercial	EI	FC cogeneration (SOFC, PECE) Efficiency increase in heat-pump Smart community, HEMS&BEMS	FC cogeneration Large efficiency increase in heat-pump Desiccant air conditioning		
	LCI	(Early penetration of rooftop PV)	(Large penetration of rooftop PV)	Mixed low carbon gas	
Industry	EI	Introduction of steam-heat-pump Introduction of low temperature heat recovery technology Friction loss reduction	Penetration of steam-heat-pump Penetration of low temperature heat recovery technology Friction loss reduction		
	LCI			Mixed low carbon gas CCS deployment	
I <sup>2</sup> CNER's enabling science for above area	EI	High pressure hydrogen storage material, Tribology research, Desiccant material, Adsorption heat pump material	Non Freon refrigerant OLED, Durability increase in FC	Pressurized SOFC Tribology research	SOFC CO2 capture
	LCI	PEM water splitting, Organic PV, Dye-Sensitized PV	Steam Electrolysis, Passive CO2 monitoring / Modeling for CCS	CO2 reduction technology (CO, Formic acid) Novel metal hydride Membran CO2 separation	Photo catalysis water splitting Catalyst for Artificial photosynthesis

### Figures on concept and result of Scenarios

- **Scenario A Base:** Development of important EI technologies and balanced deployment of renewables and CCS. About 71% CO<sub>2</sub> reduction relative to 1990 in 2050
- I<sup>2</sup>CNER's contribution to EI
  - Heat pump and FC cogeneration for residential & commercial from 2020. Low temperature heat utilization for industry from 2020. Fuel cell and hydrogen material & storage for transportation from 2020. SOFC (durability, generation efficiency and coal gas application) for power industry in 2030-2050

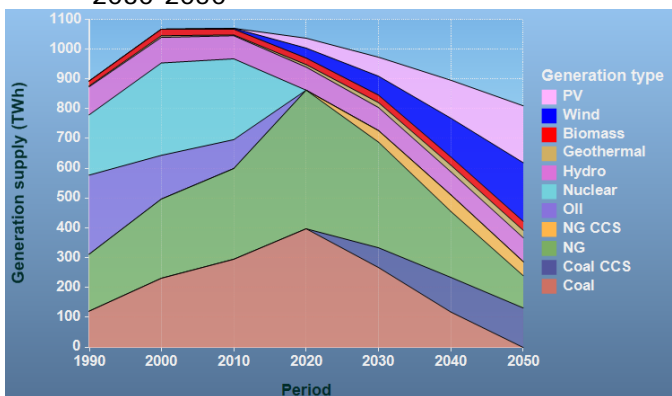


Figure 12: Power generation mix of Scenario A

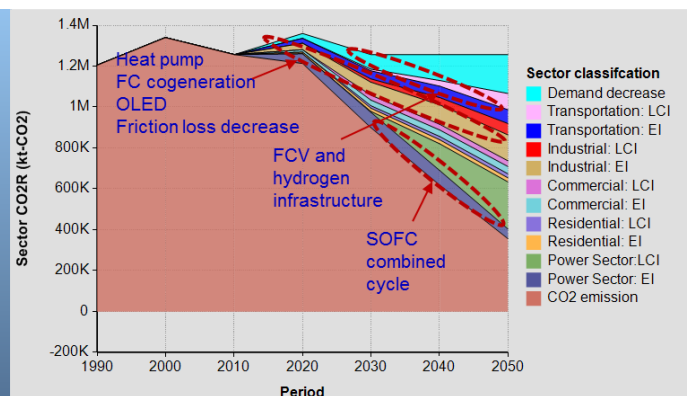


Figure 13 CO<sub>2</sub> reduction relative to 1990 by sector in Scenario A

- **Scenario B Renewables:** Very large penetration of renewables for LCI and development of important EI technologies. About 72% CO<sub>2</sub> reduction relative to 1990 in 2050
- I<sup>2</sup>CNER's contribution to renewables
  - Hydrogen storage and new battery technology to adjust intermittent PV and wind power from 2030
  - Development of electrolysis (PEM and high temperature steam) from renewable electricity to provide low carbon hydrogen from 2030

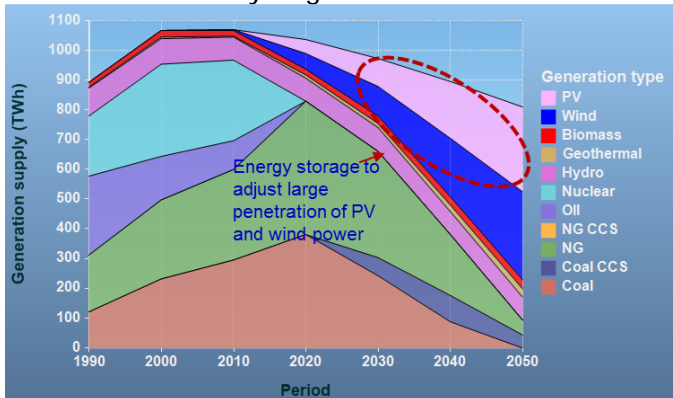


Figure 14: Power generation mix of Scenario B

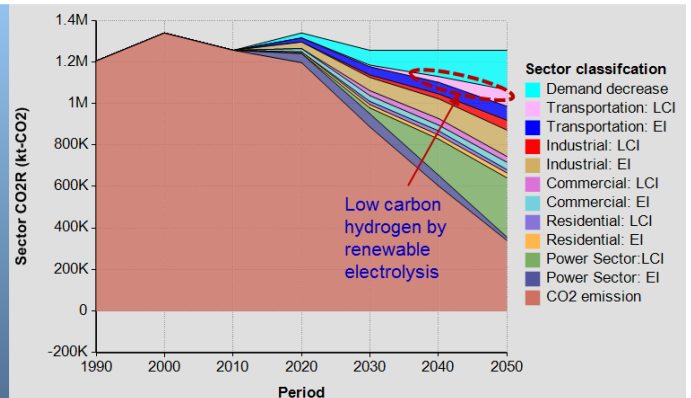


Figure 15: CO<sub>2</sub> reduction relative to 1990 by sector in Scenario B

- **Scenario C CCS:** Large deployment of CCS for power and industries, especially for coal and development of important EI technologies. About 71% CO<sub>2</sub> reduction relative to 1990 in 2050
- I<sup>2</sup>CNER's contribution to CCS
  - Low cost membrane CO<sub>2</sub> capture technology for IGCC and other fossil fuel generation from 2030
  - Low cost and highly accurate seismic monitoring and CO<sub>2</sub> simulation technology for CO<sub>2</sub> storage site characterization and monitoring from 2030

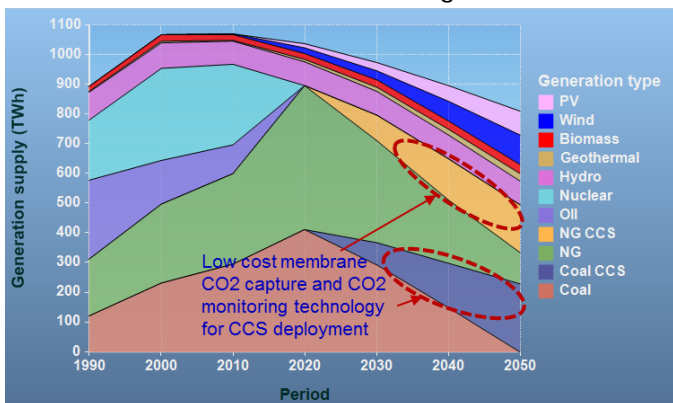


Figure 16: Power generation mix of Scenario C

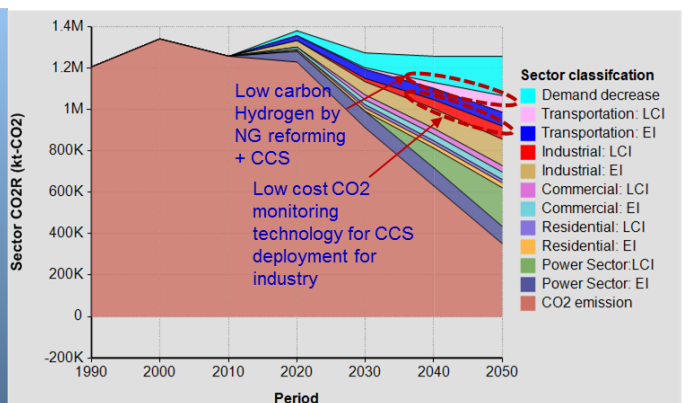


Figure 17: CO<sub>2</sub> reduction relative to 1990 by sector in Scenario C

Note: EI stands for efficiency increase in energy conversion and energy use. LCI stands for lowering of carbon intensity of fuel and electricity.

### Figures on concept and result of Scenarios (continuation)

- **Scenario D Including Some Nuclear:** Balanced application of LCI technologies including nuclear power, assuming that a part of existing nuclear plants will restart and no new plants except for the plants under construction will be used. About 71% CO<sub>2</sub> reduction relative to 1990 in 2050

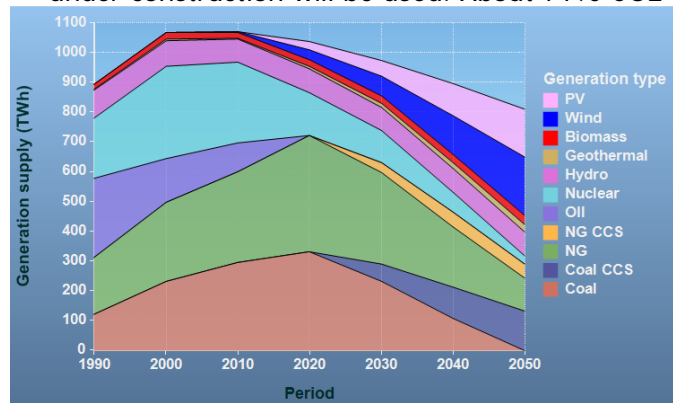


Figure 18: Power generation mix of Scenario D

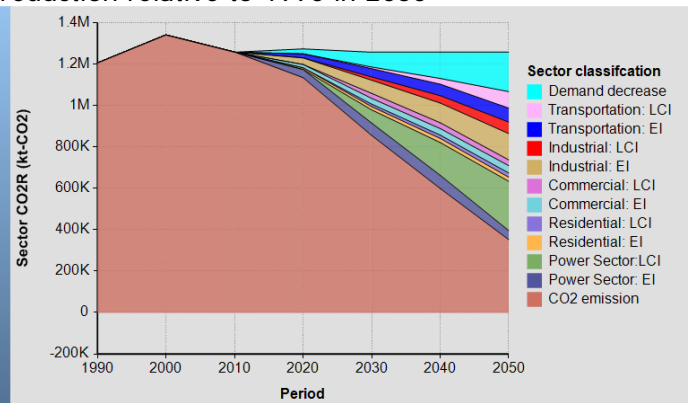


Figure 19: CO<sub>2</sub> reduction relative to 1990 by sector in Scenario D

Note: EI stands for efficiency increase in energy conversion and energy use. LCI stands for lowering of carbon intensity of fuel and electricity.

Overall, our scenario analyses show that a large deployment of renewables along with CCS can achieve low carbon intensity in the power and transportation sectors which together with a large penetration of EI technologies across the sectors results in as much as about 70% GHG emission reduction. Using existing and under construction nuclear power does not result in a large change in GHG emissions in the long run but does help GHG emissions reduction in the near future. The use of nuclear power can also help cost reduction in the technology portfolio for GHG emission reduction. Considering the possibility of sink enhancement (ex. forestation) and obtaining emission reduction credits resulting from the contribution to international emission reduction, about 70% reduction by technology development and deployment in may lead to 80% total reduction credit counted for Japan. To make a further emission reduction, a more aggressive approach to GHG emissions from industry would be necessary.

### 3-1-2. Basic research activities that contribute to the transition to a low-carbon society

*Describe the Center's achievements and outcomes in basic research that contribute to the transition to a low-carbon Society*

*-In Appendix 3-1-2, list the papers underscoring each research achievement and provide a description of each of their significance.*

I<sup>2</sup>CNER's basic research although fundamental in nature is impacting the transition to low carbon society by providing new insights for low carbon technology solutions and indicating directions to roadblock removal for such technologies. A representative sample of such basic research activities is as follows:

- 1) Pioneering research in organic light emitting diodes (OLEDs) by the Adachi group [1, 2]. The December 2008 DOE/BES Report titled "New Science for a Secure and Sustainable Future" states that switching to solid state lighting could reduce electricity use in the US by the equivalent of 100 large power plants. Preliminary calculations by the I<sup>2</sup>CNER energy analysis team indicate that such switching will save Japan about 2% in primary energy sources use.
- 2) High Performance photocatalysts that can efficiently utilize solar energy to potentially produce clean burning fuels thereby reducing carbon production at all stages of the process [3, 4].
- 3) Through mitigating the hydrogen-degradation effect on metal, alloys [5], and polymeric materials and by developing new materials with unique toughness and strength [6], application components (e.g. hydrogen compressors) in a hydrogen economy can operate safely and reliably.
- 4) Robust SOFCs provide a way of generating electricity from any fuel with efficiencies higher than those found with Carnot cycle devices and producing less carbon relative to other methods. Research in I<sup>2</sup>CNER addresses methods to inhibit poisoning (coking) of SOFCs by carbon deposits coming from the fuel [7].
- 5) I<sup>2</sup>CNER researchers developed a novel PEFC free from acid leaching with a remarkable high durability (single cell test: >400,000 cycling) together with a high power density at 120°C under a non-humidified conditions. Such performance opens the door for the next-generation PEFC for "real world" use [8].
- 6) I<sup>2</sup>CNER researchers uncovered the origin of detrimental chemical expansion in oxides commonly used in fuel cells for the first time with insight from atomistic level computational studies tied to experimental evidence, thus laying the groundwork to mitigate chemical expansion and improve fuel cell mechanical durability and lifetime [9].
- 7) Using *synchrotron methods*, I<sup>2</sup>CNER researchers are studying the oxygen reduction reaction (ORR), which is the crucial reaction for both low and high temperature fuel cells and to date operates with high overpotentials [10].
- 8) Understanding the evaporation and interaction of liquids with solid materials [11] has direct consequences on improving the efficiency of technologies such as power generation, heat pump, refrigeration systems, and thermal control.
- 9) Thermal conductivity equation of state for hydrogen has been proposed [12] for the range of temperatures from 78 K to 773 K and pressures up to 100 MPa.
- 10) Thermoelectric properties, including thermal conductivity, thermopower, and electrical conductivity of an ultralong double-walled carbon nanotube (CNT) bundle were studied from 240 K to 340 K. The determined figure of merit achieved  $10^{-3}$  is significantly larger than that reported for carbon nanotube samples [13]. CNT based thermoelectrics may be competitive in applications very sensitive to power to weight over conventional devices. 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.

- 11) TiFe, a potential candidate for hydrogen storage, was demonstrated to absorb and desorb hydrogen without activation [14] when processed by High Pressure Torsion (HPT). It is for the first time that such a result has been reported and if scaled, it may lead to technology innovation.
- 12) Understanding the reactivation and recovery mechanisms of photosystem PSII enzyme [15] is very important to the development of robust artificial photosynthetic catalysts to make hydrocarbons from water and CO<sub>2</sub>, which will directly contribute toward the realization of low-carbon society.
- 13) Research effort to remove the roadblock of using precious Pt in fuel cell technology by copying biology's ways to activate hydrogen [16].
- 14) Construction of novel hydroxide ion-conductive solids [17] for high performance alkaline fuel cells, which do not need expensive platinum catalysts, thus helping develop a lower cost fuel cell system for low carbon society.
- 15) Development of nanosized CO<sub>2</sub> separation membranes with high selectivity and flux [18, 19] is a promising means to control release of CO<sub>2</sub> emissions to the atmosphere and re-use the CO<sub>2</sub> as a carbon source for useful products (e.g. hydrocarbons). A new series of electrodes [20] and catalysts [21] for the electrochemical conversion of CO<sub>2</sub> to useful products has been developed.
- 16) Pioneering monitoring technology for detecting potential CO<sub>2</sub> leakage from sub-seabed storage reservoirs [22].

### 3-1-3. Technological Advances that Contribute to the Transition to a Low-Carbon Society

*Describe technological advances that contribute to the transition to a low-carbon society (joint research with corporations, registered/processed industrial property rights, business start-ups, etc.).*

#### Patents

Table 1 shows a list of pending patents by I<sup>2</sup>CNER researchers for which applications have been submitted after the establishment of the Center. These applications are all in areas relevant to the energy research portfolio of I<sup>2</sup>CNER. The list includes:

A new type gel agent as electrolyte for Li-air battery [1], actuation [2], tribology related fatigue life of materials [3], fuel cell reformers [4], PEFC high durability electrode materials [5, 6] and electrocatalysts [7, 8], thermal science and engineering industrial applications [9-11], thermoelectrics [12], a new hydrogen storage approach [13], a green oxidation methodology with water being the only waste [14], a new FeCo nanoalloy magnet with superb magnetization capabilities [15], Atomically-well-mixed iron-group nanoalloy catalysts [16], new catalysts for lower olefins [17], Nanothin membranes for gas separation [18].

*Table 1: Patent Applications*

	Title	Inventors	Application date	Industrial relevance
1	Gel electrolyte for Li-air battery	Ishihara, T., Mitsui, S., Miyauchi, N.	Oct.12,2012	Post Li ion battery with discharge temperature at 273K
2	Conductive Material, and its Production Method and Transducer	Matsuno, R., Takahara, A.	Mar.26,2013	Actuation
3	Prediction method for fatigue limit and fatigue life of bearings and power transmission devices	Komata, H., Ueda, T., Matsuoka, S., Matsunaga, H., Yamabe, J.	Jan. 2014	Fatigue life and strength for rolling contact of bearings.
4	Paper-structured catalysts, array of paper-structured catalysts and solid oxide fuel cells with paper-structured catalysts or with array of paper-structured catalysts	Shiratori, Y., Tran, T. Q., Kitaoka, T., Sasaki, K., Ogura, T.	July 31, 2013	Fuel cell system, reformer

5	Electrode for Fuel Cell and its Manufacturing Method, and Membrane/Electrode Assembly and Polymer Electrolyte Fuel Cell	Higashi, T., Noda, Z., Hayashi, A., Sasaki, K.	Feb. 20, 2014	High durability electrode materials for PEFC
6	High Performance Electrocatalyst of Fuel Cell Suitable for Fuel Cell Vehicle and its Manufacturing Method	Horiguchi, D., Noda, Z., Hayashi, A., Sasaki, K.	Mar. 20, 2014	High durability electrode materials for PEFC.
7	Electrocatalyst composites and their preparation methods	Nakahsima, N., and Fujigaya, T.	Feb. 2, 2012	Electrocatalyst for PEFC (JP2012-21358)
8	Electrocatalyst composites and their preparation methods	Nakahsima, N., and Fujigaya, T.	Jan. 17, 2013	Electrocatalyst for PEFC (PCT/JP2013/050748)
9	A dehumidifier and a method of dehumidification	Ng, K.C., Myat, A., Yanagi, H., Thu, K., Saha, B.B., and Leong, I.	July 23, 2012	Dehumidifiers (desiccant) for cooling and dehumidification of buildings. Several industries from Singapore and Malaysia have been negotiating for business license
10	Desalination system and method	Saha, B.B., Ng, K.C., Chakraborty, A., and Thu, K.	Oct. 1, 2013	Adsorption cycle for high quality water production from the saline or brackish water. A business license has been issued to Vegalo Ltd. of Esperidion 12, 1087 Nicosia, Cyprus.
11	Method and system for storing natural gas, PCT Indonesia	Ng, K.C., Loh, W.S., Rahman, K.A. and Saha, B.B.	Oct. 1, 2013	On storage of natural gas in portable gas bottles or cylinders, filled with solid adsorbent for applications up to 40 bar and at ambient temperature. Several industries from South Asian region have been negotiating for business license.
12	A new method for simultaneous measurement of optical absorptance and thermal conductivity of individual micro/nano wire	Wang, H., Zhang, X.	Nov. 5, 2012	Simultaneous measurement of optical absorptance and thermal conductivity of industrial micro/nano wire.
13	TiFe hydrogen storage alloys and its production methods	Horita, Z., Akiba, E., Matsuda, J., Edalat, K.	Mar. 16, 2013	Promising material for energy storage



14	Method for Substrate Oxidation	Ogo, S., Oshima, S., Hayashi, H. and Inoki, D.	Sep. 9, 2011	Green process for substrate oxidation with water being the only waste
15	Body-centered cubic (bcc)-type iron-cobalt alloy particle, its manufacturing method	Yamauchi, M.	Mar. 8, 2012	FeCo nanoalloy magnet exhibiting the largest magnetization among transition metal alloys
16	Solid carrier-supported iron group solid-solution-type alloy composite and catalyst	Yamauchi, M.	Feb. 13, 2014	Atomically-well-mixed iron-group nanoalloy catalysts
17	Manufacturing olefine having 2 to 5 carbon atoms by ficher-tropsch reaction	Yamauchi, M	Mar. 27, 2014	Catalysts for lower olefins by fischer-tropsh reaction
18	Gas separation membrane, its manufacturing method, its gas separation module, and gas separation method	Fujikawa, S.	Nov. 28, 2013	Nanometer-thick membrane for gas separation

### Industrial Projects

The following are descriptions of collaborative projects between I<sup>2</sup>CNER's researchers and Industry that are impacting real-life carbon-neutral energy solutions. All projects resulted from the Center's research activities:

#### *Polymer brush technology*

PI Takahara's research on polymer brush technology has led to many industrial projects. By way of example PI Takahara is carrying out joint research with a) Toyota on lubrication of automotive power train parts for energy efficiency, b) Sumitomo Rubber on lubrication and anti-fouling of polyolefine surface. Polyolefine is a common plastic whose functionalization will replace several energy consuming special functional polymer products whose production is energy intensive and involves a large number of chemicals, c) Chugoku Paint on energy efficient coatings for lubrication and anti-biofouling. Coating technology with excellent lubrication in sea water contributes to the fuel use reduction and CO<sub>2</sub> discharging.

#### *Catalysis*

PI Ishihara is carrying out joint research with a) Toyoda Gosei on the application of organic-dye modified concept for wide band gas nitrate on visible light usage, b) JFE Steel Corporation on the development of an active catalyst for intermediate CO<sub>2</sub> electrolysis for the re-using of CO<sub>2</sub> formed during the steel making process, c) Kansai Electric Power on the development of a new concept metal-air battery for large scale energy storage devices.

PI Ogo is a member of the organization based at Kyushu University and Fukuoka Industry-Academia Symphonicity which coordinates with industries involving DAIHATSU Motor Co., Ltd., Japan New Chisso Co., Ltd., and MITSUBISHI Gas Chemical Co., Inc. the structuring of the "Electrons from Hydrogen Network," a project aiming to create new industries in the area for functional Pt-free molecular catalysts and biocatalysts for H<sub>2</sub> activation. Such catalysts have a great potential for use in low-cost hydrogen fuel cells, accelerating hydrogen-based technology and economy.

PI Yamauchi carries out joint work Ube Industrial Ltd. on the production of novel nanoalloy catalysts. Also, PI Yamauchi developed iron-group nanoalloy catalysts for direct ethylene glycol solid alkaline fuel cells. These catalysts show high selectivity to lower olefins through the Fischer-Tropsch reaction. Presumably, the demand for lower olefins, which is important for raw materials in industrial chemicals, will exceed the supply in the near future. Plans are in place to initiate a project with industry for the development of iron-group nanoalloy catalysts for lower olefin synthesis.

### *Fuel Cells*

The lead PI of the Fuel Cells division, Prof. Kazunari Sasaki, is the director of the Next-Generation Fuel Cell Center (NEXT-FC) which is located next to the I<sup>2</sup>CNER building. Engineers and researchers from various industries such as Kyocera, Mitsubishi Hitachi Power Systems, and JX Nippon Oil and Energy are housed in the NEXT-FC carrying out work in the area of durability, reliability, and performance of fuel cells. A number of I<sup>2</sup>CNER researchers are housed in the facilities of NEXT-FC and all I<sup>2</sup>CNER researchers have access to the laboratories of the NEXT-FC. Interactions between NEXT-FC and I<sup>2</sup>CNER researchers contribute to better technology solutions since these companies are active on the commercialization of the next-generation fuel cells systems."

### *Hydrogen Storage*

I<sup>2</sup>CNER professors Lyth and Hayashi led by PI Akiba collaborate with JX Nippon Oil & Energy to synthesize nanostructured carbons with large surface area for hydrogen storage applications. This project is now entering its third year.

PI Akiba contributes to the establishment of NEDO roadmaps for hydrogen storage technologies and hydrogen storage for fuel cell vehicles. Under these activities, he has close collaborations with the car industry and the Fuel Cell Commercialization Conference of Japan (FCCJ) that is an organization established by private companies to develop and commercialize fuel cell and hydrogen technologies. The team of PI Akiba actively collaborates with various industries including automotive (TOYOTA, Nissan, and HONDA), hydrogen storage material producers, petroleum companies.

Scaling-up of the severe plastic deformation (SPD) process is crucial to the industrial production of a TiFe, our newly discovered promising candidate materials for stationary hydrogen storage. In 2013, the group of PI Horita initiated a collaboration with Nagano Forging Co. (in Nagano prefecture) to install a 500 ton SPD machine. The machine was designed based on high-pressure sliding (HPS) originally developed in Kyushu.

### *Thermophysical properties*

The database on the high pressure high temperature thermophysical properties of hydrogen has already been distributed to Japanese industries (e.g. Honda Motor, Daido Steel) as a useful design tool for hydrogen energy systems.

### *Technology transfer and commercialization: Development of a new type of metal packing for high-pressure hydrogen*

I<sup>2</sup>CNER professor M. Kubota and Y. Otsu of TOKi engineering working together overcame the challenge of developing a new seal (metal packing) for 100 MPa hydrogen gas. The resulting product is readily produced, easily installed (small tightening force and lower risk for damaging equipment), compact, reusable, highly reliable, compatible with a broad temperature range, and not susceptible to hydrogen-induced degradation. Development of this new seal can accelerate transition to hydrogen economy. After three years of R&D, the packing was commercialized in June 2013 (TOKi engineering). The shape of the packing is shown in Figure 20. The seal performance increases as hydrogen pressure increases by the self-sealing mechanism illustrated in Figure 21. During R&D, we experienced several issues such as fatigue and fretting wear failures. These issues were resolved by applying the fundamental knowledge gained during research activities such as those featured in Project 1 of the Hydrogen Materials Compatibility division. The packing was introduced into the market in June 2013.

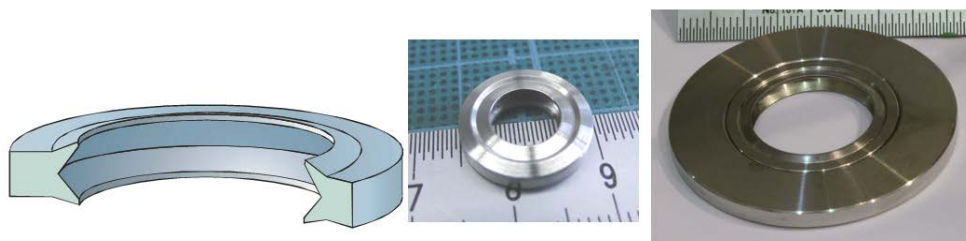
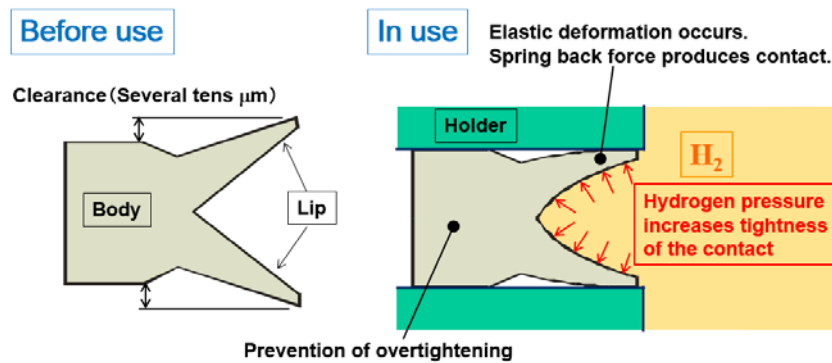


Figure 20. New metal packing for 100 MPa H<sub>2</sub> service (commercialized in June 2013)



Prevention of overtightening  
Figure 21. Principle for sealing

#### *Hydrogen embrittlement mitigation for high-strength alloys*

Lead PI Somerday, PIs Sofronis and Robertson, I<sup>2</sup>CNER postdocs Martin and Dadfarnia, and Dr. Nagao of JFE Steel studied the effect of nano-sized (Ti,Mo)C precipitates on hydrogen embrittlement of tempered lath martensitic steel. The results showed that nano-sized (Ti,Mo)C precipitates trap hydrogen and prevent intergranular fracture, thus improving the resistance of lath martensitic steel to hydrogen embrittlement. This accomplishment has brought a new concept of material design for high-performance steels with improved resistance to hydrogen embrittlement to realize safe and reliable storage and transport of hydrogen. JFE Steel Corporation has indicated interest in partnering with I<sup>2</sup>CNER to further develop this discovery toward technology.

#### *Structurally graded austenitic stainless steel*

PI Takaki is leading the field of enhancing hydrogen embrittlement resistance for high-strength austenitic stainless steels through microstructures produced by novel heat treatment. His relevant patent, No. 5055547, has been installed in a wire maker; industrial production of thin wires and wire ropes has already been successfully conducted. If this technology was extended to material products relevant to hydrogen containment components, e.g., thin plates or pipes, it would contribute to the low-carbon society by providing high-strength, low-cost austenitic stainless steels that are compatible with hydrogen gas environments.

#### *Structural health monitoring of pressure vessel*

I<sup>2</sup>CNER WPI Visiting Professor, Dr. Xu, working with AIST researchers S. Guo, N. Ueno, D. Ono, C.S. Li, Y. Sakata, and the director of the Hydrogen Energy Test and Research Center (HyTReC), S. Watanabe, successfully visualized fatigue damage in pressure vessels by applying mechanoluminescent sensor technology. These research accomplishments involved partnering with the pressure vessel company SAMTEC and HyTReC. Developing a structural health monitoring system for hydrogen gas vessels resonates with an active research area in the structural prognosis community. Such a structural health monitoring system for hydrogen pressure vessels would improve their safety and reliability as well as reduce costs by prolonging vessel replacement intervals.

#### *Nano tribo-interface for ultra-low friction*

Diamond like carbon (DLC) coatings are promising surface materials for hydrogen service (in valves for example), so an activity on this topic was started as part of the HYDROGENIUS NEDO project. DLC coatings have excellent performance in general (very low friction and wear without lubricants) so the use of these materials is expanding very quickly in automotive and other industrial areas. It is also a high-visibility research subject that is capturing the attention of many in the tribology field. Last October, the research group of PI Sugimura started new DLC research in collaboration with Tohoku University and Nagoya University for a JST project on nano tribo-interface for ultra-low friction mechanical systems. The unique expertise contributed by the PI Sugimura research group is the capability to conduct experiments in controlled gas environments to study mechanisms and improve DLC tribology. Polymers for general use are also included in this low friction project.

#### *CO<sub>2</sub> Capture by Membrane*

Gas separation by nanometer-thick and free-standing membrane is a promising approach to improve the current low permeance of a gas separation membrane, since the thickness of conventional membrane is still in the range of micron scale. Since April 2012, CO<sub>2</sub> Capture and Utilization division has an ongoing

collaboration with the NanoMembrane Inc. and Hitachi corporations to develop a nanomembrane for gas separation. Within this collaboration PI Fujikawa developed a nanomembrane with high CO<sub>2</sub>/N<sub>2</sub> selectivity which is close to the current-state-of-the art. This result has been reported in Section 2-1 and an application for a patent has been submitted [18].

Dr. Taniguchi collaborates with Mr. Tsutomu Sakai (Group leader of Environment and Chemical Process Research Laboratory, KRI, Inc., Kyoto, Japan) to fabricate PAMAM dendrimer-containing polymeric membranes with submicron thickness for enhanced CO<sub>2</sub> permeation. Involved in this research is also Prof. Taniguchi works on the development of the nano-thick membrane while KRI is doing process simulations to determine required CO<sub>2</sub> separation properties and optimize the operation conditions.

#### *Monitoring and modeling for the Tomakomai carbon capture and storage (CCS) project*

PI Tsuji and Prof. Kitamura are collaborating with the Japan CCS Corporation and analyze the geophysical and geological data (core samples) for the Tomakomai CCS project aiming to develop new monitoring methods. The collaboration addresses the critical issues related to earthquakes in the Tomakomai CCS project. By monitoring pore pressure variations around a CO<sub>2</sub> injection point, we can control the amount (or rate) of CO<sub>2</sub> injection so as to avoid generation of earthquakes. This analysis is very important and contributes to informing the public on issues related to potential CCS-induced earthquakes.

#### *Assessment of biological CCS*

PI Tsuji in collaboration with the Japan Agency for Marine Science and Technology (JAMSTEC) is investigating the potential of large-scale biological (renewable) CCS, whereby injected CO<sub>2</sub> is converted to methane within the coalbed sequence. Specifically, PI Tsuji assesses the suitability of subsurface environment for biological reaction while JAMSTEC scientists carry out laboratory analysis of the transformation rates of CO<sub>2</sub> to CH<sub>4</sub>.

#### *CO<sub>2</sub> Leakage detection and monitoring*

I<sup>2</sup>CNER professor Shitashima is funded to develop technology for CO<sub>2</sub> leakage detection/monitoring by The General Environmental Technos Co., Ltd. (KANSO Technos). KANSO has been carrying out environmental background observations at several CCS candidate sites in Japan. Work by Prof. Shitashima is contributing to the establishment of observation instruments and technology. In Feb. 2014, a mapping survey at the demonstration site of Tomakomai CCS project was conducted.

### **Training the next generation of engineers**

Teaching activities of I<sup>2</sup>CNER faculty in the Department of Automotive Sciences contribute to the preparation of the next generation of engineers and researchers for the automotive industry and in particular in the areas of fuel cells and lithium-ion batteries.

### 3-2. Achievements of Center's outreach activities

*-In Appendix 3-2, list and describe media coverage resulting from press releases and reporting.*

#### **I<sup>2</sup>CNER Annual Symposium**

Each year, the Institute holds the I<sup>2</sup>CNER Annual Symposium in order to attract world-leading researchers to I<sup>2</sup>CNER and expose them to the research that we are doing. Through his participation as a plenary lecturer in the Annual Symposium in January 2014, Professor Benny Freeman became a WPI Professor in the Institute as of April 1, 2014.

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

The Institute publishes two outreach publications, Hello! I<sup>2</sup>CNER (for high school students) and Energy Outlook (for industrial stakeholders), three times per year. Energy Outlook was established in FY 2012, and has featured interviews with several industry officials, including Katsuhiko Hirose of Toyota. Due to the regularity of its publication, high school students have begun to recognize Hello! I<sup>2</sup>CNER and we have received requests from high schools who want to participate in the "Science Café" section in upcoming issues.

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

In order to celebrate the success of the I<sup>2</sup>CNER seminar series thus far, we published the I<sup>2</sup>CNER Seminar Series Report at the end of FY 2013.

### **AAAS Annual Meeting**

Beginning in FY 2011, I<sup>2</sup>CNER has participated in the AAAS Annual Meeting each year. The I<sup>2</sup>CNER booth is always set up in the "Japan Pavilion," which is organized by the Japan Science and Technology Agency (JST). The AAAS Meeting is attended annually by a wide range of individuals, including scientists, lawmakers, administrators, national and international media, and parents and children. At the FY 2013 meeting, I<sup>2</sup>CNER Director Petros Sofronis gave a presentation about the appeal of the research environments at Japanese universities.

### **Kyushu University Soft Engineering Open Lecture "Thoughts on Energy"**

With the support of the Fukuoka City Board of Education, in the winter of 2013, I<sup>2</sup>CNER and the Kyushu University Faculty of Engineering co-hosted free, open lectures on future energy for the general public. Of the 5 lectures that were given, 2 were delivered by I<sup>2</sup>CNER researchers. Prof. Ishihara spoke about "Next Generation Battery for Energy Issues" on November 22. Prof. Sasaki gave a talk on "Towards a hydrogen energy society based on fuel cell technologies" on December 6.

### **SSH Student Workshop**

On August 7-8, 2013, I<sup>2</sup>CNER shared a booth with WPI-iCeMS at the "SSH Student Workshop." The event was held to encourage students' interest in science and technology, and students from 219 schools, including 18 international schools, participated. The event was open to the general public, as well.

### **Science Craft Festa in Kyoto**

I<sup>2</sup>CNER has participated in 2 "Science Craft Festas" in Kyoto, one in 2011 and one in 2013. These festas are organized by MEXT with the goal of exposing high school students to cutting edge research. At the 2013 Festa, I<sup>2</sup>CNER researchers presented on CO<sub>2</sub> capture and storage technology, theoretical chemistry, and graphene and fuel cells. At the 2011 Festa, we offered a demonstration of how to run a miniature hydrogen car, showed a news clip of Prof. Ogo's research achievements, and handed out visual materials on CCS technology.

### **Special Lecture at a Local High School**

On July 12, 2013, I<sup>2</sup>CNER Associate Professor Shigenori Fujikawa gave a lecture on carbon-neutral energy at a local high school.

### **I<sup>2</sup>CNER Promotion Video**

In FY 2013, I<sup>2</sup>CNER completed its first Promotion Video, which features both English and Japanese.

### **I<sup>2</sup>CNER in Tokyo Symposium**

On December 7, 2012, I<sup>2</sup>CNER hosted the "I<sup>2</sup>CNER in Tokyo" symposium in order to bring I<sup>2</sup>CNER research activities to the attention of the energy stakeholders in the capital of Japan. The symposium featured lectures by John V. Roos, then-US Ambassador to Japan; Daisuke Yoshida, then-Director-General, Research Promotion Bureau, MEXT; Monterey Gardiner, Technology Development Manager, Office of Hydrogen, Fuel Cells and Infrastructure Technologies, U.S. Department of Energy; and Katsuhiko Hirose, Project General Manager, R&D Management Division, Toyota Motor Corporation, among others. The day concluded with a panel discussion between the lecturers and the audience, which was moderated by Mark Paster.

### **5<sup>th</sup> Joint Exhibition by the Fukuoka City Children's Science & Culture Center and the Kyushu University Museum**

From July 21 to August 30, 2012, I<sup>2</sup>CNER co-hosted the 5<sup>th</sup> Joint Exhibition by the Fukuoka City Children's Science & Culture Center and the Kyushu University Museum. The exhibition, which focused on "Environment and Energy," was a fun, "hands-on" display so that the children could play while simultaneously learning about hydrogen energy and a low-carbon society. Associate Professor Tsuyohiko Fujigaya and Assistant Professor Keigo Kitamura represented I<sup>2</sup>CNER at the event. Nearly 16,000 attendees in total participated in the exhibition.

### **WPI Joint Symposium**

I<sup>2</sup>CNER organized the WPI 6 Institute Joint Symposium on Nov. 12, 2011, and Profs. Sofronis and Ogo both gave presentations. The theme of the symposium was "Cutting Edge Science & Your Future." On November 24, 2012, I<sup>2</sup>CNER co-hosted the WPI Joint Symposium along with all the other WPI

Centers. I<sup>2</sup>CNER's Associate Director, Prof. Tatsumi Ishihara, gave a lecture entitled, "the Dream of Artificial Photosynthesis; challenge to the creature."

On December 14, 2013, I<sup>2</sup>CNER co-hosted the WPI Science Talk Live 2013 along with all the other WPI Centers. The event included presentations by WPI researchers and high school students. Admission was free and the event was open to the public. Simultaneous interpretation in English and Japanese were provided.

### **I<sup>2</sup>CNER Annual Report**

The Institute publishes an Annual Report each year to update the community on our activities and progress.

#### 4. Interdisciplinary Research Activities (within 3 pages)

##### 4-1. State of Strategic (or "Top-down") Undertakings toward Creating New Interdisciplinary Domains

#### **Start-up Funding for Interdisciplinary Research**

To promote interdisciplinary research across division boundaries, the SSC introduced a new program titled "Start-up Funding for Interdisciplinary Research" to solicit research proposals for start-up funding. Only joint proposals by faculty from at least two divisions were considered for review. In FY2011, nine (9) proposals were selected after rigorous screening. In FY2012, all 9 projects were required to submit progress reports and give seminar presentations in order to be considered for funding in the second call for interdisciplinary research proposals. In this second call, several projects which were initiated in FY 2011 were halted, and a total of five (5) projects were selected, of which one (1) was a new project and four (4) projects were renewals. The five selected projects for FY 2012 were:

- 1) Hydrogen Adsorption on Graphene Nanofoam  
(*Profs. Lyth and Shao*)
- 2) Nano Processing and Properties of Mg-based Materials for Energy Storage  
(*Profs. Shao, Akiba, Takata, Bishop, Lyth, and Fujikawa*)
- 3) Investigation of proton conducting amorphous oxides for pre-combustion CO<sub>2</sub> separation  
(*Profs. Fujikawa and Bishop*)
- 4) Direct Investigation of physical characteristics of super critical CO<sub>2</sub> toward monitoring of CO<sub>2</sub> behavior in geological reservoir  
(*Profs. Kitamura and Fujikawa*)
- 5) A novel nanostructured electrode by combining nanotitania and mesoporous carbon  
(*Profs. Matsumoto and Hayashi*)

In FY2012, the total budget allocated to these five projects was \$85,500 USD (1USD=100 JPY), which is a reduction by more than 50% relative to the FY2011 budget, the reason being an overall lack of substantial accomplishments. Overall, the program resulted in the following interdisciplinary publications:

- 1) Lyth, S. M., Shao, H., Liu, J., Sasaki, K. and Akiba, E. (2014), Hydrogen adsorption on grapheme foam synthesized by combustion of sodium ethoxide, *International Journal of Hydrogen Energy*, 39 (1), 376-380.
- 2) Shao, H., Ma, W., Kohno, M., Takata, Y., Xin, G., Fujikawa, S., Fujino, F., Bishop, S. R. and Li, X. (2014), Hydrogen storage and thermal conductivity properties of Mg-based materials with different structures, *International Journal of Hydrogen Energy*, in press (<http://dx.doi.org/10.1016/j.ijhydene.2014.02.063>).

#### **Distribution of Funding to Young Faculty**

A portion of the funds which were conserved through the budget cuts for the Interdisciplinary Research Projects has been allocated for a new initiative designed to help support young faculty. Beginning April 1, 2013, each of the young faculty members was automatically allocated 1.5 million JPY to support their research programs with specific instructions that the funds should be used to advance interdisciplinary research.

### **Competitive-funding Allocation**

In FY 2013, a new program, titled "I<sup>2</sup>CNER Competitive Funding" was initiated. Through this program, we aim to cultivate fusion/interdisciplinary research by maintaining rigorous standards for the allocation of funds, which are used to increase financial support only for productive research teams that achieve results such as publishing fusion papers in high impact-factor journals. The allocation of funds (Total amount: 150,000 USD in FY 2013/ 1 USD=100JPY) is administered by the Director in consultation with the two Associate Directors and the IPRC, after the programs of all I<sup>2</sup>CNER faculty have been reviewed. In FY 2013, funding was allocated to those faculty members who were productive and whose achievements were relevant to I<sup>2</sup>CNER's fusion research (including papers, awards, external research funds, etc.). The program is ongoing and its first assessment will be done in FY2014.

#### **4-2. State of "Bottom-up" Undertakings from the Center's researchers toward Creating New Interdisciplinary Domains**

\*I<sup>2</sup>CNER's "Bottom-up" Interdisciplinary Research Undertakings have been initiated in several ways over the years. Examples of the most common strategies/circumstances for initiating "bottom-up" interdisciplinary projects are listed below.

### **Mutual Presence in I<sup>2</sup>CNER Building 1**

The new I<sup>2</sup>CNER building brought our researchers under the same roof and this instigated collaborations across the disciplines. One example is the collaboration between PI Tatsumi Ishihara, PI John Kilner, Satellite Faculty Angus Rockett, and postdoc John Druce. This collaboration was the result of a tour of the Kyushu I<sup>2</sup>CNER facilities taken by Professor Rockett. The unique capabilities of both the I<sup>2</sup>CNER faculty and staff, and the Low Energy Ion Scattering (LEIS) instrument in I<sup>2</sup>CNER brought to the fore the potential to answer long-standing questions about a key energy generating photovoltaic material. The collaboration combines physics (Kilner), materials science (Rockett), and inorganic chemistry (Ishihara).

### **Division Retreats (requested by the Director)**

Starting Fall 2013, the Director and Associate Directors required each research division of the Institute to host a division retreat at a location away from KU/the I<sup>2</sup>CNER building so that each research division could consider carefully its research themes and collaborative projects, with a central focus on cross-cutting issues. Examples of the interdisciplinary collaborations which emerged are:

- 1) The collaboration between PI Ken Sakai and Satellite Faculty Lane Martin on "High-Efficiency Hybrid Organic/Inorganic Photocatalysis Systems." This work stands at the forefront of advanced materials science and chemistry.
- 2) The collaboration between Professors Hidehisa Hagiwara and Aleksandar Staykov, PI Tatsumi Ishihara, and Satellite Faculty Elif Ertekin on "A hybrid molecular switch for ultra-efficient photocatalytic charge separation." This work is fusion of solid state photocatalysis with molecular chemistry.

### **IISS Presentations**

Since its inception, young researchers have been giving presentations at the Institute Interest Seminar Series (IISS) with the goal of initiating cross-division collaborations. Examples of collaborations which have emerged are:

- 1) The collaboration between Professors Masamichi Nishihara and Aleksandar Staykov, which resulted in a joint journal publication in the Journal of Polymer Science Part B: Polymer Physics (2014), 52, 293–298. This project fuses polymer chemistry, solid state materials science, computational chemistry, and electrochemistry.
- 2) Molly Jhong (Illinois graduate student) from the group of Satellite Faculty Paul Kenis presented her research before the groups of PIs Naotoshi Nakashima and Kazunari Sasaki. I<sup>2</sup>CNER Professor Stephen Lyth approached Ms. Jhong after the presentation to suggest that she try some of his N-doped carbon materials for CO<sub>2</sub> conversion. A joint collaboration on materials synthesis and electrochemistry is ongoing.

### **Unofficial Seminars on "Computational Materials Science"**

In October 2013, young faculty, led by Professor Aleksandar Staykov, put forward a new, unofficial initiative on "Computational Materials Science" in order to advance exchange and collaboration in molecular and

materials chemistry across division boundaries. The effort, which involves informal seminar presentations and discussion, gives researchers from molecular chemistry and materials chemistry the opportunity to meet and exchange ideas, and share computational techniques and knowledge in the emerging interdisciplinary fields of organic/inorganic interface chemistry and the fields of surface chemistry and material interfaces. These meetings, which have attracted both theoreticians and experimentalists, have led to collaborations between members of the Fuel Cells, Hydrogen Production, and Hydrogen Materials Compatibility divisions. Although the members of this initiative have not asked for financial support, the Director supports and endorses it.

### **I<sup>2</sup>CNER Events & Initiatives amongst Researchers**

Various I<sup>2</sup>CNER events have led to interdisciplinary collaborations. Occasionally these projects may also emerge from initiatives amongst researchers. Examples of such collaborations are as follows:

- 1) During the I<sup>2</sup>CNER Kick-Off Symposium in February 2011, PI Brian Somerday presented experimental results for gas impurity inhibition of hydrogen gas-accelerated fatigue crack growth. I<sup>2</sup>CNER Professor Aleksandar Staykov was in the audience for this talk, and this led to discussions on how the mechanisms for inhibition could be explored theoretically by applying density function theory (DFT) modeling. The work resulted in a joint publication entitled "Effect of hydrogen gas impurities on the hydrogen dissociation on iron surface" in *the International Journal of Quantum Chemistry*, 114 (10), 626-635, 2014.
- 2) During an I<sup>2</sup>CNER meeting on high pressure torsion for hydrogen storage materials, Satellite Faculty David Cahill and PIs Yasuyuki Takata and Zenji Horita decided to consider the very new idea that bulk processing can be applied to semiconductors to reduce their thermal conductivity. By traveling between Kyushu and Illinois, I<sup>2</sup>CNER Professor Masamichi Kohno served as link for this highly collaborative project which resulted in a joint paper titled "Reduction in Thermal Conductivity of Crystalline Silicon Processed by High-Pressure Torsion." This paper is currently under review in *Nanoscale Research Letters*.
- 3) Due to their scientific stature, PIs Harry Tuller and John Kilner have been instrumental on instigating interdisciplinary research amongst I<sup>2</sup>CNER faculty. Examples of joint publications which have emerged as a result of the initiative of these two PIs are in *Advanced Functional Materials*, 22 (9), 1958-1965, 2012 and the *Journal of Materials Chemistry A*, 1 (26), 7673-7680, 2013.

#### 4-3. State of Advancing Interdisciplinary Research that can be expected to accelerate the Transition to a Low-Carbon Society

*-In Appendix 4-3, list papers published on the Center's interdisciplinary research and provide a description of each of their significance.*

### **Creating a "Culture" of Interdisciplinary Research**

The Administration of I<sup>2</sup>CNER has worked very hard to integrate a "culture" of interdisciplinary research into the very structure and operations of the Institute. For example, having an overall view of the progress and activities of the full time I<sup>2</sup>CNER faculty and researchers, the Director has at his disposal the I<sup>2</sup>CNER Competitive Fund (Section 4-1) and discretionary funds, which are both intended to foster and advance interdisciplinary research. The importance of interdisciplinary research is emphasized consistently in the letters that all I<sup>2</sup>CNER full-time faculty receive as part of their annual evaluation. In addition, all I<sup>2</sup>CNER faculty know that interdisciplinary research is a requirement for promotion and tenure within the Institute, a fact that is clearly stated in the Institute's governing document on Faculty Promotion.

#### 5. International Research Environment (within 4 pages)

##### 5-1. International Circulation of the Best Brains

###### 5-1-1. State of Linkage with the Illinois Satellite Institute, and of Joint Research with them

*Describe the roles of the satellite organizations and the personnel make-up and system, collaborative framework, and joint research results with them.*

*-In Appendix 5-1-1, list the status of collaboration with the satellite.*

### **Satellite Personnel Make-up**

- Administration:
  - Prof. Petros Sofronis (Director, PI, Hydrogen Materials Compatibility Division)



- Prof. Kenneth Christensen (Associate Director, PI, CO<sub>2</sub> Storage Division)
- Mr. William Dick (Executive Advisor to the Director on University of Illinois Project Regulations)
- Faculty:
  - Prof. Andrew Gewirth (IPRC Chair, PI, Fuel Cells Division)
  - Profs. Angus Rockett, Elif Ertekin, Lane Martin, and *Xiuling Li* (Satellite Faculty, Hydrogen Production Division)
  - Prof. David Cahill (Satellite Faculty, Thermal Science and Engineering Division)
  - Prof. Thomas Rauchfuss (Satellite Faculty, Catalytic Materials Transformations Division)
  - Prof. Paul Kenis (Satellite Faculty, CO<sub>2</sub> Capture and Utilization Division)
  - Prof. Dimitrios Kyritsis (Satellite Faculty, CO<sub>2</sub> Storage Division, appointment ended as of July 16, 2013)
  - Prof. Arne Pearlstein (Satellite Faculty, CO<sub>2</sub> Storage Division, appointment ending as of August 16, 2014)
  - *Prof. Albert Valocchi* (Satellite Faculty, CO<sub>2</sub> Storage Division)
  - Prof. James Stubbins (Satellite Faculty, Energy Analysis Division)
- EAC Members:
  - Prof. Robert Finley (CO<sub>2</sub> Storage Division)
- Administrative Support:
  - Ms. Jessica Dalhaus (Project Coordinator, Assistant to the Director)
  - Ms. Yvonne Shaw (Grants & Contracts Coordinator)

*Individuals listed in italics are funded directly by the University of Illinois College of Engineering in order to support and strengthen I<sup>2</sup>CNER's computational capabilities in the areas of modeling and simulation of CO<sub>2</sub> storage, and devices for photoelectrochemical production of hydrogen.*

### **Collaborative Framework**

The Illinois Satellite faculty members are all internationally recognized researchers in their respective areas of expertise. They were specifically invited to complement the I<sup>2</sup>CNER research activities at Kyushu. Professors Andrew Gewirth and Kenneth Christensen currently serve as I<sup>2</sup>CNER PIs.

### **Satellite Office**

The I<sup>2</sup>CNER Satellite has been allocated a spacious office suite housed within the UIUC Department of Mechanical Science and Engineering. Office space is available for Japanese researchers during their visits to the Illinois campus.

### **Consistent Contact with KU Faculty**

The Illinois Satellite held an international workshop on “Catalytic Concepts for Fuel Cells” in September 2013 which involved speakers from both KU and Illinois. Through such I<sup>2</sup>CNER events and mutual visits of faculty and students between the two universities, researchers from both universities have opportunities to directly exchange and discuss research ideas for interaction and collaboration, in addition to their regular communications via email and teleconferencing.

### **Visiting Students**

In order to facilitate active exchange of students between Kyushu University and the University of Illinois (I<sup>2</sup>CNER Satellite Institute), and other collaborating institutions overseas, the Institute accepts short-term students from overseas as “Visiting Students” at Kyushu University. As of March 31, 2014, the Institute has hosted a total of 14 graduate students from Illinois (5 in FY 2011, 5 in FY 2012, and 4 in FY 2013). 1 Illinois student is already planning to visit KU in the summer of 2014.

### **I<sup>2</sup>CNER Undergraduate Exchange Pilot Program**

From February 25-March 26, 2014, 5 Kyushu University undergraduate students from the Faculty of Engineering traveled to the University of Illinois at Urbana-Champaign as part of the I<sup>2</sup>CNER Undergraduate Exchange pilot program. The students observed and assisted with research in UIUC laboratories under the supervision of Satellite Faculty and graduate students, participated in group meetings, completed weekly “check-ins” with the Director/Associate Director of the Satellite, took tours of 3 local engineering companies, and interacted heavily with the Center for East Asian and Pacific Studies (CEAPS) to enhance their cultural experience of the university. In order to continue offering

engineering students cross-cultural experiences, an MOU for undergraduate exchange between the University of Illinois and Kyushu University is currently being negotiated.

### **GRIPT Project & Collaborative Library Efforts**

The Grainger Engineering Library Information Center at the University of Illinois (Profs. William H. Mischo and Mary C. Schlembach) has been working closely with the Kyushu University Library (Mr. Kenshi Hyodo, Senior Librarian) to develop a set of scholarly information services that provide enhanced access to a myriad of online information resources available to I<sup>2</sup>CNER researchers. In particular, work has focused on the development of a custom Group Information Productivity Tool (GRIPT) that offers access to I<sup>2</sup>CNER researcher publications by group and author, key subject journals, specific known item journal articles, pre-stored customizable topical search results, highly cited articles and papers, and articles citing a specific article. This tool is customized for on-campus and remote access by both Illinois and Kyushu researchers. This project involves visits by the Illinois Librarians to Kyushu University. (URLs: <http://hades.grainger.uiuc.edu/guy/pip7j.asp?i2cner> and [http://hades.grainger.uiuc.edu/sarina/i2cner\\_scopus/i2cner\\_search.asp](http://hades.grainger.uiuc.edu/sarina/i2cner_scopus/i2cner_search.asp))

### **Special Seminar Presentation on Life at the Illinois Satellite**

In order to encourage KU researchers to make the trip to Illinois, Prof. Masamichi Kohno, one of the first KU researchers to travel to the Satellite for an extended stay, gave a special seminar presentation about what it is like to live on the Illinois campus. In his presentation, Prof. Kohno explained many details, including the local bus service, the guest housing facility, the train system, easy access to Chicago, history of the University of Illinois, various available laboratory facilities, a typical agenda for a day at Illinois, and on- and off-campus attractions.

### **Joint Research**

#### *Hydrogen Production*

- In a collaborative activity Prof. Rockett (Illinois), Dr. Druce, Prof. Kilner and Prof. Ishihara (Steam Electrolysis group, Hydrogen Production Division), and Dr. Helena Tellez (Imperial College, London, UK) have been investigating the effects of several sample preparation methods for different Cu(In,Ga)Se<sub>2</sub> (CIGS) single crystal epitaxial films by low-energy ion scattering (LEIS) analysis of the outermost surface. Devices produced from these materials can serve as the key energy source for driving hydrogen production as well as having potential as components of hybrid photoelectrochemical cell electrodes. Because LEIS is sensitive to the very outer atomic layer of a sample, it is critical that appropriate cleaning in-situ be performed for the preparation of the sample. Typically, this can be accomplished by exposure to atomic oxygen, hydrogen or low energy sputtering. The first joint publication addresses the effects of each of these treatments on the surface composition of Cu(In,Ga)Se<sub>2</sub> (CIGS) photovoltaics and identifies the optimal preparation method for future studies of the composition of these surfaces which make the heterojunction which controls performance of semiconductor photovoltaic devices.
  - Tellez, H., Druce, J., Liao, D., Hall, A., Ishihara, T., Kilner, J., and Rockett, A., Low Energy Ion Scattering: Surface Preparation and Analysis of Cu(In,Ga)Se<sub>2</sub> for Photovoltaic Applications, submitted, *Progress in Photovoltaics*.
- In an ongoing collaboration between Prof. Rockett (Illinois) and PI Takahara, and Dr. Y. Higaki (Kyushu) are studying chemical reactions and phase equilibria in Cu<sub>2</sub>ZnSnSe<sub>4</sub>, a compound of great interest as an alternative to CuInGaSe<sub>2</sub> made from earth-abundant elements using temperature programmed synchrotron x-ray diffraction analysis. Samples were sent from Illinois to Kyushu and analysis was conducted recently. Data analysis is in progress and joint publications are expected based on the results of this and future experiments.
- Collaboration between the groups of PI Gewirth (Illinois) and Ishihara (Kyushu) addressed the photoelectrochemical activity of oxysulfide material Bi<sub>2</sub>O<sub>2</sub>S as a photocatalyst. The material was synthesized by the Kyushu Group and the activity was measured by the Illinois group. The work resulted in a joint publication:
  - Pacquette, A. L., Hagiwara, H., Ishihara, T. and Gewirth, A. (2014), Fabrication of an oxysulfide of bismuth Bi<sub>2</sub>O<sub>2</sub>S and its photocatalytic activity in a Bi<sub>2</sub>O<sub>2</sub>S/In<sub>2</sub>O<sub>3</sub> composite, *Journal of Photochemistry and Photobiology A: Chemistry* 277, 27-36.

- In an ongoing collaboration, Prof. Ertekin (Illinois) and Prof. Staykov (Kyushu) work on design of a hybrid organic/inorganic switching mechanism based on a heterojunction between a porphyrin molecule and the  $\text{KTaO}_3$  oxide. The system was synthesized by the Kyushu team, and subsequent characterization suggested that nearly 100% efficient charge carrier separation takes place across the interface. The joint computational electronic structure analysis revealed the molecular switching mechanism that enables uni-directional electron transfer. This high computational demand of this work was provided by the Blue Waters high-performance computing framework, a petascale computational facility housed at the NCSA at Illinois. Several aspects of the computational predictions have been confirmed by surface studies carried out by Prof. Kilner and John Druce on the LEIS. This work is now being prepared for submission to an archival journal: Staykov, A., Jain, C. A. and Ertekin, E., "A hybrid molecular switch for ultra-efficient photocatalytic charge separation."

#### Hydrogen Storage

- The group of Kyushu PI Horita initiated collaboration with Prof. Ian Robertson in Wisconsin-Madison and PI Sofronis. The topic of this collaboration is to investigate the effect of high Pressure Torsion (HPT) (i.e., heavy deformation) on microstructural evolution of hydrogen-charged pure Ni and 304 stainless steel. An Illinois graduate student, Megan Emigh, stayed in Kyushu from June to August 2013 to carry out the collaborating study. Using facilities in Kyushu, she prepared samples for hydrogen charge and HPT processing and evaluated some basic microstructures. The sample analyses are now continued at Illinois for further evaluation of the microstructures and mechanical properties.
- The evolved microstructure and the influence of hydrogen will be determined for materials subjected to high pressure torsion. These tests offer the advantage that the strain and strain rate can be determined and there is no cracking of the samples, which avoids the complex stress state associated with a crack. Characterization efforts are in progress.

#### Fuel Cells

- A viable electrochemical process for the conversion of  $\text{CO}_2$  to CO requires electrodes that exhibit excellent electrochemical performance and are durable. The structure of the catalyst layer is key, as it determines catalytic activity, loading, and selectivity. In a joint research, the groups of Profs. P. Kenis and A. Gewirth (Illinois) in collaboration with PI Nakashima's group (Kyushu) achieved a high selectivity for CO over  $\text{H}_2$  (80-92%) upon the electrochemical reduction of  $\text{CO}_2$  to CO using Au nanoparticles supported on polymer-wrapped multiwall carbon nanotubes (MWNTs). By using this new class of catalyst developed in Nakashima group, it also exhibits high activity: a maximum partial current density for CO of  $160 \text{ mA/cm}^2$ , and an up to 8.8x higher current density for CO at intermediate cathode potentials ( $V = -1.39 \text{ V vs. Ag/AgCl}$ ) compared to the state-of-the-art silver nanoparticle-based catalysts normally used under identical experimental conditions. Furthermore, such good performance can be achieved with a very low catalyst loading of  $0.17 \text{ mg Au/cm}^2$ , suggesting that Au nanoparticles are highly dispersed on MWNTs, resulting in high electrochemically-active surface area ( $23 \text{ m}^2/\text{g Au}$ ). Reducing loadings of precious metal catalysts without sacrificing activity and selectivity offers promise for electrochemical  $\text{CO}_2$  reduction to become an economically viable process. The work has been submitted for joint publication:
  - Jhong, H.-R. M., Tornow, C. E., Kim, C., Anderson, P. S., Gewirth, A. A., Fujigaya, T., Nakashima, N. and Kenis, P. J. A., Gold Nanoparticles on Polymer-Wrapped Carbon Nanotubes: An Efficient and Selective Catalyst for  $\text{CO}_2$  Reduction. *Manuscript in preparation.*
- Current catalysts for electrochemical conversion of  $\text{CO}_2$  to CO are typically based on precious metals, which are costly, and of limited availability in lights of application at large scale. In this project the group of Prof. Kenis (Illinois) working with Prof. S. Lyth (Kyushu) explored nitrogen-doped carbon-based catalysts that do not contain precious metals, or any other metals, to hopefully identify a very active, durable, but also comparatively cheap catalyst. The collaboration started based on an idea of prof. S. Lyth (Kyushu) and Molly Jhong (Illinois graduate student) during Jhong's stay at Kyushu. The team synthesized and tested a carbonitride-based catalyst, which exhibited identical performance ( $90 \text{ mA/cm}^2$  current density,  $>90\%$  Faradaic efficiency for CO product) to the state of the art Ag nanoparticle catalyst. This accomplishment is significant because this catalyst eliminates the need for precious metal catalysts, immediately reducing a significant

cost factor of such a process if commercialized. The work resulted in a manuscript that is currently under review:

- Jhong, H.-R. M., Kenis, P. J. A. and Lyth, S. M., Nitrogen-Doped Carbon Catalyst for Electrochemical CO<sub>2</sub> Conversion to CO, *Journal of the American Chemical Society*, submitted

#### *Thermal Science and Engineering*

- Prof. D. Cahill (Illinois) is working with PI Takata to establish experimental capabilities at Kyushu University for pump-probe measurements of thermophysical properties. The collaboration includes development of in-situ measurements of thermophysical properties in both electrochemical and high pressure environments and high-throughput/high-precision measurements of GHz surface acoustic wave velocity and damping to characterize thin film elastic properties, and the near-surface region of materials that have been degraded by environmental effects and wear.
- In another joint effort, Prof. Cahill and PIs Takata and Horita (Kyushu) investigated the reduction in the thermal conductivity of a model semiconductor crystal by severe plastic deformation. Processing by high pressure torsion was performed at Kyushu and measurements were done at both Illinois and at Kyushu using the new experimental capabilities that have been established by the I<sup>2</sup>CNER collaboration. An extension to thermoelectric materials may provide a cost-effective method of creating nanostructured materials to improve the thermal efficiency of thermoelectric energy conversion. The work has been submitted for publication:
  - Harish, S., Tabara, M., Ikoma, Y., Horita, Z., Takata, Y., Cahill, D. G. and Kohno, M., Reduction in Thermal Conductivity of Crystalline Silicon Processed by High-Pressure Torsion, submitted for publication in *Nanoscale Research Letters*.

#### *Catalytic Materials Transformations*

- PI Yamauchi (Kyushu) utilizes a new synthetic technique to prepare nanoalloy catalysts involving ordered structures that have never been applied to CO<sub>2</sub> reduction before. Mr. Sichao Ma (Illinois graduate student in Prof. P. Kenis' group) (visited Yamauchi's group from Nov. 18 to Dec. 2 to synthesize ordered CuPd and AuCu nanoalloy catalysts, i.e., B2-type CuPd and L10-type AuCu nanoalloys supported on glassy carbon. He is currently carrying out catalytic tests of those synthesized samples at the University of Illinois.
- One of the goals of PI Yamauchi group is to promote energy cycles that do not release CO<sub>2</sub> to the atmosphere, so called "Carbon-Neutral Energy Cycle (CN cycle)". The oxidation part has been recently studied (e.g. Platinum-free direct ethylene glycol fuel cells). However, the reduction part has not been investigated sufficiently to date. Prof. Kenis' group (Illinois) has explored original electrochemical cells for CO<sub>2</sub> reduction. These electrochemical cells could possibly be applicable to the reduction of wastes from the CN cycles. Prof. Sadakiyo (Kyushu) is focusing on the electrochemical synthesis of ethanol/ethylene glycol from acetic acid/oxalic acid, which is the waste of the CN cycle. He synthesized various kinds of metal catalysts supported on carbon at Kyushu University and visited Kenis' group in Illinois University from Feb. 6 to Mar. 14 to learn how to evaluate catalysts for the acetic acid reduction reaction. Specifically, he learned about the structure of the cell and analysis techniques for the reaction. He is currently examining his catalysts and further developing catalysts for fuel reproduction by taking advantages of Kenis' methods.
- One of the goals of PI Ogo's group is to decipher how hydrogenases work on a molecular level. The leading group in the area of hydrogenase modeling is Rauchfuss's at Illinois. A second area of overlap and cross fertilization is the design of molecular fuel cells, in which bio-inspired catalysts convert O<sub>2</sub> and H<sub>2</sub> to water. The guiding examples came from Rauchfuss's work on the reactions of O<sub>2</sub> with [Cp\*<sub>2</sub>Ru(NiS<sub>2</sub>N<sub>2</sub>)]<sup>+</sup> and Cp\*<sub>2</sub>Ir(H)(TsHDPEN-). The I<sup>2</sup>CNER interchange was critical in Ogo's implementation of these or similar components into molecular catalysts. So successful has been this work that Rauchfuss has recruited a Japanese-speaking graduate student Michaela Carlson. She is just beginning her PhD research by first spending a few weeks in Ogo's Labs. She brings new cutting edge methodology related to photo-activation of the hydrogenase-inspired catalysts.

#### *Hydrogen Materials Compatibility*

- The division's significant accomplishment described in section 2-1, *Elucidating the variables affecting accelerated fatigue crack growth of steels in hydrogen gas with low oxygen concentrations*,

represents joint research between involving Prof. Alex Staykov (Kyushu) and Prof. Petros Sofronis (Kyushu, Illinois). The collaboration team developed a physics-based analytical model that quantified the interplay between several environmental and mechanical variables affecting oxygen-modified, hydrogen-accelerated crack growth. In addition, the team defined the basic mechanisms for trace oxygen inhibition of hydrogen uptake into steels using density functional theory (DFT) modeling. The effort resulted in the following publications

- Staykov, A., Yamabe, J. and Somerday, B. P. (2014), Effect of Hydrogen Gas Impurities on the Hydrogen Dissociation on Iron Surface, *International Journal of Quantum Chemistry*, 114 (10), 626-635
- Somerday, B. P., Sofronis, P., Nibur, K.A., San Marchi, C., and Kirchheim, R. (2013), Elucidating the Variables Affecting Accelerated Fatigue Crack Growth of Steels in Hydrogen Gas with Low Oxygen Concentrations, *Acta Materialia*, 61 (16), 6153-6170.
- In a collaborative activity, PIs Sofronis and Robertson hosted WPI Visiting Scholar Dr. Akihide Nagao (JFE Steel, Japan). This collaboration focused on applying a recently developed technique that combines focused-ion beam machining and transmission electron microscopy to discover and analyze the microstructure immediately beneath the fracture surface at site-specific locations. Using this new microscopy approach, it was shown that hydrogen-induced intergranular fracture at prior austenite grain boundaries and “quasi-cleavage” fracture at lath boundaries in martensitic steel are driven by a hydrogen-enhanced and plasticity-mediated decohesion mechanism. This collaboration resulted in the following publications:
  - 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.
  - Nagao, A., Smith, C. D., Dadfarnia, M., Sofronis, P. and Robertson, I. M., Interpretation of hydrogen-induced fracture surface morphologies for lath martensitic steel, *Procedia Materials Science*, accepted for publication
  - Nagao, A., Smith, C. D., Sofronis, P. and Robertson, I.M. (2012), The role of hydrogen in hydrogen-induced “quasi-cleavage” fracture of lath martensitic steel, *CAMP-ISIJ*, 25, 441.
  - Nagao, A., Smith, C. D., Dadfarnia, M., Sofronis, P. and Robertson, I. M. (2013), The role of hydrogen in hydrogen-induced intergranular fracture of lath martensitic steel, *CAMP-ISIJ*, 26, 331.
- The collaboration between PIs Sofronis and Robertson and WPI Visiting Scholar Dr. Akihide Nagao (JFE Steel, Japan) also focused on the effect of nano-sized (Ti,Mo)C precipitates in hydrogen embrittlement of tempered lath martensitic steel. Four-point bend tests and hydrogen thermal desorption analysis of baseline steel without addition of Ti and Ti-added steel showed that nano-sized (Ti,Mo)C precipitates trap hydrogen and prevent intergranular fracture, improving the resistance of lath martensitic steel to hydrogen embrittlement. With increasing hydrogen concentration, the benefit of hydrogen trapping at (Ti,Mo)C precipitates decreases as they become saturated with hydrogen. This collaboration resulted in the following publications:
  - Nagao, A., Martin, M. L., Dadfarnia, M., Sofronis, P. and Robertson, I. M., The effect of nano-sized (Ti,Mo)C precipitates on hydrogen embrittlement of tempered lath martensitic steel, *Acta Materialia*, in print.
  - Nagao, A., Eftink, B. P., Dadfarnia, M., Somerday, B. P. and Sofronis, P. (2012), The effect of nano-sized TiC precipitates on hydrogen embrittlement of tempered lath martensitic steel, *International Hydrogen Conference Proceedings*, 127-135
  - Nagao, A., Eftink, B. P., Dadfarnia, M., Somerday, B. P. and Sofronis, P. (2014), The effect of nano-sized (Ti,Mo)C precipitates on hydrogen embrittlement of tempered lath martensitic steel, *CAMP-ISIJ*, 27, 427

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

- Using an automated setup for deposition of catalyst inks on the micro-porous layer of a gas diffusion electrode, Prof. Kenis's group were able to create very thin, crack free, uniform catalyst layers, for example comprised of Ag nanoparticles. This is significant because these electrodes performed significantly better in CO<sub>2</sub> conversion (>50% improvement in current density) than electrodes prepared by hand painting, while at the same time the catalyst loading was reduced 10-fold. This effort, which was featured prominently on the cover of *Advanced Energy Materials*, was a result of progressive achievements building on FY 2011 work toward improved electrodes. As

a follow up effort, Kenis is now working closely with Fujikawa to further improve these gas diffusion electrodes. Fujikawa uses his expertise for the development of membranes with desired physical properties (permeability to CO<sub>2</sub> and CO; wettability to maintain gas-liquid separation; durability; ...) that can be used as the microporous layer and catalyst support layer, to replace the thick Teflon-like layers present in the commercially available gas diffusion electrodes that we use right now.

- Jhong, H.-R. M., Brushett, F. R. and Kenis, P. J. A. (2013), The effects of catalyst layer deposition methodology on electrode performance, *Advanced Energy Materials*, 3 (5), 589-599.
- One of the challenges of electrochemical CO<sub>2</sub> conversion is the need for precious metal catalysts to achieve reasonable rates of conversion. In this work, Prof. Kenis's group sought to use TiO<sub>2</sub> as a support for Ag nanoparticles, to thereby hopefully achieve the same or better performance than with plain silver nanoparticles. In their electrochemical flow reactor (electrolyzer) the group were able to achieve identical performance with the Ag/TiO<sub>2</sub> catalyst as with the plain Ag nanoparticle catalyst; in other words, identical performance with much less precious Ag catalyst mass. Furthermore, the group found strong indications that the support material stabilizes one or more of the intermediates in the reduction of CO<sub>2</sub>. In preceding work, Prof. Kenis already had achieved similar results, using Ag-based organometallic catalysts, also achieving a much higher activity per unit mass of Ag. In ongoing work of Kenis with Lyth and with Nakashima, the catalyst performance is further improved by using catalyst based upon: (i) immobilized gold nanoparticles on polymer wrapped nanotubes (with Nakashima, manuscript in preparation), and (ii) nitrogen-doped carbon materials that are more active than Ag catalyst, cheaper (no precious metal!), and presumably more durable (with Lyth, manuscript submitted for publication).
  - Ma, S., Lan, Y., Perez, G. M. J., Moniri, S. and Kenis, P. J. A. (2014), Silver supported on titania as an active catalyst for electrochemical carbon dioxide reduction, *ChemSusChem*, 7 (3), 866-874.
  - Tornow, C. E., Thorson, M. R., Ma, S., Gewirth, A. A. and Kenis, P. J. A. (2012), Nitrogen-based catalysts for the electrochemical reduction of CO<sub>2</sub> to CO, *Journal of the American Chemical Society*, 134 (48), 19520-19523.
  - Jhong, H.-R. M., Kenis, P. J. A. and Lyth, S. M., Nitrogen-Doped Carbon Catalyst for Electrochemical CO<sub>2</sub> Conversion to CO, submitted, *Journal of the American Chemical Society*.
- Prof. Kenis and collaborators were recently invited to contribute two reviews on the status of (electro-) catalysis for CO<sub>2</sub> conversion.
  - Jhong, H.-R. M., Ma, S. and Kenis, P. J. A. (2013), Electrochemical Conversion of CO<sub>2</sub> to Useful Chemicals: Current Status, Remaining Challenges, and Future Opportunities (Review), *Current Opinion in Chemical Engineering*, 2 (2), 191-199.
  - Appel, A. M., Bercaw, J. E., Bocarsly, A. B., Dobbek, H., Dubois, D. L., Dupuis, M., Ferry, J. G., Fujita, E., Hille, R., Kenis, P. J. A., Kerfeld, C. A., Morris, R. H., Peden, C. H. F., Portis, A. R., Ragsdale, S. W., Rauchfuss, T. B., Reek, J. N. H., Seefeldt, L. C., Thauer, R. K. and Waldrop, G.L., (2013) Frontiers, Opportunities, and Challenges in Biochemical and Chemical Catalysis of CO<sub>2</sub> Fixation (Review), *Chemical Reviews*, 113 (8), 6621-6658.

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

- The Illinois group of PI Christensen (Prof. A. Valocchi, Dr. G. Blois, Mr. F. Kazemifar) collaborates with the Kyushu group of PI Tsuji (Prof. K. Kitamura, Dr. F. Jiang) on geophysical experiments and hydrological analysis for CO<sub>2</sub> and water flow mechanisms in porous sandstone. The team developed methods for monitoring the complex fluid flow around small scale heterogeneity by geophysical parameters. The team also simulated two-phase fluid flow around the small-scale heterogeneity by using the LBM method. These results indicate the strong effect of small-scale heterogeneity on multi-phase fluid flow mechanism. This study is related to the research project (1-1) "Reservoir characterization and CO<sub>2</sub> dynamic modeling."
- PI Christensen's research effort is focused on the quantification of flow processes associated with drainage and imbibition of CO<sub>2</sub> in complex porous micromodels under reservoir conditions. A unique experimental protocol was recently developed to allow quantification of flow processes associated with interactions between two immiscible fluids in porous micromodels relevant to drainage and imbibition interactions between resident brine and injected CO<sub>2</sub> in porous geological formations during sequestration. A manuscript describing this experimental protocol is under consideration for publication in *Microfluidics and Nanofluidics*. In parallel, Prof. Christensen has developed a

high-pressure test facility that allows for obtaining quantitative velocity data in multi-phase flow of supercritical/liquid CO<sub>2</sub> and water in two-dimensional porous micromodels at reservoir thermodynamic conditions (pressure and temperature). The geometry of the porous micromodels is presently periodic arrays of circular and/or elliptic posts but they have now begun fabrication of micromodels reflecting the heterogeneity of actual geologic formations. The micromodels are fabricated by dry-etching silicon and anodic bonding to glass. A pressure-cell enables sustainment of liquid/supercritical CO<sub>2</sub> and water at pressures up to approximately 100 bar. The aforementioned experimental protocol is presently being utilized in these high-pressure experiments to study the flow dynamics of liquid/supercritical CO<sub>2</sub> drainage and imbibition, particularly dynamic events that lead to “bursts” of fluid displacement at such high velocities that the presumed dominance of capillary and viscous effects in the pore spaces may give way to significant inertial effects. The latter are completely ignored in the most sophisticated models of residual trapping of CO<sub>2</sub>, meaning that the true displacement dynamics of drainage and imbibition are not faithfully represented in reservoir-scale simulations of CO<sub>2</sub> fate. This work is related to Research project (1-1) “Reservoir characterization and CO<sub>2</sub> dynamic modeling.”

#### *Energy Analysis*

- Prof. P. Kenis (Illinois), in a collaboration with Profs. Stubbins (Illinois) and Itaoka (Kyushu), and Paster (Kyushu), have executed a full scale economic analysis whether the current performance achieved in electrochemical conversion of CO<sub>2</sub> to CO can be economically viable in the production of liquid fuels through the Fischer-Tropsch process, or, if not, this effort will indicate by how much we need to improve the electrochemical conversion process for the overall process to become economically feasible.

#### 5-1-2. Results of International Joint Research (other than with the University of Illinois)

- 1) **Imperial College, London, UK (J. A. Kilner, T. Ishihara)**: Discovery that Na<sub>0.5</sub>Bi<sub>0.5</sub>TiO<sub>3</sub> (NBT) based materials can be a completely new family of oxide ion conductors with potential applications to intermediate-temperature SOFCs used in steam electrolysis. It also opens up a new direction to design oxide ion conductors in perovskite oxides; Surface analysis of energy materials through low-energy ion scattering (LEIS). I<sup>2</sup>CNER hosts one of the eight commercial LEIS instruments that are currently operating worldwide fitted with the new toroidal energy analysers and high-brightness plasma sources.
- 2) **University of Perth (J. Jiang, T. Ishihara)**: Fundamental understanding of the effect of impurities such as boron on the degradation of advanced SOFC cathodes.
- 3) **Seoul National University (S. Y. Park, K. Sakai)**: Fundamental studies to understand the mechanism underlying the water splitting active site of a single molecular catalyst from an artificial photosynthesis perspective.
- 4) **Texas A&M University (H.-J. Sue, A. Takahara)**: Composite functionalization of polymers for the development of novel carbon nano-tube/polypropylene composite materials with improved durability and long-term lubrication properties.
- 5) **Stony Brook University (T. Koga, A. Takahara)**: The plasticization effect of compressed CO<sub>2</sub> gas on semi-crystalline fluorinated polymer brushes (lubrication films for friction reduction) was demonstrated even at low temperature and pressure conditions. The supercritical CO<sub>2</sub> based processing could be used as an alternative, low temperature and environmentally green means for the improvement of the interior crystalline structures of these brushes and the associated macroscopic surface wettability and properties.
- 6) **ECOSTORE project by EU (E. Akiba)**: Educational program for young European scientists. Agreement between I<sup>2</sup>CNER through Kyushu University and ECOSTORE.
- 7) **Dalian Institute of Chemical Physics (DICP), Chinese Academy of Sciences (P. Chen, E. Akiba)**: Amides and borohydrides with high hydrogen storage capacity were explored as a promising new class of hydrogen storage materials. Insights on material design and kinetics improvement for practical applications were presented.
- 8) **Peking University (X. Li, H. Shao)**: It was found that nanostructure and nanocatalysts could

dramatically enhance kinetics. But desorption thermodynamics (desorption enthalpy and entropy) does not change with size and catalysts in the range of 5 to 300 nm.

- 9) **MIT (H. Tuller, S. Bishop, N. Perry)**: Understanding of the origin of chemical expansion in SOFCs and developing new materials with reduced chemical expansion. This is a multi-university and interdisciplinary approach that led to the discovery of the origins of the chemical expansion; it derives from the larger size of the reduced cation after an oxide ion is removed from the lattice. In addition, the group demonstrated that charge localization on reduced cations plays a significant role in enhancing chemical expansion.
- 10) **MIT (H. Tuller, N. Perry, S. Bishop, K. Sasaki, J. Kilner)**: Interdisciplinary probing of the relationship between electrochemical properties and surface chemistry of SOFC electrodes. Sluggish reaction rates at the electrodes of SOFCs are known to be one of the key barriers to improving the efficiency of SOFCs. Achievements include identification of additional phases (e.g. La oxide) that dramatically enhance the oxygen exchange rate as compared to the “aged” CeO<sub>2</sub> based film without the added phase, as well as finding that addition of La to (La,Sr)(Ti,Fe)O<sub>3</sub> solid solutions modifies the segregation rate of Sr to the surface with consequent changes in the electrochemical performance degradation. In related work at MIT, Yildiz and Tuller demonstrated, by in situ scanning tunnelling microscopy/spectroscopy (STM/STS), the important and detrimental impact of Sr segregation in SrTi<sub>1-x</sub>Fe<sub>x</sub>O<sub>3</sub> (STF), a model perovskite system, on the surface electronic structure at high temperature. The results demonstrate that Sr segregation in STF can deteriorate oxygen reduction kinetics through two mechanisms – inhibition of electron transfer from STF to oxygen species adsorbing onto the surface and the smaller concentration of oxygen vacancies available on the surface for incorporating oxygen into the lattice.
- 11) **MIT (B. Yildiz, D. Marrochelli), Technical University of Denmark (C. M. Mogensen, C. Chatzichristodoulou), University of Maryland, (E. Wachsman)**: Contributions to the research reported in #9 above.
- 12) **Tsinghua University (X. Zhang, Y. Takata)**: Measurement of the optical absorptance of an individual multi-walled carbon nanotube (CNT) which are devices to be used in energy systems. Knowledge of optical absorptance coupled with thermal conductivity measurements helps to further understand thermal transport at the nanoscale. Optical absorptance is an important property but has rarely been accurately measured for nanomaterials. The study was carried out by laser beam irradiation along with measurement of the temperature rise.
- 13) **Griffith University (P. L. Woodfield, Y. Takata)**: Measurements of thermal conductivity of helium and hydrogen using a transient short-hot-wire method; correlation equations for high temperature and high pressure.
- 14) **University of Edinburgh (K. Sefiane, Y. Takata) and University of Maryland (J. Kim)**: Experimental measurements by infrared thermography, reported for the first time, of temperature and heat flux at a liquid/wall interface during evaporation.
- 15) **University of Göttingen and Sandia National Laboratories (R. Kirchheim, B. P. Somerday, P. Sofronis)**: The team developed a physics-based analytical model that quantified the interplay between several environmental and mechanical variables affecting oxygen-modified, hydrogen-accelerated crack growth. In addition, the team defined the basic mechanisms for trace oxygen inhibition of hydrogen uptake into steels using density functional theory (DFT) modeling.
- 16) **JFE Steel (A. Nagao), University of Wisconsin-Madison (I. M. Robertson), Sandia National Laboratories (B. P. Somerday)**: Improving the resistance of lath martensitic steel to hydrogen embrittlement by (Ti, Mo)C precipitates.
- 17) **Bandung Institute of Technology (W. Kadir, T. Tsuji)**: The team carried out reservoir simulations to model and identify suitable CO<sub>2</sub> injection sites in the Gundih area of Java Island. The simulations were conducted by using laboratory measurements of hydrological properties and subsurface structure properties extracted from seismic data (geometry of the Ngrayong formation).
- 18) **University of Bergen (T. A. Johansen, T. Tsuji)**: The team developed an accurate methodology to measure CO<sub>2</sub> saturation and pore fluid pressure separately for reservoir characterization by using information for the S-wave velocity distribution.



- 19) **QICS Project, Plymouth Marine Laboratory (J. Blackford, K. Shitashima)**: It is for the first time that a sub-seabed CO<sub>2</sub> release experiment in the world was carried out in 2012. This project funded by the Natural Environment Research Council of the UK is ongoing. It was demonstrated that the biological impact and footprint of this small leak analogue (<1 ton CO<sub>2</sub> d-1) is confined to a few decades of meters. Migration of CO<sub>2</sub> to the seafloor is constrained by sediment structure and by the dissolution and re-precipitation of calcium carbonate naturally present in the sediments.

#### 5-1-3. State of Top World-level Researchers residing at the Center

*Describe the participation of overseas Principle Investigators, the short-term stays of joint researchers, and the state of participation in symposiums sponsored by the Center.*

*-In Appendix 5-1-3, enter the number of researchers from abroad within the total number of the Center's researchers, and their annual transition*

#### **Participation of Overseas PIs and Researchers**

All 8 of our overseas Principal Investigators actively participate in I<sup>2</sup>CNER. They all visit I<sup>2</sup>CNER at least once a year, spending between one and four weeks at Kyushu to participate in events and exchange opinions for collaborative research projects. Aside from PIs, we host WPI Professors, WPI Visiting Professors, and a WPI Associate Professor from overseas on a regular basis.

#### **WPI Faculty Fellows Program**

We have implemented the WPI Faculty Fellow Program. For full details, please refer to Section 2-2.

#### **Recruitment of Permanent-staying Foreign PIs**

The Institute's Faculty Recruiting Committee (FRC) has conducted an extensive recruiting campaign to hire permanent-staying foreign principal investigator(s), including 1) Advertising in international journals, 2) Accessing faculty candidate files from the Mechanical Science and Engineering Department of the University of Illinois, 3) Contacting the head-hunting agency UIUC uses, 4) Requesting that all divisions nominate potential candidates, and 5) Instituting a "Faculty Fellows Program," as mentioned above. The Institute has devoted maximum effort to recruit foreign PIs who would reside at I<sup>2</sup>CNER.

#### 5-1-4. Utilization and Employment Situation of Young Researchers

*Describe the utilization and employment situation of young researchers including postdoctoral researchers.*

*-In Appendix 5-1-4, enter the following:*

- The status of international recruitment for postdoctoral researchers, applications received, and selections made*
- The percentage of postdoctoral researchers from abroad*
- The state of postdoctoral researchers employment*

#### **Faculty Recruiting Committee (FRC) & Postdoc Hiring**

Upon the announcement of the award and before the launching of the Institute, I<sup>2</sup>CNER initiated an aggressive open international recruitment campaign, which it has continued in subsequent years. At the junior level, I<sup>2</sup>CNER seeks to hire researchers who demonstrate promise for future international recognition. The recruitment process is administered by the Faculty Recruiting Committee (FRC), which includes key members of the Institute and any other faculty who can provide input for cases of targeted hiring. In addition, each WPI Principal Investigator was allocated 1 postdoctoral research associate line in FY 2012 in order to increase the overall number of postdocs at the Institute. These postdocs are hired following the normal screening by the FRC. For additional specific details about postdoctoral researchers, please see Section 9 of this report.

#### **Tenure Committee**

The Director convenes a tenure committee on an ad-hoc basis when outstanding young researchers of the Institute are identified as deserving consideration for tenure. The tenure process follows exactly the same protocol as the promotion process, and again involves confidential evaluation by world-leading scientists. Through such an ad-hoc Tenure Committee, two of the Institute's junior Principal Investigators, who serve as the Division Lead PIs of their respective research divisions, will be appointed as tenured Associate Professors as of April 1, 2014.

#### **Faculty Excellence Program**

The Director instituted the "Faculty Excellence Program" soon after the launching of the Institute in order

to attract and recruit individuals who will contribute to transformation and positive change within their research division and across the Institute. Individuals recruited through this program have an outstanding record of accomplishment, and clearly enhance our capacity to achieve strategic objectives and promote interdisciplinary research activities. Through this program, we have hired two outstanding young researchers; one (female) Associate Professor as a PI in FY 2011 and a Full Professor in FY 2013.

### **Faculty Promotion**

The Institute follows a process for promoting faculty which breaks away from the Japanese tradition and instead applies the same standards as top US universities, as outlined in the governing document "18. Faculty Promotion." The first faculty promotion considerations following this process are underway for 3 of our young faculty and will be completed in FY 2014. The process involves a confidential assessment by world-leading scientists from the international community in the candidate's area of expertise. The process is also carried out by a promotions committee which is interdisciplinary and involves senior faculty from both Kyushu University and the University of Illinois.

### **Independence of Assistant and Associate Professors**

I<sup>2</sup>CNER's Assistant and Associate Professors are encouraged to develop their own research programs, independent of senior faculty, to serve the Institute's research objectives. While each assistant or associate professor is housed in a specific division and may interact with full professors, principal investigators, or the Division Lead Principal Investigator, he or she is wholly responsible for his or her own research program/group.

#### 5-1-5. Other

*Describe the Center's policy for sending Japanese researchers overseas to gain international experience, and give examples of how the Center is working to create career paths for its researchers within a global environment of researcher mobility.*

### **Collaborative Foreign Exchange Program**

In July 2013, I<sup>2</sup>CNER established a "Collaborative Foreign Exchange Program" in order to encourage young researchers, especially Japanese, to more actively visit our overseas collaborating institutions. The program requires that interested researchers submit a 2-page proposal to be reviewed by the SSC, and if approved, submit a 1-page summary report after the visit is complete. Researchers are also required to give a presentation in the Institute Interest Seminar Series (IISS) after the travel is complete. As of March 31, 2014, 7 young researchers (6 Japanese, 1 non-Japanese) had their proposals approved and 6 of them visited the Illinois Satellite through this program. So far, visits have ranged from 1 week to a few months long, but they are expected to be longer as the collaborative research advances. Beginning in April 2014, one of our female assistant professors will start her 6-month stay at Sandia National Laboratories.

### **Post-I<sup>2</sup>CNER Employment of Young Researchers**

To date, 3 I<sup>2</sup>CNER postdocs have leveraged their appointments at the Institute to advance their professional careers. I<sup>2</sup>CNER postdoctoral researcher, Dr. Yuki Naganawa, accepted a position as an Assistant Professor at Nagoya University beginning June 1, 2012. I<sup>2</sup>CNER postdoctoral researcher, Dr. Takeshi Matsumoto, accepted an Assistant Professor position at Chuo University beginning April 1, 2014. In addition, I<sup>2</sup>CNER EAD postdoctoral researcher, Dr. Seiichiro Kimura, left the Institute to become an associate at the Matsushita Institute of Government and Management. Beginning April 1, 2014, Dr. Kimura's appointment in the Institute changed to WPI Visiting Scholar.

### **Humboldt Research Fellowship Winner**

- I<sup>2</sup>CNER postdoctoral researcher, Dr. May Martin, who as a graduate student, repeatedly visited Kyushu University for extended periods of time in order to bridge the Satellite research activities with KU, won the prestigious Humboldt Research Fellowship from Germany.

#### 5-2. Creating the Center's Environment

##### 5-2-1. Holding International Research Meetings

*Describe the results obtained from holding the Center's main international research meetings.*

*-In Appendix 5-2-1, indicate the number of international research conferences or symposiums held and give up to major examples of the most representative ones for each fiscal year.*

### **I<sup>2</sup>CNER Kick-off Symposium**

The Kick-off Symposium for the International Institute for Carbon-Neutral Energy Research (I<sup>2</sup>CNER) of Kyushu University (KU) was held Tuesday, February 1, 2011, at Kyushu University's Inamori Frontier Research Center, Ito Campus. The symposium was attended by Mr. Takafumi Goda, Director-General of the Science & Technology Policy Bureau of MEXT; Mr. Tadashi Higashi, Secretary-General of the Fukuoka Strategy Conference for Hydrogen Energy; Dr. Anne Emig, Head, National Science Foundation (NSF) Tokyo Regional Office; and Dr. Toshio Kuroki, WPI Program Director, among others. The event provided an ideal opportunity for researchers from KU, the University of Illinois at Urbana-Champaign, and the Institute's other international partners to converge and begin exchanging ideas and engaging in debate about carbon-neutral energy issues.

### **I<sup>2</sup>CNER Annual Symposium and International Workshop 2012**

On January 31, 2012, I<sup>2</sup>CNER held its first Annual Symposium on Kyushu University's Ito Campus. KU President Setsuo Arikawa, MEXT Director Mitsuyuki Ueda; and WPI Program Director Dr. Toshio Kuroki were in attendance at the event. The symposium was attended by approximately 170 foreign and domestic researchers. The Annual Symposium was followed by the I<sup>2</sup>CNER International Workshop and Joint Research Symposium with the Research Center for Hydrogen Industrial Use and Storage (HYDROGENIUS) on February 2, 2012. At the International Workshop, I<sup>2</sup>CNER's researchers were able to participate in and move freely between nine concurrent sessions related to the Institute's research themes.

### **I<sup>2</sup>CNER Satellite Kick-off Symposium**

The I<sup>2</sup>CNER Satellite hosted its kick-off symposium at the University of Illinois at Urbana-Champaign March 6-7, 2012. The symposium was attended by WPI Program Director Toshio Kuroki, KU President Setsuo Arikawa, KU Vice President Yukio Fujiki, UIUC Provost Professor Richard Wheeler, and UIUC Dean of the College of Engineering Professor Ilesanmi Adesida. Day 1 of the symposium featured lectures by many prominent researchers, including Sam Baldwin, Chief Science Officer, Office of Energy Efficiency & Renewable Energy, U.S. Department of Energy; George Crabtree, Argonne National Laboratory; Michael Wang, Center for Transportation Research, Argonne National Laboratory; David Greene, Energy & Transportation Science Division, Oak Ridge National Laboratory; Walter Short, Former Manager of the Energy Forecasting & Modeling Group, US National Renewable Energy Laboratory; Robert Carling, Director, Transportation Energy Center, Sandia National Laboratories; Katsuhiko Hirose, Project General Manager, Strategic Planning & Administration Department of the Fuel Cell System Engineering Division of Toyota Motor Corporation; and K. Scott Weil, Fuel Cell Technologies Program, US Department of Energy. Day 1 concluded with a panel discussion which was moderated by Mark Paster, Former Technology Development Manager, US Department of Energy. Day 2 of the symposium featured lectures by I<sup>2</sup>CNER's KU and Satellite researchers, toward the goal of familiarizing the researchers of the Institute with one another's work and encouraging discussion on future research directions. A total of 30 researchers from Kyushu University travelled to Illinois to participate in this event.

### **I<sup>2</sup>CNER in Tokyo Symposium**

Please refer to Section 3-2 of this report for details.

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

On January 29, 2013, I<sup>2</sup>CNER hosted its New Building Completion Ceremony & Annual Symposium 2013. The event was attended by over 200 people, including Dr. Hiroo Imura, Chairperson of the 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. Monterey Gardiner, Technology Development Manager, Office of Hydrogen, Fuel Cells and Infrastructure Technologies, US Department of Energy; Professor Setsuo Arikawa, President of Kyushu University; Dr. Toshio Kuroki, WPI Program Director; and Prof. Peter Schiffer, Vice Chancellor for Research at the University of Illinois at Urbana-Champaign. Keynote lectures at the Annual Symposium were given by Dr. Eiichi Harada, Associate Office and Deputy General Manager of the Corporate Technology Planning Center of Kawasaki Heavy Industries, and Dr. George Crabtree, Director of the Joint Center for Energy Storage Research (JCESR), Argonne National Laboratory, and winner of the US Department of Energy (DOE) Energy Innovation Hub.

### **I<sup>2</sup>CNER Catalytic Concepts for Energy Symposium**

The I<sup>2</sup>CNER Satellite hosted the “Catalytic Concepts for Energy Symposium” at the University of Illinois at Urbana-Champaign on September 13, 2013. The symposium featured a diverse group of both national and international researchers specializing in catalysis issues. Invited speakers included Dr. Vojislav Stamenkovic, Argonne National Laboratory; Prof. Naotoshi Nakashima, Kyushu University; Prof. Aleksandar Staykov, Kyushu University; Prof. Tom Jaramillo, Stanford University; Dr. Etsuko Fujita, Brookhaven National Laboratory; Prof. Dan Scherson, Case Western Reserve University; Prof. Sharon Hammes-Schiffer, UIUC; and Prof. Takahiro Matsumoto, Kyushu University. The keynote lecture was delivered by Prof. Fraser Armstrong, University of Oxford. Also in attendance was the UIUC Dean of the College of Engineering, Prof. Andreas Cangelaris. The topics covered included proton, oxygen, nitrate, and carbon dioxide reduction; non-platinum metal electrodes for catalysis; alloys and composite materials for catalysis; mass spectrometry; and electrochemical methods. Not only did the Catalytic Concepts for Energy Symposium introduce I<sup>2</sup>CNER as a stakeholder in the field of catalysis to some of the experts in the field and vice versa, it also allowed all participants a unique opportunity to interface and explore possible new research directions. In particular, the I<sup>2</sup>CNER hosts have reported that they used this event like a think tank to brainstorm about I<sup>2</sup>CNER’s present and future research efforts on catalysis.

#### **I<sup>2</sup>CNER & ACT-C Joint Symposium 2014**

On January 30, 2014, the International Institute for Carbon-Neutral Energy Research (I<sup>2</sup>CNER) co-organized the “I<sup>2</sup>CNER & ACT-C Joint Symposium 2014” with the Advanced Catalytic Transformation program for Carbon utilization (ACT-C) of the Japan Science and Technology Agency (JST). The symposium was held in I<sup>2</sup>CNER Hall on the Ito Campus of Kyushu University and was attended by 177 people, including many international guests. Opening remarks were given by the Executive Vice President of Kyushu University, Prof. Yukio Fujiki. The plenary lectures were given by Prof. Ei-ichi Negishi of Purdue University, 2010 Nobel Prize Laureate in Chemistry, and Prof. Benny D. Freeman of the University of Texas at Austin. In the afternoon session, various researchers of I<sup>2</sup>CNER and ACT-C gave presentations on their latest research findings. The symposium concluded with a poster session in which participants actively exchanged ideas concerning their research activities.

#### **1<sup>st</sup> International Symposium on Chemical Energy Conversion Processes (ISCECP-1)**

I<sup>2</sup>CNER Professor Ken Sakai organized the first ever International Symposium on Chemical Energy Conversion Processes (ISCECP-1) June 12-13, 2013. The scope of the symposium included most topical issues correlated with energy conversion processes, such as solar energy conversion by adopting water splitting or carbon dioxide reduction, or energy consumption processes such as fuel cell related chemical conversion processes catalyzed by various molecular as well as heterogeneous systems, etc. The goal of the event was to establish a forum in which to exchange ideas, experiences, and research results on chemical energy conversion issues.

#### **Innovative Materials for Processes in Energy Systems (IMPRES) 2013**

I<sup>2</sup>CNER Associate Director and Thermal Science & Engineering Division Lead PI, Prof. Yasuyuki Takata, Associate Professor Masamichi Kohno, and Professors Bidyut Baran Saha and Michihisa Koyama organized the 3<sup>rd</sup> International Symposium on Innovative Materials for Processes in Energy Systems (IMPRES2013) September 4-6 2013. Topics covered in IMPRES included theories, experiments, and simulations on the development of functional materials for fuel cells, heat pumps, heat storage, sorption systems, and their applied aspects.

### 5-2-2. Support System for Overseas Researchers

#### **Administrative Support for the Transition into Japanese Society for Foreign Researchers**

The Administrative Office is in close communication with the existing International Student and Researchers Support Center of Kyushu University, and offers full-time support to international researchers in the area of invitation procedures, including visa application processing and accommodations on campus. In cooperation with the International Affairs Division at Kyushu University, English versions of various applications and other forms have been introduced. Additional training and workshop opportunities are offered to assist in the transition for international researchers while they are conducting research at I<sup>2</sup>CNER. Additionally, the I<sup>2</sup>CNER Administrative Office provides extensive living support and assistance with medical checkups, private accommodations, family support, travel arrangements, and introduction to the Japanese social insurance system, including medical, just to name a few.

### **Living Arrangements for Foreign Researchers**

Currently, we have introduced university facilities to accommodate for invited national and international researchers, or have made arrangements for fully-furnished private apartments with easy-access to Kyushu University.

### **Ito Guest House**

"Ito Guest House," an on-campus housing accommodation for short-stay researchers from overseas, was newly built and opened on April 6, 2012 on Ito campus, where I<sup>2</sup>CNER is located.

### **English Bus Schedules & Cafeteria Menus**

International initiatives such as a bilingual display (Japanese and English) of bus time tables at campus bus stops and destination signs of buses running between the nearest train station and campus, in addition to cafeteria menus, are in place for the convenience of foreign researchers.

### **Campus Loop & Campus Shuttle Bus Stops**

A new bus stop on the Ito Campus Loop bus has been established in front of the I<sup>2</sup>CNER building as of February 1, 2013. A bus stop on the Campus Shuttle bus has been established in front of the new "Shiiki Hall," which is adjacent to the I<sup>2</sup>CNER building, as of April 1, 2014.

### **Fuse News**

In order to facilitate a comfortable exchange environment, the I<sup>2</sup>CNER Administrative Office and the Satellite Support Staff cooperatively publish "Fuse News." "Fuse News" is an internal publication of I<sup>2</sup>CNER which is intended to help the researchers become familiar with one another's research programs, as well as the cultures and campuses at Kyushu University and UIUC. Since "Fuse News" was started, a total of 7 volumes have been published (3 in FY 2011, 2 in FY 2012, and 2 in FY 2013).

## **6. Implementing Organizational Reforms (within 3 pages)**

### **6-1. Operation carried out under the Center Director's Leadership**

*Describe the division of roles and authority between the Center and its host institution, and the state of the Center director's presence at the Center.*

#### **Distribution of Authority**

Institute regulations and rules give the authority for the administrative operations to the Institute Director, and the appointment/dismissal of the Institute Director is authorized by the President of the host institution. The Director is assisted by two Associate Directors.

#### **The Science Steering Committee (SSC)**

The Science Steering Committee (SSC) was established upon the launching of the Institute. The committee 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. In FY 2013, two of our outstanding Associate Professors, Fujikawa and Tsuji, joined the SSC as new lead PIs of their respective divisions. In addition, as of November 1, 2013, Prof. Kenshi Itaoka has been invited to represent the EAD in the SSC as Acting Division Leader (non-voting member). The Director's decision-making authority, in consultation with the Science Steering Committee, has been established by preparing applicable Governing Documents.

#### **Decision-Making Process**

In order to specify the decision-making process in the Director's absence and to clarify the roles and responsibilities of the administrators of the Institute, document "22. Institutional Management and Administration" was written and officially added to the governing documents of the Institute in FY 2012.

#### **I<sup>2</sup>CNER Administration Meetings**

In order to promote excellent communication and understanding amongst I<sup>2</sup>CNER's administrators, regularly scheduled administrative meetings between the Director, the Associate Directors, and the

Administrative Director have been established. This face to face meeting is intended to supplement the existing communication system which includes daily emails, telephone calls, video-conferencing, etc.

### **Director's Physical Presence**

The Director's physical presence at I<sup>2</sup>CNER increased from 46% in FY 2012 to 48% in FY 2013. Specifically, in FY 2013, the Director made ten (10) trips and spent a total of 108 days of his time in Japan. By comparison, he made 10 trips totaling 103 days in Japan in FY 2012, and he made 5 trips totaling 54 days in Japan in FY 2011 (24%).

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

In FY 2012, the Director began publishing a newsletter entitled "I<sup>2</sup>CNER P.I.peline" in order to open a direct line of communication between the Director and the researchers of the Institute. Moreover, this publication was started in the spirit of keeping the researchers of the Institute informed of important events and changes that are happening within I<sup>2</sup>CNER. So far, three issues of I<sup>2</sup>CNER P.I.peline have been published (vol. 1-1: Dec 2012, vol. 2-1: May 2013, vol. 2-2: Dec 2013).

### **Ad-hoc Committee on Future Research Directions**

In FY 2013, the Director formed an ad-hoc committee chaired by Prof. H. Matsumoto, whose goal was to provide input to the Administration for the plan for the future of the Institute. The committee was asked to go beyond I<sup>2</sup>CNER's current research portfolio. The findings of the Committee were presented at the retreat with the External Advisory Committee (EAC) on March 26, 2014.

## 6-2. Administrative Personnel who facilitate the use of English in the Work Process

### **Administrative Director**

As of April 1, 2013, Prof. Kazuo Funaki took over the post of Administrative Director, which includes responsibility for the Administrative Office and other duties as assigned by the Director. Prof. Funaki served at Kyushu University for many years as a full professor, and has extensive experience and knowledge of the university.

### **Composition of Administrative Staff**

As of April 1, 2014, the administrative staff includes 18 members, and is divided into four groups:

1. General Affairs and Human Resources (6 members)
2. Accounting and Contracting (5 members)
3. Research Support and International Affairs (3 members)
4. Public Relations (2 members)

These four groups act as a support system to the Institute's researchers and administration under the supervision of the Administrative Director and the Associate Administrative Director. Kyushu University staff members have a good command of English, technical knowledge of general affairs and human resources, and those in the accounting and budget section are also highly experienced.

## 6-3. System Reforms and Their Ripple Effect within the Host Institution

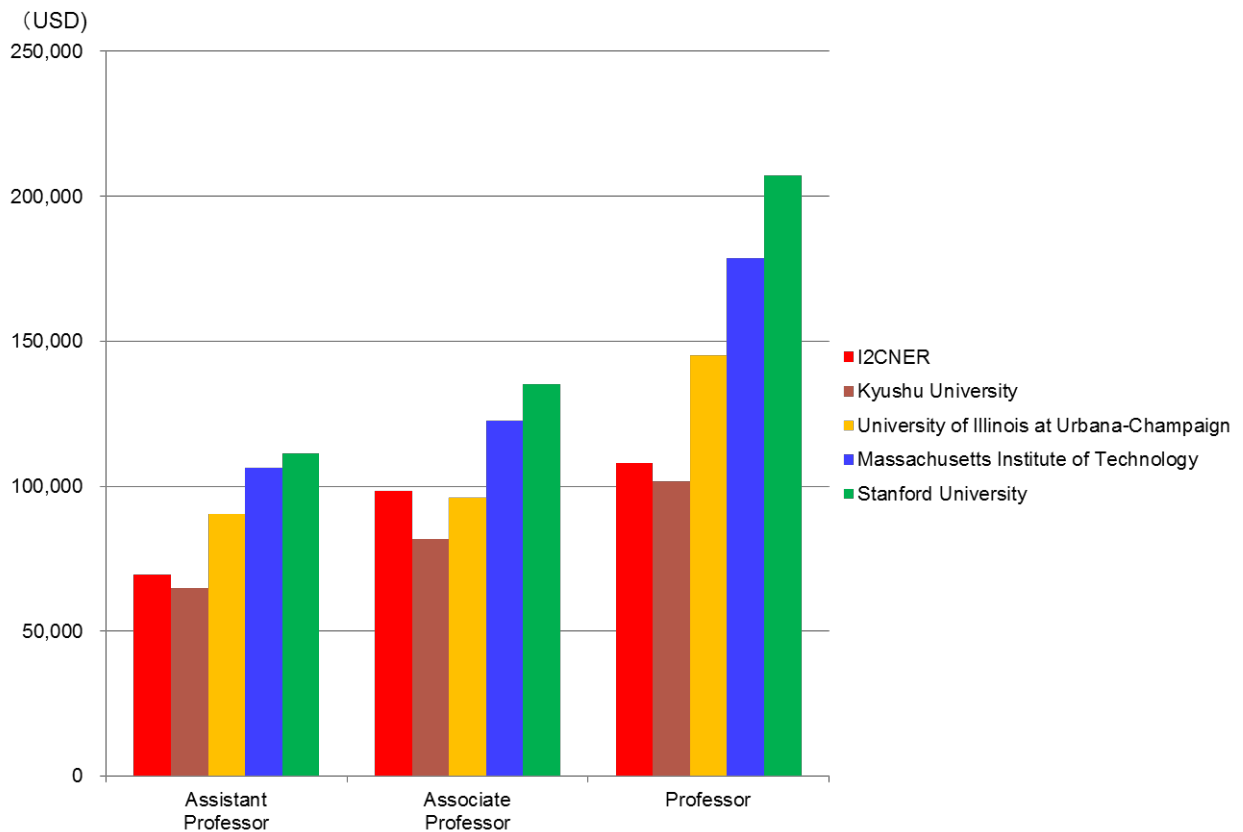
*Describe the following:*

- Reforms to the Center's research operation advanced by way of the WPI Program's research-results evaluation system
- Reforms to the Center's operation made by introducing a merit-based salary system
- Ripple effects of the Center's system reforms within the host institution

### **Merit-based Salary System**

Compensation considerations are based upon a special agreement between I<sup>2</sup>CNER and Kyushu University entitled "Regulations on Special Measures on the Hiring of National University Corporation Kyushu University International Institute for Carbon-Neutral Energy Research Employees." As a result of this special agreement, the Institute follows a special merit-based salary system which deviates from the established salary ranges. Individual faculty and researcher salaries are determined based on individual accomplishments and contributions to the interests of the Institute, as decided by the Director, in consultation with the two Associate Directors. Chart 1 below shows a comparison of I<sup>2</sup>CNER faculty salaries with those of faculty at Kyushu University, the University of Illinois at Urbana-Champaign, MIT, and Stanford.

Chart 1: I<sup>2</sup>CNER Faculty Salary Comparison



### “Ripple Effects” within Kyushu University

#### *New Merit-based Annual Salary System*

In order to promote revitalization and secure diverse, competent personnel within the university, Kyushu University introduced a new merit-based annual salary system for faculty members in November 2011. Furthermore, KU went a step ahead of the MEXT “National University Reform Plan,” and decided that the renewed system shall start in March 2014. Kyushu University aims to continuously review and improve this system for the purpose of integrating an attractive annual salary system with a sensible performance evaluation system.

#### *Stanford Satellite*

As part of its global strategy, Kyushu University has decided to establish an additional satellite institute at Stanford University, using the Illinois Satellite as a model for the establishment of KU overseas research and education centers, while also strengthening the entire operation of the original Illinois Satellite.

#### *I<sup>2</sup>CNER Research Hub*

Following the completion of I<sup>2</sup>CNER building 1, which was built at the heart of the Center Zone on Ito campus, Kyushu University approved the development of I<sup>2</sup>CNER building 2, as well as the Center of Innovation (COI), in the same vicinity. In sum, the areas surrounding I<sup>2</sup>CNER building 1 are being developed rapidly in order to transform the Center Zone into Kyushu University’s new research hub/industry-academia zone. In April 2014, the university’s administration moved into the newly-built Shiiki Hall, which is adjacent to I<sup>2</sup>CNER building 1.

#### *Cross-Appointment*

In view of the successful model of Director Sofronis’ cross-appointment case, which was the first ever at Kyushu University, a plan to institutionalize an employment system by cross-appointment is now under consideration by KU.

#### *Travel Expenses for Inviting Researchers from Overseas*

When inviting renowned researchers from overseas, I<sup>2</sup>CNER has established a practice of flexibly handling their travel expenses where appropriate. Beginning April 1, 2014, this will become an approved/common practice across all units of Kyushu University.

### *Intra-University Faculty Transfer System*

In order to enable flexibility in allocating faculty within the University while further improving the standards of education and research conducted at Kyushu University, KU established rules on the Intra-University Faculty Transfer System, which went into effect December 1, 2012. Utilizing this personnel- system reform, 9 senior-level Kyushu PIs were transferred to the Institute from the Faculty of Engineering as of April 1, 2013, and as a result, their main affiliation is now with I<sup>2</sup>CNER, which has helped improve mindset. Their transfer is extended on an annual basis, and all 9 of them will continue to serve as the core Kyushu-based principal investigators of I<sup>2</sup>CNER for FY 2014. In addition, the "Institute of Mathematics for Industry" of Kyushu University has started personnel transfers using the Intra-University Faculty Transfer System.

#### 6-4. Support by Host Institution

*Besides the state and effectiveness of the host institution's support for the Center, describe the Center's positioning within the host institution's mid- to long-term plans.*

*-In Appendix 6-4, describe specific support measures being taken by the host institution.*

#### **Kyushu University Education and Research Council**

The I<sup>2</sup>CNER Director is a member of the Education and Research Council which is administered by the KU President. When the Director is absent from KU, a representative attends the Council on his behalf.

#### **Faculty Council**

As part of the ongoing transition of I<sup>2</sup>CNER into a permanent unit of the Kyushu University system, a Faculty Council was established on April 1, 2013. The establishment of the Faculty Council helped to facilitate the transfer of 9 PIs from the Faculty of Engineering, which was mentioned above.

#### **Mid-term Plan of Kyushu University**

In the mid-term plan of Kyushu University, it has been decided to specify that "Kyushu University will advance the cutting-edge research in carbon-neutral energy-related areas in collaboration with the University of Illinois," that is being conducted at I<sup>2</sup>CNER, "the WPI Center that possesses the strength and features of Kyushu University." At the same time, Kyushu University will also take measures to further promote its collaborative research with the Illinois Satellite, "which is to be conducted at the University of Illinois."

#### **Tenured Positions**

As of March 31, 2014, the KU President has made 5 tenured positions for associate professors available to I<sup>2</sup>CNER. Of these, 1 female associate professor (also serves as PI) was hired in FY 2011, and as of April 1, 2014, two of our Division Lead PIs have been promoted to tenured associate professor positions. In addition, I<sup>2</sup>CNER competes for tenured positions in the University Reform Revitalization Program by submitting a proposal each year. In FY 2013, one full professor position was granted and it has already been filled.

#### **"Agreement on Academic Cooperation between KU and Illinois"**

In order to promote relations and mutual understanding between the two universities, an "Agreement on Academic Cooperation between KU and Illinois" has been drawn up. The specific purpose of this agreement is to develop scientific, academic, and educational cooperation on the basis of equality and reciprocity. Both universities are moving forward with the necessary procedures to enter into this agreement.

#### **"Student Exchange Program Agreement"**

Active discussions regarding a "Student Exchange Program Agreement" are currently underway between Kyushu University and the University of Illinois at Urbana-Champaign. The purpose of the agreement is to institutionalize the process of student exchange and to promote "traffic" across the Pacific between the Kyushu University School/Graduate School of Engineering and the UIUC College of Engineering in the future. Prof. Watanabe, Vice Dean of the Faculty of Engineering of Kyushu University, and Prof. Ken Christensen, Associate Director of the Illinois Satellite, are working cooperatively to facilitate/negotiate this agreement.



## **KU Public Relations Center**

It has been decided that Kyushu University will establish a Public Relations Center, which will be directed by the KU President. This PR Center is designed to institutionalize the Office for Public Relations Strategy and the Public Relations Strategy Council (both of which will be newly organized and placed under the PR Center), as well as collaborating faculty members. The PR Center will collaborate with the PR sections of each KU unit, including the PR Group in the I<sup>2</sup>CNER Administrative Office, in order to reinforce the university's PR functions as a whole.

### 6-5. Others

#### 6-5-1. Efforts to Foster Young Researchers (e.g., start-up funding)

##### **Evaluation Letters to Young Investigators**

The research progress of all young faculty members is reviewed by the Director, Associate Directors, and the corresponding Division Lead PI on an annual basis, including an individual face-to-face interview with the Director and Associate Directors in the month of February. Following these Annual Interviews and Assessments of Young Faculty and post-docs, feedback is provided to the young investigators in the form of a specific, individualized assessment and evaluation letter from the Director.

##### **Director's Discretionary Funding**

The Director set aside additional discretionary funds in FY 2013. Please see Section 4-3 for more details.

##### **Start-up funding for interdisciplinary research**

In FY2011, the administration of the Institute launched "Start-up funding for interdisciplinary research" to encourage inter-division research within I<sup>2</sup>CNER. The program was continued in FY 2012. For full details, please refer to Section 4-1 of this report.

##### **FY 2013 Funding for Young Faculty**

In FY 2013, it was decided that the "Start-up Funding for Interdisciplinary Research" program had not produced sufficient results to justify continuation. Instead, a portion of the funds which were conserved through the budget cuts for the Interdisciplinary Research Projects was allocated for a new initiative designed to help support young faculty. Beginning April 1, 2013, each of the young faculty members was automatically allocated 1.5 million JPY to support their research programs.

##### **General Start-up Research Funding**

In FY 2011, general Start-up research funding was allocated to newly hired I<sup>2</sup>CNER full-time researchers to develop their research environment. The total budget allocated to them was 2,228,383 USD (1USD=100 JPY).

In FY 2012, general Start-up research funding up to 40,000 USD was allocated to full-time faculty and post-docs. The total budget allocated to them was 565,000 USD (1USD=100JPY).

In FY 2013, general Start-up research funding was allocated to full-time faculty, part-time faculty, and postdocs. The total budget allocated to them was 527,500 USD (1USD=100JPY).

##### **Competitive-funding Allocation**

I<sup>2</sup>CNER Competitive Funding was established in FY2013. For full details, please refer to Section 4-1 of this report.

##### **Teaching Opportunities for Young Faculty**

Following the increase in the number of full-time PIs in April 2013, we have already provided opportunities for the young faculty members to collaboratively teach/advise PhD students under the supervision of the PIs.

##### **New Educational and Research Field**

In summer 2013, 3 new education and research fields were established in collaboration with the School/Graduate School of Engineering ("Energy International Education") and the Graduate School of Integrated Frontier Sciences ("Automotive Carbon-Neutral Energy") so that our young, full-time faculty members could be involved in teaching and supervising both undergraduate and graduate students. In the Fall 2013 semester, 15 faculty members (9 Japanese and 6 non-Japanese, including Director

Sofronis) gave lectures to “Global 30” students of the School of Engineering (“Advanced Engineering A,” 2 credit hours). For the upcoming FY 2014 Fall semester, 7 of I<sup>2</sup>CNER’s faculty members (5 Japanese and 2 non-Japanese) are scheduled to give lectures to the students of the Graduate School of Integrated Frontier Sciences (both Japanese and non-Japanese) in English. We will continue our efforts to strengthen our relationship with the above 3 departments in order to further solidify the framework for our young faculty to positively engage in energy-related education at Kyushu University.

### **Collaborative Foreign Exchange Program**

I<sup>2</sup>CNER’s “Collaborative Foreign Exchange Program,” designed specifically to encourage young Japanese researchers to visit our overseas collaborating institutions, was established in July 2013. For full details, please refer to Section 5-1-5 of this report.

### **Institute Interest Seminar Series (IISS)**

In order to foster a climate of collaboration and interdisciplinary research that cross-cuts division boundaries, the Institute regularly hosts the “Institute Interest Seminar Series (IISS).” For complete details, please refer to Section 2-2.

### **SRA Program**

I<sup>2</sup>CNER instituted the “Super Research Assistants (SRA)” Program in order to recruit and support excellent graduate students to carry out PhD thesis work under the supervision of our WPI assistant, associate, and full professors within the various divisions of the Institute. All SRAs are required to make presentations in English at the Institute Interest Seminar Series, submit progress reports, and give an additional presentation before the Institute’s SRA Selection Committee for the renewal of their SRA status. The quality of I<sup>2</sup>CNER SRAs is demonstrated by the fact that two former SRAs from FY 2012 were hired as JSPS fellows (i.e. Research Fellowship for Young Scientists: doctoral course students), beginning April 1, 2013. I<sup>2</sup>CNER employed 4 SRAs in FY 2011, 7 in FY 2012, 7 in FY 2013, and will employ 8 in FY 2014.

### **Skill Building Seminars**

The Institute holds special seminars for young researchers on a regular basis to help them improve their proposal-writing skills. To date, the Institute has hosted 2 KAKENHI Seminars and one special seminar. The first KAKENHI Seminar, given by Prof. Koji Takahashi of the Thermal Science and Engineering Division, was hosted on August 30, 2013 and attended by 31 researchers. The second KAKENHI Seminar on October 2, 2013 was given by Prof. Michihisa Koyama of the Energy Analysis Division and attended by 22 researchers. On February 5, 2014, the Institute hosted a special seminar given by Dr. Vincent Dusastre, the Chief Editor of Nature Materials. The seminar was attended by 60 researchers.

#### **6-5-2. Appointment of Female Researchers**

*-In Appendix 6-5-2, give the transition in the number of female researchers.*

### **Efforts to Hire Female Researchers**

In general, it is a priority within the Institute to hire and maintain top-tier female researchers. The Director specifically reviews every female applicant for any postdoc or faculty position. 1 of our female researchers was hired through the Faculty Excellence Program, which expedites the normal hiring process for faculty with international acclaim and a proven record that he/she can bring about transformational change across division boundaries, as mentioned in Section 5-1-4. As of April 1, 2014, I<sup>2</sup>CNER employs a total of 19 female researchers: 7 at KU, 9 at Illinois, and 3 at international partner institutions.

## **7. Future Vistas (within 2 pages)**

### **7-1. Future Policies and Plans for Advancing the Center’s Operation and Project**

I<sup>2</sup>CNER is at the center of Kyushu University’s (KU) mid-term plan, which specifies that “Kyushu University will advance the cutting-edge research in carbon-neutral energy-related areas in collaboration with the University of Illinois.” In addition, I<sup>2</sup>CNER can be a unique asset for KU’s globalization efforts in the context of the University Reform Revitalization Program. Further, the Institute’s faculty members are instructors in the G30 Engineering Project, which KU plans to expand by establishing an education

program that involves energy, the "Global Education Course." I<sup>2</sup>CNER will be the main driver of this energy component.

As part of Kyushu University's "Leaping into the World's Top 100" Action Plan (KU Globalization Strategy), the establishment of a new international course, "Carbon-Neutral Energy International Education," will be supported in FY 2014 in order to advance undergraduate education taught in English. The plan for this English undergraduate course is for it to be offered within the International School of Liberal Arts and Science, and further developed to be part of graduate education in the future. This will enable I<sup>2</sup>CNER and its faculty members to get further engaged, not only in research, but in education at Kyushu University, thus expanding I<sup>2</sup>CNER's portfolio in carbon-neutral energy.

Within the globalization initiative, KU is planning to negotiate a program with the University of Illinois to send KU researchers from all disciplines to spend time in residence at Illinois for extended periods of time (e.g. an academic semester).

These encompassing measures/initiatives of KU are warranting indicators of the future of I<sup>2</sup>CNER as a permanent unit of KU.

#### 7-2. Measures to sustain the center as a World Premier International Research Center after Program Funding Ends

As of April 1, 2014, I<sup>2</sup>CNER has 6 tenured faculty positions (1 full professor and 5 associate professors). With the aim of placing at least 1 tenured faculty member in each of the 9 research divisions, I<sup>2</sup>CNER will continue to submit proposals to the Kyushu University Reform Revitalization Program. In addition, the introduction of the Intra-University Faculty Transfer System helps I<sup>2</sup>CNER to maintain and expand its faculty strength. Between these two systems, we aim to secure about 20 faculty members.

With regard to additional funding sources for the operation of I<sup>2</sup>CNER, the following financial measures are under consideration:

- 1) In addition to the KU management expense grants, which are spent for the operation of I<sup>2</sup>CNER, external funding acquired by the above-mentioned 20 researchers will be allotted to management, personnel, research, and any other expenditures of their own research activities.
- 2) Corporation-supported non-tenured faculty members whose research is impactful to the corporation's operations (an example is the former employment arrangement of Prof. Kubota through an Air Liquide grant).
- 3) Resources from technology transfer or patent sales. The KU office for technology transfer (IMAO) is expected to play an active role in this development.
- 4) Foundations associated with KU could contribute to I<sup>2</sup>CNER's sustainability. Example cases within KU are the Inamori Frontier Research Center, which is supported by Kyocera, and the support for research the Gas Association of Japan provides to the Faculty of Engineering.
- 5) Leverage the initiatives of the Government of Japan for globalization of the National Universities. Thanks to its linkage with the University of Illinois, I<sup>2</sup>CNER, along with KU, is in a unique position to utilize these government initiatives for resources and future expansion.

#### 8. Others (within 1 page)

*\* In addition to the above 1-7 evaluation items, only if there is anything else that deserves mention regarding the center project's progress, please note it.*

#### **External Advisory Committee (EAC)**

Upon the official launching of the Institute, the Director consulted with senior authorities in the field of renewable energy and CO<sub>2</sub> sequestration and storage as well as members of the US Department of Energy to establish the External Advisory Committee (EAC). Following the first EAC meeting in February 2012 at Kyushu University, the 2<sup>nd</sup> I<sup>2</sup>CNER Retreat with the EAC at the University of Illinois at Urbana-Champaign was held May 30-31, 2013, and the EAC submitted the report to the Director on June 19<sup>th</sup> prior to the FY 2013 Site Visit. The 3<sup>rd</sup> EAC Retreat was held on March 26, 2014 at Kyushu University to discuss the Institute's future

research directions. The report from the most recent retreat is expected by May 15, 2014. As of March 31, 2014, the External Advisory Committee (EAC) had eight members:

- Prof. Ronald J. Adrian (Chair), Arizona State University, USA
- Dr. Deborah Myers (Co-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, Retired, 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)

### **Chief Science Advisor**

Prof. Ian Robertson, Dean of Engineering at the University of Wisconsin-Madison, not only serves as a Principal Investigator of the Hydrogen Materials Compatibility Division and a member of the IPRC, but also as Chief Science Advisor to the Director in order to further strengthen the management of the Institute in relation to its research activities.

### **International Partner Researchers**

Participating Personnel and collaborating divisions are:

- Prof. John Kilner, Hydrogen Production Division, Imperial College London, PI
- Dr. Brian P. Somerday, Hydrogen Materials Compatibility Division, Sandia National Laboratories, PI
- Prof. Nikolaos Aravas, Hydrogen Materials Compatibility Division, University of Thessaly, WPI Professor
- Prof. Robert O. Ritchie, Hydrogen Materials Compatibility Division, University of California at Berkeley, WPI Professor
- Prof. Reiner Kirchheim, Hydrogen Materials Compatibility Division, University of Göttingen, PI
- Prof. Kanao Fukuda, Hydrogen Materials Compatibility Division, Malaysia-Japan International Institute of Technology, Universiti Teknologi Malaysia, WPI Visiting Professor
- Dr. Chao-Nan Xu, Hydrogen Materials Compatibility Division, AIST, WPI Visiting Professor
- Prof. Harry L. Tuller, Fuel Cells Division, Massachusetts Institute of Technology, PI
- Dr. Dario Marrocchelli, Prof. Graeme Watson, Prof. Bilge Yildiz, Fuel Cells Division, Trinity College Dublin at Massachusetts Institute of Technology
- Assistant Prof. Jennifer Rupp, Fuel Cells Division, Swiss Federal Institute of Technology Zurich (ETH), WPI Associate Professor
- Dr. Toyoki Kunitake, Fuel Cells Division, Kitakyushu Foundation for the Advancement of Industry Science and Technology, WPI Visiting Professor
- Prof. Xing Zhang, Thermal Science and Engineering Division, Tsinghua University, PI
- Dr. Ping Chen, Hydrogen Storage Division, Dalian Institute of Chemical Physics, WPI Professor
- Emeritus Prof. Louis Schlapbac, Hydrogen Storage Division, retired from ETH, WPI Visiting Professor
- Dr. Peter McGrail, CO<sub>2</sub> Capture and Utilization Division, Pacific Northwest National Laboratory
- Prof. Benny Freeman, CO<sub>2</sub> Capture and Utilization Division, University of Texas at Austin, WPI Professor
- Prof. Katsuki Kusakabe, CO<sub>2</sub> Capture and Utilization Division, Sojo University, WPI Visiting Professor
- Prof. Tor Arne Johansen, CO<sub>2</sub> Storage Division, University of Bergen
- Prof. Wawan Gunawan A. Kadir, CO<sub>2</sub> Storage Division, Bandung Institute of Technology
- Dr. Ziqui Xue, CO<sub>2</sub> Storage Division, Research Institute of Innovative Technology for the Earth (RITE), WPI Visiting Professor
- Dr. Mark Paster, Energy Analysis Division, former energy analysis employee of the U.S. DOE, WPI Visiting Professor
- Dr. Kuniaki Honda, Energy Analysis Division, formerly with the Gas and Power Co., Ltd., Japan, WPI Visiting Professor
- Prof. Ken Okazaki, Tokyo Institute of Technology, WPI Visiting Professor

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

In order to promote engagement with leaders of the national and international community, and enhance its visibility, the Institute launched the "I<sup>2</sup>CNER Seminar Series" in March 2011. This seminar series features distinguished and internationally-recognized researchers from academia, national laboratories, and industry, as well as policy makers in government agencies. As of March 31, 2014, the Institute has hosted a total of 64

I<sup>2</sup>CNER Seminars (2 in FY 2010, 17 in FY 2011, 23 in FY 2012, and 22 in FY 2013). More than 50% of the speakers in this series have been non-Japanese.

## **I<sup>2</sup>CNER CO<sup>2</sup>**

A regular networking event, I<sup>2</sup>CNER CO<sup>2</sup> (Coffee and Collaboration) was established in January 2013 upon the inauguration of I<sup>2</sup>CNER Building 1. I<sup>2</sup>CNER CO<sup>2</sup> gives the Institute's researchers the opportunity to meet casually over coffee to discuss basic science issues, the details of their collaborations, etc., in front of electronic blackboards.

### **9. Center's Response to Results of FY2013 Follow-up (including Site Visit Results) (Use as Many Pages as needed.)**

*Describe the Center's Response to Results of FY2013 Follow-up. Note: If you have already provided this information, please indicate where in the report.*

#### **FY2013 Follow-up, "3. Recommendations"**

##### **Director's Physical Presence**

- *In 2012, Director Sofronis made 10 trips to Japan, spending 103 days or 46% of his time. Although this is clearly good improvement, it is important to maintain his physical presence at more than 50%.*
  - Please see response under Section "6-1."

##### **Recruitment of Permanent-staying Foreign PIs**

- *A particular effort should be made to appoint world-leading top scientists as PIs residing at I<sup>2</sup>CNER. The Faculty Recruiting Committee should move much more proactively to identify and invite such scientists. Administrative Division should also work to help in close cooperation with its counterpart in Illinois.*
  - The Institute's Faculty Recruiting Committee (FRC) has conducted an extensive recruiting campaign to hire permanent-staying foreign principal investigator(s). For full details, please see Section 5-1-3 of this report.

##### **Kyushu-Illinois Researcher Exchange**

- *The mutual exchange of researchers between KU and University of Illinois (UI) is not enough in numbers and in their lengths of stay. In FY2012, five researchers visited UI from KU and only two of them stayed for more than one month, while from UI twenty visited KU but stayed for less than one week.*
  - In FY 2013, 23 researchers from KU visited UIUC, of which 16 stayed for under 1 week, 5 stayed between 1 week and 1 month, and 2 stayed for a period longer than 1 month. 22 researchers from UIUC visited KU in FY 2013, of which 19 stayed for a period of less than 1 week, and 3 stayed between 1 week and 1 month. Further details are provided in Appendix 5-1-1.

##### **Post-doc Appointment**

- *The efforts to increase the number of post-docs are ongoing straightforward. One post-doc line has been allocated to each Kyushu PI, but clearly this appointment procedure needs rigorous evaluation of each candidate.*
  - Candidates for the PI Postdoctoral lines must undergo a screening by the Faculty Recruiting Committee (FRC) just like every other researcher who is hired in the Institute. If the FRC does not approve the hiring of a candidate for a PI Postdoctoral line, the PI is asked to select a different candidate for the position, and the screening starts again when a suitable candidate is identified by the PI. For more information, please see Section 5-1-4.

##### **Division Research Themes/Projects & Research Work by Young Faculty**

- *Fuel Cell Division should seek for some high-risk research themes. Thermo physical Properties Division needs to reconsider their short-term and long-term research themes in relevance to carbon neutral concept. The research project on electro-fuel utilizing captured CO<sub>2</sub> should be carefully examined if it is a central issue for realizing a carbon neutral society. It should be noted that some of the research work carried out by young faculties do not seem to be at top-levels in the relevant fields. They should discuss on their research subjects more extensively with senior researchers or Lead PI's in their fields.*

- The Fuel Cells division working closely with the Energy Analysis Division has radically refocused its research efforts, e.g. work on fuel processing for low temperature SOFCs (LT-SOFC) has been terminated. The new roadmap of the division that was constructed in close collaboration with the energy analysis division includes only two projects with clearly defined and focused objectives: a) Development of a higher temperature ( $> 100^{\circ}\text{C}$ ) hydrogen PEM fuel cell with higher efficiency and better durability by developing alternative materials; b) Development of long-term chemically durable SOFCs for ambient operation and for pressurized operation with much higher efficiencies. For FY2013, the division takes pride in a number of discoveries that are reported in section 2-1. By way of example, it was discovered that i) nanotube based electrocatalysts with Polybenzimidazole membranes have enabled high power densities for 400,000 cycles at  $120^{\circ}\text{C}$ , a dramatic advance relative to current-state-of-the-art ( $< 80,000$  cycles); ii) charge localization on reduced cations after an oxide ion is removed from the lattice is the origin of the detrimental chemical expansion in oxides commonly used in SOFCs.
- As recommended, the techno-economics of the electrochemical reduction of  $\text{CO}_2$  for the production of fuel and useful products has been carried out for the conversion of  $\text{CO}_2$  produced by a 500 MW power plant into CO, using an electrolyzer for CO formation driven by electricity from the grid and using water electrolysis driven by the same electrical grid for the production of  $\text{H}_2$  needed. The results demonstrate that with the use of electricity from renewables implementation is possible if one considers the baseline of continuously rising cost for fossil fuels in the future, say, 20 years from now.
- In FY 2013, the young researchers participated in a number of meetings with the energy analysis division for the maturation of their division's roadmaps. We believe it is now clear to all of them how their research efforts are associated with specific division projects with clear milestones and ultimate targets. This, along with support from division PIs provides, helps them focus their research activities.

## **Site Visit Results, "7. Actions required and recommendations"**

### **Director's Physical Presence**

1. *In 2012, Director Sofronis made 10 trips to Japan, spending 103 days or 46% of his time. Although this is clearly good improvement, it is important to maintain his physical presence at more than 50%.*
  - Please see response under Director's Physical Presence above.

### **Recruitment of Permanent-staying Foreign PIs**

2. *A particular effort should be made to appoint world-leading top scientists as PIs residing at I<sup>2</sup>CNER. The Faculty Recruiting Committee should move much more proactively to identify and invite such scientists. Administrative Division should also work to help in close cooperation with its counterpart in Illinois. Even more should be done on publicity in recruiting young faculty and PhD students worldwide.*
  - Please see response under Recruitment of Permanent-staying Foreign PIs above.

### **Internal Programs Review Committee (IPRC)**

3. *The Internal Programs Review Committee functions well in identifying relevant and well-designed research projects in I<sup>2</sup>CNER. It should be one of the standing committees, and utilized to continuously review the composition of Divisions and redesign them as appropriate. It is essential to (1) take a deep dive review, and (2) work toward a sustaining strategy that will most effectively match the mission of the center.*
  - The Internal Programs Review Committee (IPRC) was made into a standing committee of the Institute in FY 2013. For full details, please see Section 2-2 of this report.

### **EAD/Roadmap Maturation**

4. *The work of Energy Analysis Division as well as the roadmaps of research divisions should be continuously refined and tuned to produce a consistent scenario of emission reduction and pathway toward a carbon neutral society on an annual basis. The impact of each technology target should also be assessed quantitatively with its uncertainty level gradually reduced. Each division should aim at a reasonable balance between fundamental and application-oriented research, while strengthening fusions and collaborations.*

- Please see Sections 2-2 and 3-1-1 of this report respectively for challenges related to the operation of the Energy Analysis Division (EAD) and its overall research effort toward formulating I<sup>2</sup>CNER's energy vision for a carbon-neutral society (CNS).

In FY 2013, Prof. Itaoka was appointed Acting Leader of the EAD. Prof. Itaoka coordinated effectively a series of productive meetings between the EAD and each and every technical division throughout the year. Remarkably each of these meetings were attended by all division researchers—from postdocs to PIs. With input from the EAD, through division retreats whose main goal was the maturation of roadmaps, and accounting for the recommendations from the institute retreat with the External Advisory Committee in May of 2013, the divisions submitted revised roadmaps in early January 2014. In parallel, the EAD worked throughout the year to develop an energy vision for CNS and make sure that the I<sup>2</sup>CNER research division roadmaps are intimately tied through short-, mid-, and long-term milestones to the development and deployment timing of promising set of technology options—energy scenarios—for a large reduction of greenhouse gas (GHG) emissions (70-80%) by 2050 from 1990 levels. A second series of meetings between the EAD and the divisions led to the harmonization of the energy scenarios for a CNS with the individual division roadmaps.

### **Review and Redesign of Existing Research Projects**

5. *Thorough review and redesign of existing Divisions' research projects is necessary with the help of the IPRC and the EAD. Fuel Cell Division should seek for some high-risk, disruptive research themes. Thermophysical Properties Division needs to reconsider their short-term and long-term research themes in relevance to carbon neutral concept. The research project on electro-fuel utilizing captured CO<sub>2</sub> should be carefully examined if it is a central issue for realizing a carbon neutral society.*

- As described in "EAD/Roadmap Maturation," through input from the EAD, the Thermal Science and Engineering division recast its research efforts into new and focused projects with well-defined objectives, milestones, and ultimate targets. For the Fuel Cells division and the techno-economic analysis of the electrochemical conversion of CO<sub>2</sub>, please see response under "Division Research Themes/Projects & Research Work by Young Faculty" and "Internal Programs Review Committee (IPRC)" above.

### **International Collaboration**

6. *The international collaboration should be enhanced to be even more productive. I<sup>2</sup>CNER should be regarded as a unique opportunity to take for all individuals including PhD students, researchers, faculty members and administration staffs to visit overseas research institutions for a substantial period. PDs, particularly Japanese, should be encouraged to more actively seek for an opportunity to work abroad for a relatively long period of a year or two. When developing research collaborations, balanced focus on regions including Europe and research topics should be made.*

- Please see response in Section 6-4 under "Agreement on Academic Cooperation between KU and Illinois" and "Student Exchange Program Agreement," and in section 6-5-1 under "Collaborative Foreign Exchange Program." Also a detailed description of the linkage between KU and Illinois through travel of post-doc and young faculty is given in section 5-1-5. Additional partnership that have been initiated in FY 2013 will offer more opportunities to postdocs and young faculty to carry out research in the US and Europe. Already a group of I<sup>2</sup>CNER researchers visited the University of California, Irvine last February and identified three projects for collaboration between I<sup>2</sup>CNER and the National Fuel Cell Research Center (NFCRC). The signed MoU between I<sup>2</sup>CNER and NTNU/SINTEF last March opens new opportunities for young Japanese researchers to visit Trondheim, given that already this partnership has been initiated through a joint grant by the Research Council of Norway. In general a number of researchers have traveled to many institutions around the world, e.g. Indonesia.

### **Level of Research by Young Faculty**

7. *It should be noted that some of the research work carried out by young faculties do not seem to be at top-levels in the relevant fields. They should discuss on their research subjects more extensively with senior researchers or Lead PI's in their fields.*

- Please see response under Division Research Themes/Projects & Research Work by Young Faculty above.

## **The following are the recommendations for which concrete actions should be taken.**

### **Metrics of Success**

1. *WPI program generally aims at basic research, but their outcome in application or innovation is also appreciated. Hence, in evaluation of I<sup>2</sup>CNER, some new measures should be developed to qualify and quantify their achievement in terms of applied research, IPs, market introduction and even innovation. Note that I<sup>2</sup>CNER was started under the STI policy of "Green Innovation."*
  - I<sup>2</sup>CNER is a mission-driven (Green Innovation) research center but is focused on basic science. As such, it can be evaluated on the basis of the following metrics:
    - 1) Relevance of the I<sup>2</sup>CNER research efforts and objectives to enable the green innovation initiative of the government of Japan
    - 2) Approach to carrying out research. This can be evaluated by the quality of the publications in high impact, discipline-oriented journals. By publishing in such journals, a stringent review process which will address whether the research advances what is considered state-of-the-art by a community of experts is ensured.
    - 3) Degree of realization of milestones and targets in research roadmaps
    - 4) Level of collaboration with international research centers and efforts and degree of research interdisciplinarity.
    - 5) Number and quality of participating industrial partners
    - 6) Filing for patents
    - 7) Technology transition events. It is our understanding that Technology transition events are more important than number of patents pending.
    - 8) The overriding metric is that quality needs to pervade all I<sup>2</sup>CNER operations.

### **Technology Transfer**

2. *In addition to the traditional collaborations with the industry, encouragement and support of patents with the help of technology licensing office should be made by I<sup>2</sup>CNER. Clear attributions of success must be defined that can be presented in the highlights for all divisions, quantifying technology transfer (just like high impact publications and their highlights quantify science achievements). This will be a fair process across the center if all divisions target the same set of attributes with some doing better in science development and some better in technology development.*
  - In FY 2013, I<sup>2</sup>CNER contacted both the Kyushu University Intellectual Property Management Center (IMAQ) and the University of Illinois Office of Technology Management (OTM) to begin discussions on a technology transfer process for the Institute. Along with Director Sofronis, Lesley Millar, OTM Director, and Professor K. Furukawa of IMAQ, spearheaded this effort. IMAQ and OTM had several joint meetings via videoconference in which they discussed the general operations and strengths of both offices in order to start collaborating. All of the assistance that OTM can offer, including IP agreements, disclosures, patent applications, etc. are available to all I<sup>2</sup>CNER Faculty. Similarly, IMAQ is prepared to help all KU researchers with patent and IP issues. OTM and IMAQ are prepared to work together on any joint research projects between Kyushu and Illinois which may need assistance with technology transfer.
  - From the inception of I<sup>2</sup>CNER, there have been 18 applications for patents (see Table 1 of section 3-1-3), one (1) technology transfer event to TOKi Engineering (see section 3-1-3 under "Industrial Projects"), one licensing event (No. 10 in Table 1 of Section 3-1-3), and negotiations for licensing (No. 11 in Table 1 of section 3-1-3). All patent applications are in areas relevant to the energy research agenda of I<sup>2</sup>CNER.
  - Although this was an event that happened in FY 2014 and this report is to include materials through the end of FY 2013, an I<sup>2</sup>CNER-industry event took place in Tokyo on April 11, 2014. The event was part of I<sup>2</sup>CNER's initiative to establish a process with industry whereby we host regular meetings, showcase our research activities, and jointly explore aspects of our research that could lead to technology transfer. 21 corporations participated in the April 11 event, including Nissan Motor Co.,



Tokyo Gas Co., Air Liquide Japan, Nippon Steel & Sumitomo Metal Corporation, Toyota Motor Corporation, Toshiba Corporation, and JX Nippon Oil & Energy Corporation.

### Further Network Development

3. *It is hoped that I<sup>2</sup>CNER will develop strong networking with top players in the world. One way is to identify key individuals and stakeholders, and reach out to them, i.e., use the outreach to fully introduce and explain I<sup>2</sup>CNER, request a critical review of I<sup>2</sup>CNER roadmap, significantly increase the strength of I<sup>2</sup>CNER program, and substantially increase I<sup>2</sup>CNER initiatives.*

- The Institute signed an agreement with the National Fuel Cell Research Center (NFCRC) at the University of California, Irvine on December 31, 2013. Contact between researchers was initiated on February 25, 2014.
- The Institute is in the process of negotiating a "Letter of Understanding" with the Air Resources Board of the State of California (CARB) in order to reinforce common ideas of green innovation.
- After over a year of mutual effort, the Institute signed an MOU with the Norwegian University of Science and Technology (NTNU) and SINTEF on March 17, 2014. A joint research proposal between I<sup>2</sup>CNER and NTNU has been awarded by the Norway Research Council.
- I<sup>2</sup>CNER has remained in close contact with the US Department of Energy (DOE) Office of Energy Efficiency and Renewable Energy (EERE) in order to gather feedback and advice on its research agenda. A formal meeting to discuss metrics, roadmap maturation, and possible future research topics was held in Washington, D.C. on February 12, 2014.
- The Institute has received a request for collaboration from EaStCHEM, a joint Chemistry Research School between the Universities of Edinburgh and St. Andrews. EaStCHEM is ranked amongst the top 4 Chemistry departments in the United Kingdom. Possible areas of collaboration include fuel cells, porous materials for energy storage and gas, solar materials, and homogeneous and heterogeneous catalysis.
- The Institute and HEmS (Hydrogen in metals- from fundamentals to the design of new steels) of the University of Oxford, which is a 5 year project with over \$8 million USD in funding per year, had meetings to explore the possibilities for collaboration. The Director is currently on the Strategic Advisory Panel of HEmS.
- Beginning October 1, 2013, I<sup>2</sup>CNER had a four year "Consortium Agreement" with the "ECOSTORE," which is an EU-supported consortium project. (The agreement will conclude on September 30, 2017). The aim of the project is to bring together senior and junior scientists from in and outside of Europe through education about hydrogen storage. International exchange of young researchers is also a priority of the ECOSTORE. Prof. Estuo Akiba (Hydrogen Storage Division Lead Principal Investigator) serves as an Associated Partner on the project. The ECOSTORE workshop in March 2015 will be held at I<sup>2</sup>CNER. It is expected that more than 10 graduate students and postdocs from Europe will participate in the workshop.  
(<http://inano.au.dk/news-events/news/show/artikel/international-ecostore-project-four-million-euro-for-research-into-energy-storage-using-hydrogen-an/>)

## World Premier International Research Center Initiative (WPI)

### 1. FY 2013 List of Principal Investigators

**NOTE:**

- *Underline names of investigators who belong to an overseas research institution. Place an asterisk (\*) by names of investigators considered to be ranked among world's top researchers.*
- *In case of researchers not listed in initial plan, attach "Biographical Sketch" for those participating as principal investigators.*
- **※1 shows PIs who transfer from the Faculty of Engineering to I<sup>2</sup>CNER from April 1, 2013.**

< Results at the end of FY2013 >									
Principal Investigators Total:26									
Name (Age)	Affiliation (Position title, department, organization)	Academic degree, specialty	Working hours (Total working hours: 100%)				Starting date of project participation	Status of project participation (Describe in concrete terms)	Contributions by PIs from overseas research institutions
			Work on center project		Others				
			Research activities	Other activities	Research activities	Other activities			
Center director  <u>Petros Sofronis</u> (56)*	Prof., International Institute for Carbon-Neutral Energy Research, Kyushu University	Ph.D., Micromechanics of materials, Environmental degradation of materials	15%	70%	10%	5%	2010, Dec.1 <sup>st</sup>	<ul style="list-style-type: none"> <li>• Manages the Institute from IL Satellite</li> <li>• Travels to the Institute to participate in events and exchange with researchers (48% time)</li> <li>• Promotes I<sup>2</sup>CNER's interests to various research institutions and industries on a daily basis</li> <li>• Daily exchange of e-mails</li> <li>• Participates in meetings/events via videoconference system</li> </ul>	<ul style="list-style-type: none"> <li>• Manages and directs I<sup>2</sup>CNER's operations</li> </ul>
Tsutomu Katsuki (67)*	Prof., International Institute for Carbon-Neutral Energy Research, Kyushu University	Dr. of Science, Sustainable chemical transformation, Catalysis	90%	10%	0%	0%	2010, Dec.1 <sup>st</sup>	<ul style="list-style-type: none"> <li>• Located at I<sup>2</sup>CNER</li> <li>• Participates in research/events</li> </ul>	/
Tatsumi Ishihara (52)*	Prof., International Institute for Carbon-Neutral Energy Research, Kyushu University ※1	Dr. of Eng., Catalyst and solid state electrochemistry	90%	10%	0%	0%	2010, Dec.1 <sup>st</sup>	<ul style="list-style-type: none"> <li>• Located at I<sup>2</sup>CNER</li> <li>• Participates in research/events as Associate Director, Head of Hydrogen Production Division</li> </ul>	/

Chihaya Adachi (50)*	Prof., Department of Applied Chemistry, Kyushu University	Dr. of Eng., Materials science and device physics	60%	20%	10%	10%	2010, Dec.1 <sup>st</sup>	<ul style="list-style-type: none"> <li>• Located at I<sup>2</sup>CNER</li> <li>• Participates in research/events</li> </ul>	
Atsushi Takahara (58)*	Prof., Institute for Materials Chemistry and Engineering, Kyushu University,	Dr. of Eng., Surface and Interface Characterization	60%	20%	10%	10%	2010, Dec.1 <sup>st</sup>	<ul style="list-style-type: none"> <li>• Located at I<sup>2</sup>CNER</li> <li>• Participates in research/events</li> </ul>	
Seiji Ogo (50)*	Prof., International Institute for Carbon-Neutral Energy Research, Kyushu University ※1	Dr. of Science, Green Chemistry	90%	10%	0%	0%	2010, Dec.1 <sup>st</sup>	<ul style="list-style-type: none"> <li>• Located at I<sup>2</sup>CNER</li> <li>• Participates in research/events as Head of Catalytic Materials Transformations Division</li> </ul>	
Katsuki Kusakabe (59)*	Prof., Department of Nanoscience, Sojo University	Dr. of Eng., Reaction engineering, Catalyst	50%	10%	20%	20%	2010, Dec.1 <sup>st</sup>	<ul style="list-style-type: none"> <li>• Primarily located at partner institution</li> <li>• Located at I<sup>2</sup>CNER part time</li> <li>• Participates in meetings/events at I<sup>2</sup>CNER twice a month</li> <li>• Appointment will change to WPI Visiting Professor as of April 1, 2014</li> </ul>	
Zenji Horita (60)*	Prof., International Institute for Carbon-Neutral Energy Research, Kyushu University ※1	Ph.D., Dr. of Eng., Materials Science	90%	10%	0%	0%	2010, Dec.1 <sup>st</sup>	<ul style="list-style-type: none"> <li>• Located at I<sup>2</sup>CNER</li> <li>• Participates in research/events</li> </ul>	
Naotoshi Nakashima (62)*	Prof., International Institute for Carbon-Neutral Energy Research, Kyushu University ※1	Ph. D., Nanocarbon science, Supramolecular science	85%	15%	0%	0%	2010, Dec.1 <sup>st</sup>	<ul style="list-style-type: none"> <li>• Located at I<sup>2</sup>CNER</li> <li>• Participates in research/events</li> </ul>	

Kazunari Sasaki (49)*	Prof., International Institute for Carbon-Neutral Energy Research, Kyushu University ※1	Dr. of Science and technology, Fuel cell materials, Inorganic materials	90%	10%	0%	0%	2010, Dec.1 <sup>st</sup>	<ul style="list-style-type: none"> <li>• Located at I<sup>2</sup>CNER</li> <li>• Participates in research/events as Head of Fuel Cell Division</li> </ul>	
Etsuo Akiba (62)*	Prof., International Institute for Carbon-Neutral Energy Research, Kyushu University ※1	Dr. of Science, Materials science	70%	30%	0%	0%	2010, Dec.1 <sup>st</sup>	<ul style="list-style-type: none"> <li>• Located at I<sup>2</sup>CNER</li> <li>• Participates in research/events as Head of Hydrogen Storage Division</li> </ul>	
<u>Harry L. Tuller</u> (68)*	Prof. Department of Materials Science and Engineering, Massachusetts Institute of Technology	Eng. Sc. D., Functional electroceramic materials	35%	5%	45%	15%	2010, Dec.1 <sup>st</sup>	<ul style="list-style-type: none"> <li>• Primarily located at partner institution</li> <li>• Participates in research</li> <li>• Visited I<sup>2</sup>CNER for four weeks to participate in events and exchange opinions for collaborative research projects</li> <li>• Discussion via Internet</li> </ul>	<ul style="list-style-type: none"> <li>• None besides what is mentioned on the left</li> </ul>
<u>John A Kilner</u> (67)*	Prof., Department of Materials, Imperial College, London	PhD., Materials for solid oxide fuel cells and electrolysers	35%	5%	45%	15%	2010, Dec.1 <sup>st</sup>	<ul style="list-style-type: none"> <li>• Primarily located at partner institution</li> <li>• Participates in research</li> <li>• Visited I<sup>2</sup>CNER for four weeks for research to participate in events and exchange opinions for collaboration</li> <li>• Regular discussion via Internet</li> </ul>	<ul style="list-style-type: none"> <li>• None besides what is mentioned on the left</li> </ul>
Joichi Sugimura (56)	Prof., International Institute for Carbon-Neutral Energy Research, Kyushu University ※1	Dr. of Eng., Tribology and Machine Design	70%	30%	0%	0%	2010, Dec.1 <sup>st</sup>	<ul style="list-style-type: none"> <li>• Located at I<sup>2</sup>CNER</li> <li>• Participates in research/events</li> <li>• Hosted students from UIUC</li> </ul>	
Yasuyuki Takata (57)	Prof., International Institute for Carbon-Neutral Energy Research, Kyushu University ※1	Dr. of Eng., Thermal Engineering	70%	30%	0%	0%	2010, Dec.1 <sup>st</sup>	<ul style="list-style-type: none"> <li>• Located at I<sup>2</sup>CNER</li> <li>• Participates in research/events as Associate Director, Head of Thermal Sciences and Engineering Division</li> </ul>	

<u>Xing Zhang</u> (52)	Prof., Department of Engineering Mechanics, Tsinghua University	Ph.D., Thermal Science	10%	10%	45%	35%	2010, Dec.1 <sup>st</sup>	<ul style="list-style-type: none"> <li>Primarily located at partner institution</li> <li>Participates in research/events</li> <li>Visited I<sup>2</sup>CNER for three weeks to conduct research, participate in events, and exchange opinions for collaboration</li> <li>Discussion via Internet</li> </ul>	<ul style="list-style-type: none"> <li>None besides what is mentioned on the left</li> </ul>
<u>Brian P. Somerday</u> (45)*	Dr., Sandia National Laboratory	Ph.D., Materials Science and Engineering	20%	15%	35%	30%	2010, Dec.1 <sup>st</sup>	<ul style="list-style-type: none"> <li>Primarily located at partner institution</li> <li>Participates in research as Head of Hydrogen Materials Compatibility Division</li> <li>Stayed at I<sup>2</sup>CNER for two weeks to participate in events and exchange opinions for collaboration</li> <li>Participates in meetings/events via videoconference system</li> </ul>	<ul style="list-style-type: none"> <li>Accepting researchers from I<sup>2</sup>CNER</li> </ul>
Setsuo Takaki (61)	Prof., International Institute for Carbon-Neutral Energy Research, Kyushu University ※1	Dr. of Engineering	90%	10%	0%	0%	2011, April.1 <sup>st</sup>	<ul style="list-style-type: none"> <li>Located at I<sup>2</sup>CNER</li> <li>Participates in research/events</li> </ul>	
<u>Reiner Kirchheim</u> (70)*	Prof., The Institut für Metallphysik, University of Göttingen	Ph.D.	20%	20%	40%	20%	2011, April.1 <sup>st</sup>	<ul style="list-style-type: none"> <li>Primarily located at partner institution</li> <li>Participates in research</li> <li>Stayed at I<sup>2</sup>CNER for two weeks to participate in events and exchange opinions for collaboration</li> <li>Discussion via Internet</li> </ul>	<ul style="list-style-type: none"> <li>None besides what is mentioned on the left</li> </ul>
Miho Yamauchi (40)	Associate Prof., International Institute for Carbon-Neutral Energy Research, Kyushu University	Dr. of Science, Chemistry	100%	0%	0%	0%	2012, Jan. 1 <sup>st</sup>	<ul style="list-style-type: none"> <li>Located at I<sup>2</sup>CNER</li> <li>Participates in research/events</li> <li>Hosted a student from UIUC</li> </ul>	
Ken Sakai (52)	Prof., Department of Chemistry Faculty of Sciences, Kyushu University	Ph.D., Inorganic Chemistry	80%	10%	0%	10%	2012, Jan.16 <sup>th</sup>	<ul style="list-style-type: none"> <li>Located at I<sup>2</sup>CNER</li> <li>Participates in research/events</li> </ul>	

<u>Ian Robertson</u> (56)	Prof., Dean of Engineering, University of Wisconsin-Madison, Chief Science Advisor to the Director	Ph.D., Metallurgy	20%	5%	25%	50%		2012, April.1 <sup>st</sup>	<ul style="list-style-type: none"> <li>• Primarily located at partner institution</li> <li>• Participates in research/events as Chief Science Advisor to the Director</li> <li>• Visited I<sup>2</sup>CNER for one week to participate in events and exchange opinions for collaboration</li> <li>• Discussion via Internet</li> </ul>	<ul style="list-style-type: none"> <li>• Sent graduate students to Institute</li> </ul>
<u>Andrew A. Gewirth</u> (54)	Prof., Chemistry, University of Illinois	Ph.D., Chemistry	20%	5%	60%	15%		2012, April.1 <sup>st</sup>	<ul style="list-style-type: none"> <li>• Primarily located at partner institution</li> <li>• Participates in research</li> <li>• Visited I<sup>2</sup>CNER for one week to participate in events and exchange opinions for collaboration</li> <li>• Discussion via Internet</li> </ul>	<ul style="list-style-type: none"> <li>• None besides what is mentioned on the left</li> </ul>
<u>Kenneth T. Christensen</u> (40)	Prof. and Kritzer Faculty Scholar, Mechanical Science and Engineering, Aerospace Engineering and Geology Depts., University of Illinois, Associate Director of the I <sup>2</sup> CNER Satellite Institute	Ph.D., Theoretical and Applied Mechanics specializing in experimental fluid mechanics	20%	25%	35%	20%		2012, April.1 <sup>st</sup>	<ul style="list-style-type: none"> <li>• Primarily located at partner institution</li> <li>• Participates in research/events as Associate Director of the Illinois Satellite</li> <li>• Visited I<sup>2</sup>CNER for one week to participate in events and exchange opinions for collaboration</li> <li>• Discussion via Internet</li> </ul>	<ul style="list-style-type: none"> <li>• None besides what is mentioned on the left</li> </ul>
Shigenori Fujikawa (43)	Associate Prof., International Institute for Carbon-Neutral Energy Research, Kyushu University	Dr. of Eng., Nanoscience and engineering	100	0	0	0		2013, June.1 <sup>st</sup>	<ul style="list-style-type: none"> <li>• Located at I<sup>2</sup>CNER</li> <li>• Participates in research/events as Head of CO<sub>2</sub> Capture and Utilization Division</li> </ul>	
Takeshi Tsuji (34)	Associate Prof., International Institute for Carbon-Neutral Energy Research, Kyushu University	Dr. of Science, Earth and Planetary Science; Resource engineering; Space exploration	95	5	0	0		2013, June.1 <sup>st</sup>	<ul style="list-style-type: none"> <li>• Located at I<sup>2</sup>CNER</li> <li>• Participates in research/events as Head of CO<sub>2</sub> Storage Division</li> </ul>	

**Researchers unable to participate in project in FY 2013**

Name	Affiliation (Position title, department, organization)	Starting date of project participation	Reasons	Measures taken
Yukitaka Murakami	Prof., International Institute for Carbon-Neutral Energy Research, Kyushu University	2010, Dec.1 <sup>st</sup>	Resigned	
Saburo Matsuoka	Prof., Department of Mechanical Engineering, Kyushu University	2010, Dec.1 <sup>st</sup>	Retired	
Yoshinori Naruta	Prof., Institute for Materials chemistry and Engineering, Kyushu University	2010, Dec.1 <sup>st</sup>	Retired	
Masaki Minemoto	Prof., Department of Chemical Engineering, Kyushu University	2010, Dec.1 <sup>st</sup>	Retired	Shigenori Fujikawa was newly appointed as PI (as mentioned above)
Tetsuo Yanagi	Prof., Research Institute for Applied Mechanics, Kyushu University	2010, Dec.1 <sup>st</sup>	Retired	Takeshi Tsuji was newly appointed as PI (as mentioned above)
Kiminori Shitashima	Associate Prof., International Institute for Carbon-Neutral Energy Research, Kyushu University	2012, Jan.16 <sup>th</sup>	Appointment changed to WPI Associate Professor (following an annual review)	
Robert O. Ritchie	Prof., Department of Materials Science and Engineering, University of California, Berkeley	2010, Dec.1 <sup>st</sup>	Appointment changed to WPI Professor (following an annual review)	
Ludwig J. Gauckler	Prof., Department of Materials, Swiss Federal Institute of Technology	2010, Dec.1 <sup>st</sup>	Resigned	
Louis Schlapbach	Deputy Director-General, Global Research Center for Environment and Energy based on Nanomaterials Science, National Institute for Materials Science	2010, Dec.1 <sup>st</sup>	Appointment changed to WPI Visiting Professor (following an annual review)	
Ping Chen	Dalian Institute of Chemical Physics	2010, Dec.1 <sup>st</sup>	Appointment changed to WPI Professor (following an annual review)	

Chen-Tung Arthur Chen	National Sun Yat-sen University	2010, Dec.1 <sup>st</sup>	Appointment terminated (following an annual review)	
Angus Rockett	Prof., Materials Science & Engineering, University of Illinois	2012, April.1 <sup>st</sup>	Appointment changed to Satellite Faculty (following an annual review)	
Elif Ertekin	Assistant Prof., Department of Mechanical Science & Engineering, University of Illinois	2012, April.1 <sup>st</sup>	Appointment changed to Satellite Faculty (following an annual review)	
Lane W. Martin	Assistant Prof., Materials Science and Engineering, University of Illinois	2012, April.1 <sup>st</sup>	Appointment changed to Satellite Faculty (following an annual review)	
David Cahill	Prof., Department Head, Materials Science and Engineering, University of Illinois	2012, April.1 <sup>st</sup>	Appointment changed to Satellite Faculty (following an annual review)	
Thomas B. Rauchfuss	Prof., Department of Chemistry, University of Illinois	2012, April.1 <sup>st</sup>	Appointment changed to Satellite Faculty (following an annual review)	
Paul J.A. Kenis	Prof. and Head, Department of Chemical & Biomolecular Engineering, University of Illinois	2012, April.1 <sup>st</sup>	Appointment changed to Satellite Faculty (following an annual review)	
Dimitrios Kyritsis	Associate Prof., Department of Mechanical Science and Engineering, University of Illinois	2012, April.1 <sup>st</sup>	Appointment changed to Satellite Faculty (following an annual review)	
Robert J. Finley	Principal Geologist and Director, Advanced Energy Technology Initiative Illinois State Geological Survey, University of Illinois	2012, April.1 <sup>st</sup>	Appointment changed to Satellite Faculty (following an annual review)	
Arne J. Pearlstein	Prof., Mechanical Science and Engineering, University of Illinois	2012, April.1 <sup>st</sup>	Appointment changed to Satellite Faculty (following an annual review)	
James F. Stubbins	Prof. and Head, Department of Nuclear, Plasma and Radiological Engineering, University of Illinois	2012, April.1 <sup>st</sup>	Appointment changed to Satellite Faculty (following an annual review)	



## Biographical Sketch of a New Principal Investigator

Name (Age)	Shigenori Fujikawa (43)
<i>NOTE: Place an asterisk (*) by the name of investigators considered to be ranked among the world's top researchers.</i>	
Current affiliation (Position title, department, organization)	Associate Professor, International Institute for Carbon-Neutral Energy Research (I <sup>2</sup> CNER), Kyushu University
Academic degree, specialty	Dr. of Engineering, Nanoscience and Engineering
<p>Research and education history</p> <p>(Education)</p> <p>1999            Ph.D. Engineering, Kyushu University</p> <p>1996            M.S. Engineering, Kyushu University</p> <p>1994            B.S. Engineering, Kyushu University</p> <p>(Research)</p> <p>2011-present   Associate Professor, Lead Principal Investigator of the CO<sub>2</sub> Capture and Utilization Division (July 2013-present) International Institute for Carbon-Neutral Energy Research (I<sup>2</sup>CNER)</p> <p>2011-present   Visiting Principal Investigator, RIKEN (Saitama, Japan)</p> <p>2008-2012      Deputy of Laboratory Head (Principal Investigator) Interfacial Nanostructure Research Lab., Innovation center, RIKEN</p> <p>2008-2012      Adjunct Associate Professor Depart of electronic Chemistry, Tokyo Institute Technology (Kanagawa, Japan)</p> <p>2007-present   Partner, External Board Member NanoMembrane Technologies Inc. (Saitama, Japan)</p> <p>2007-2009      Team Leader (Principal Investigator) Nanocompartment Engineering Lab., Advanced Science Institute, RIKEN</p> <p>2004-2008      Deputy of Laboratory Head (Principal Investigator) Innovative Nanopatterning Research Lab., Frontier Research System, RIKEN</p> <p>2000-2007      Special Postdoctoral Researcher (2000-2004) Topochemical Design Laboratory, Frontier Research System, RIKEN</p> <p>1999-2000      Research Fellow of the Japan Society for the Promotion of Science Department of Chemistry, Yale University (Connecticut, USA)</p>	
<p>Achievements and highlights of past research activities</p> <p>(1) Development of free-standing nanomembranes for selective molecular transport. Membranes play an important role in industrial chemical purification and its important function is selective transportation of molecules and ions. Ultimate thinning of a membrane is a direct approach, we first developed free-standing membranes with only a few tens of nanometers in thickness. By designing the membrane materials, we have succeeded to introduce the selective filtration function to a membrane for precise transportation of small molecules and ions. (ex. <i>Langmuir</i> <b>2009</b>, 25, 19, 11563-11568)</p> <p>(2) Surface nanofabrication for the creation of a large scale array of metal nanostructures We have developed a novel nanofabrication process based on the achievements of nanometer-thick membranes. In this research direction, metallic nanostructure array with a high aspect ratio, such as nanofin, nanowire, and related structures exhibits unique behaviors. (ex. <i>Langmuir</i> <b>2006</b>, 22, 21, 9057-9061; <i>Nano Letters</i> <b>2011</b>, 11(1), 8-15; <i>Angew. Chem. Int. Ed.</i> <b>2014</b>, 53, 1, 127-131)</p>	

## Achievements

## (1) International influence

- a) *Guest speaker, chair, director, or honorary member of a major international academic society in the subject field,*
- b) *Holder of a prestigious lectureship,*
- c) *Member of a scholarly academy in a major country,*  
*American Chemical Society, The Chemical Society of Japan, The Society of Polymer Science, Japan, Material Research Society, The Japan Society of Applied Physics*
- d) *Recipient of an international award(s) ,*
1. *The Nanofabrication Technology award of International Nanotechnology Exhibition and Conference, 2007*
  2. *Gordon Bell Prize Honorable Mention, Peak Performance, "A 185 Tflop/s Simulation of Amyloid-forming Peptides from Yeast Prion Sup35 with the Special-purpose Computer System MD-GRAPE2" in US Supercomputing Conference, 2006*
- e) *Editor of an influential journal, etc.*

## (2) Receipt of large-scale competitive fundings (over past 5 years)

(2013)

1. Hitachi collaboration fund, 2,100,000 JPY, 2013/6-2014/3, 2013
2. MEXT, Grant-in-Aid for Scientific Research on Innovative Areas (2010-2015), 5,710,000 JPY (for 2013), 2012/4-2015/3,2010
3. JST, ACT-C, 5,700,000 JPY (for 2013), 2012/10-2017/3, 2012
4. JST, ALCA, 2,000,000 JPY (for 2013), 2013/10-2018/3, 2013

(2012)

5. JST, ACT-C, 5,700,000 JPY (for 2012), 2012/10-2017/3, 2012
6. Hitachi collaboration fund, 2,100,000 JPY, 2012/6-2013/3, 2012
7. MEXT, Grant-in-Aid for Scientific Research on Innovative Areas (2010-2015), 6,000,000 JPY (for 2012), 2012/4-2013/3,2010
8. JST, CREST,1,700,000 (for 2012), 2007/10-2013/3, 2007

(2011)

9. MEXT, Grant-in-Aid for Scientific Research on Innovative Areas (2010-2015), 8,200,000 JPY (for 2012), 2012/4-2013/3,2010
10. JST, CREST,7,000,000 (for 2011), 2007/10-2013/3, 2007

(2010)

11. MEXT, Grant-in-Aid for Scientific Research on Innovative Areas (2010-2015), 9,200,000 JPY (for 2012), 2012/4-2013/3,2010
12. JST, CREST,7,000,000 (for 2010), 2007/10-2013/3, 2007

(2009)

13. JST, CREST,7,000,000 (for 2009), 2007/10-2013/3, 2007

## (3) Article citations (Titles of major publications, and number of citations.)

1. Hybrid of Palladium Nanoparticles and Silicon Nanowire Array: A Platform for Catalytic Heterogeneous Reactions  
Y. M.A. Yamada, Y. Yuyama, T. Sato, S. Fujikawa, Y. Uozumi,  
*Angew. Chem. Int. Ed.* 2013, accepted (0 citations)
2. o-Phenylene Octamers as Surface Modifiers for Homeotropic Columnar Ordering of Discotic Liquid Crystals.  
T. Kajitani, Y. Suna, A. Kosaka, T. Osawa, S. Fujikawa, M. Takata, T. Fukushima, T. Aida.  
*J. Am. Chem. Soc.* 2013, 135 (39), 14564–14567 (0 citations)

3. Molecular Insight into Different Denaturing Efficiency of Urea, Guanidinium, and Methanol: A Comparative Simulation Study.  
T. Koishi, K. Yasuoka, S. Y. Willow, S. Fujikawa, X. C. Zeng  
*J. Chem. Theory and Comp.* 2013, 9(6), 2540-2551. (2 citations)
4. Sensitivity to refractive index of high-aspect-ratio nanofins with optical vortex  
E. Maeda, Y. Lee, Y. Kobayashi, A. Taino, M. Koizumi, S. Fujikawa, J.-J. Delaunay  
*Nanotechnology* 2012, 23(50), 505502 (1 citations)
5. Enzymatic direct electron transfer at ascorbate oxidase-modified gold electrode prepared by one-step galvanostatic method,  
B. Patil, S. Fujikawa, T. Okajima, T. Ohsaka, Takeo,  
*Int. J. Electrochem. Sci.* 2012, 7(6), 5012-5019 (2 citations)
6. Controlled polymerization and self-assembly of halogen-bridged diruthenium complexes in organic media and their dielectrophoretic alignment  
R. Kuwahara, S. Fujikawa, K. Kuroiwa, N. Kimizuka  
*J. Am. Chem. Soc.* 2012, 134(2), 1192-1199 (6 citations)
7. Measurement of Contact-Angle Hysteresis for Droplets on Nanopillared Surface and in the Cassie and Wenzel States: A Molecular Dynamics Simulation Study  
T. Koishi, K. Yasuoka, S. Fujikawa, X. C. Zeng,  
*ACS Nano* 2011, 5(9), 6834-6842. (16 citations)
8. Au double nanopillars with nanogap for plasmonic sensor  
W. Kubo, S. Fujikawa\*  
*Nano Letters* 2011, 11(1), 8-15 (36 citations)
9. Size-controlled simple fabrication of Free-standing, ultralong metal nanobelt array  
W. Kubo, H. Hayakawa, K. Miyoshi, S. Fujikawa\*  
*J. Nanosci. Nanotech* 2011, 11(1), 131-137 (2 citations)
10. Molecular dynamics simulations of urea-water binary droplets on flat and pillared hydrophobic surfaces.  
T. Koishi, K. Yasuoka, X.-C. Zeng, S. Fujikawa  
*Faraday Discuss.* 2010, 146, 185-193 (9 citations)
11. Manipulation of a one dimensional molecular assembly of helical superstructures by dielectrophoresis.  
W. Kubo, S. Fujikawa\*  
*Appl. Phys. Lett.* 2009, 95, 16, 163110/1-163110/3 (0 citations)
12. Coexistence and transition between Cassie and Wenzel state on pillared hydrophobic surface.  
T. Koishi, K. Yasuoka, S. Fujikawa, T. Ebisuzaki X.-C. Zeng  
*Proc. Natl. Acad. Sci. U. S. A.* 2009, 106, 21, 8435-8440 (77 citations)
13. Nanochannel Design by Molecular Imprinting on a Free-Standing Ultrathin Titania Membrane.  
S. Fujikawa,\* E. Muto, T. Kunitake  
*Langmuir* 2009, 25, 19, 11563-11568 (7 citations)
14. Embedding of a gold nanofin array in a polymer film to create transparent, flexible and anisotropic electrodes.  
W. Kubo, S. Fujikawa\*  
*J. Mater. Chem.* 2009, 19, 15, 2154-2158 (6 citations)
15. Fabrication of nanoline arrays of noble metals by electroless plating and selective etching process.  
K. Miyoshi, S. Fujikawa,\* T. Kunitake  
*Colloids Surf., A* 2008, 321, 1-3, 238-243 (5 citations)
16. Fabrication of nanofins of TiO<sub>2</sub> and other metal oxides via the surface sol-gel process and selective dry etching.  
R. Takaki, H. Takemoto, S. Fujikawa,\* T. Kunitake  
*Colloids Surf., A* 2008, 321, 1-3, 227-232 (2 citations)

17. Facile Fabrication of Silver Nanofin Array via Electroless Plating.  
K. Miyoshi, Y. Aoki, T. Kunitake, S. Fujikawa\*  
*Langmuir* 2008, 24, 8, 4205-4208 (12 citations)
18. Photoluminescence Modification in 3D-Ordered Films of Fluorescent Microspheres.  
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*Langmuir* 2007, 23, 17, 9109-9113 (18 citations)
19. Rapid fabrication of a smooth hollow-spheres array.  
S. Matsushita, S. Fujikawa, S. Onoue, T. Kunitake, M. Shimomura  
*Bull. Chem. Soc. Jpn.* 2007, 80, 6, 1226-1228 (6 citations)
20. Embedding of Individual Ferritin Molecules in Large, Self-Supporting Silica Nanofilms.  
S. Fujikawa,\* E. Muto, T. Kunitake  
*Langmuir* 2007, 23, 8, 4629-4633 (6 citations)
21. Fabrication of Arrays of Sub-20-nm Silica Walls via Photolithography and Solution-Based Molecular Coating.  
S. Fujikawa,\* R. Takaki, T. Kunitake  
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22. Efficient Fabrication and Enhanced Photocatalytic Activities of 3D-Ordered Films of Titania Hollow Spheres.  
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23. Efficient fabrication of large, robust films of 3D-ordered polystyrene latex.  
Y. Li, T. Kunitake, S. Fujikawa, K. Ozasa  
*Colloids Surf., A* 2006, 275, 1-3, 209-217 (8 citations)
24. 3D nanoarchitecture from ultrathin titania film via surface sol-gel process and photolithography.  
S. Fujikawa, T. Kunitake  
*Chem. Lett.* 2005, 34, 10, 1414-1415 (1 citations)
25. Nanocopying of Individual DNA Strands and Formation of the Corresponding Surface Pattern of Titania Nanotube.  
S. Fujikawa,\* R. Takaki, T. Kunitake  
*Langmuir* 2005, 21, 19, 8899-8904 (16 citations)
26. Preparation of hollow structures composed of titania nanocrystal assembly.  
S. Fujikawa, T. Kunitake  
*Int. J. Nanosci.* 2002, 1, 5 & 6, 617-620 (1 citations)
27. Synthesis of metal and metal oxide nanoparticles in the nanospace of ultrathin TiO<sub>2</sub>-gel films: role of the ion-exchange site.  
J. He, I. Ichinose, S. Fujikawa, T. Kunitake  
*Int. J. Nanosci.* 2002, 1, 5 & 6, 507-513 (0 citations)
28. Nanocopying as a Means of 3D Nanofabrication: Scope and Prospects.  
T. Kunitake, S. Fujikawa  
*Aust. J. Chem.* 2003, 56, 10, 1001-1003 (8 citations)
29. Preparation of Porous and Nonporous Silica Nanofilms from Aqueous Sodium Silicate.  
J. He, I. Ichinose, S. Fujikawa, T. Kunitake, A. Nakao  
*Chem. Mater.* 2003, 15, 17, 3308-3313 (19 citations)
30. Surface Fabrication of Hollow Nanoarchitectures of Ultrathin Titania Layers from Assembled Latex Particles and Tobacco Mosaic Viruses as Templates.  
S. Fujikawa, T. Kunitake  
*Langmuir* 2003, 19, 16, 6545-6552 (58 citations)

31. Surface fabrication of interconnected hollow spheres of nm-thick titania shell.  
S. Fujikawa, T. Kunitake  
*Chem. Lett.* 2002, 11, 1134-1135 (8 citations)
32. Reversible conversion of nanoparticles of metallic silver and silver oxide in ultrathin TiO<sub>2</sub> films: a chemical transformation in nano-space.  
J. He, I. Ichinose, S. Fujikawa, T. Kunitake, A. Nakao  
*Chem. Commun.* 2002, 17, 1910-1911 (27 citations)
33. A General, Efficient Method of Incorporation of Metal Ions into Ultrathin TiO<sub>2</sub> Films.  
J. He, I. Ichinose, S. Fujikawa, T. Kunitake, A. Nakao  
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34. Ultrathin composite films: An indispensable resource for nanotechnology.  
Ichinose, J. He, S. Fujikawa, M. Hashizume, J. Huang, T. Kunitake  
*RIKEN Rev.* 2001, 37, 34-37 (2 citations)
35. Organization of hydrophilic nanoparticles on a hydrogel surface and their gel-assisted transfer to solid substrates.  
N. Kimizuka, S. Fujikawa, T. Kunitake  
*Adv. Mater.* 1998, 10, 16, 1373-1376 (3 citations)
36. AFM observation of organogel nanostructures on graphite in the gel-assisted transfer technique.  
N. Kimizuka, M. Shimizu, S. Fujikawa, K. Fujimura, M. Sano, T. Kunitake  
*Chem. Lett.* 1998, 10, 967-968 (16 citations)
37. Protein assembly on solid surfaces by gel-assisted transfer (GAT) technique.  
N. Kimizuka, S. Fujikawa, T. Kunitake  
*Chem. Lett.* 1998, 8, 821-822 (2 citations)
38. Mesoscopic supramolecular assembly of a 'Janus' molecule and a melamine derivative via complementary hydrogen bonds.  
N. Kimizuka, S. Fujikawa, H. Kuwahara, T. Kunitake, A. Marsh and J.-M. Lehn  
*J. Chem. Soc., Chem. Commun.* 1995, 20, 2103-4 (52 citations)

(4) Others (*Other achievements that indicate qualification as a top-caliber researcher, if any.*)

## Biographical Sketch of a New Principal Investigator

Name (Age)	Takeshi Tsuji (34)
<i>NOTE: Place an asterisk (*) by the name of investigators considered to be ranked among the world's top researchers.</i>	
Current affiliation (Position title, department, organization)	Associate Professor, International Institute for Carbon-Neutral Energy Research (I <sup>2</sup> CNER), Kyushu University
Academic degree, specialty	Dr of Science, Earth and Planetary Science
<p>Research and education history</p> <p>(Education)</p> <p>2007 Ph.D. Earth and Planetary Science, the University of Tokyo</p> <p>2004 M.S. Earth and Planetary Science, the University of Tokyo</p> <p>2002 B.S. Resources and Environmental Engineering, Waseda University</p> <p>(Research)</p> <p>2013-present Lead Principal Investigator of the CO<sub>2</sub> Storage Division, Associate Professor (2012-present), International Institute for Carbon-Neutral Energy Research (I<sup>2</sup>CNER)</p> <p>2013 Senior Visiting Scientist, Japan Agency for Marine-Earth Science and Technology (JAMSTEC)</p> <p>2011-2012 Pre-Project Scientist, Japan Aerospace Exploration Agency (JAXA)</p> <p>2008-2012 Visiting Lecturer, Kansai University</p> <p>2007-2012 Assistant Professor, Graduate School of Engineering, Kyoto University</p> <p>2007-2012 Visiting Scientist, Japan Agency for Marine-Earth Science and Technology (JAMSTEC)</p> <p>2010-2011 Visiting Scholar, Department of Geophysics, Stanford University</p> <p>2010 Co-Chief Scientist, Integrated Ocean Drilling Program (IODP) Expedition 327, Juan de Fuca hydrology</p> <p>2009 Committee member, Research Institute for of Innovative Technology for the Earth (RITE)</p> <p>2007 Postdoctoral Research Associate, Institute for Frontier Research on Earth Evolution, Japan Agency for Marine-Earth Science and Technology (JAMSTEC)</p> <p>2004-2007 JOI Alliance/Lamont-Doherty Earth Observatory Logging Staff Scientist</p> <p>2006-2007 Japan Society for the Promotion of Science Research Fellow (DC)</p>	
<p>Achievements and highlights of past research activities <i>(Describe qualifications as a top-caliber researcher if he/she is considered to be ranked among the world's top researchers.)</i></p> <ul style="list-style-type: none"> <li>Selected as co-chief scientist of International drilling project “Integrated Ocean Drilling Program (IODP)” and led twenty of international scientists in the drilling cruise. This program is mainly funded by NSF and MEXT.</li> </ul>	

## Achievements

## (1) International influence

a) Guest speaker, chair, director, or honorary member of a major international academic society in the subject field,

b) Holder of a prestigious lectureship,

- Lecturer in CCOP CO<sub>2</sub> Storage Mapping Program (CCSM) Seminar, March 18, 2014.
- Lecturer in Nagoya University, November 1, 2013.
- Lecturer in University of Tokyo, September 27, 2013.
- Lecturer in University of Tokyo, May 27, 2013.
- Lecturer in Ritsumeikan University, July 19, 2012.
- Lecture in JAMSTEC, November 30, 2011.
- Lecture in JOGMEC, November 9, 2011.
- University of California (UCSC; Whole Earth Seminar), October 26, 2010.

c) Member of a scholarly academy in a major country,

d) Recipient of an international award(s) ,

e) Editor of an influential journal, etc.

## (2) Receipt of large-scale competitive fundings (over past 5 years)

1. Collaborative research with RITE, "Development of water-alternating-gas technology using microbubble CO<sub>2</sub> injection, Principal-Investigator, US\$20,000 (JPN¥2,000,000) in FY2013, 2013.
2. Japan Science and Technology Agency (JST), SATREPS, "Pilot study for Carbon Sequestration and Monitoring in Gundih Area – Central Java Province, Indonesia", Co-Investigator, US\$39,000 (JPN¥3,900,000) in FY2013, 2013-2015.
3. Collaborative research with Fukada Geological Institute, "Fault evaluation for CO<sub>2</sub> storage", Principal-Investigator, US\$25,800 (JPN¥2,580,000) in FY2013, 2013.
4. Collaborative research with Shikoku Research Institute. Inc., "Deep geological structures around the Median Tectonic Line revealed by PS logging data and seismic data", Principal-Investigator, US\$6,000 (JPN¥600,000) in FY2013, 2013.
5. Grant-in-Aid for Scientific Research on Innovative Areas (MEXT), "New perspective of great subduction-zone earthquakes from the super deep drilling", Co-Investigator, US\$13,000 (JPN ¥1,300,000) in FY2013, 2009-2013.
6. The Sumitomo Foundation, "Seismic monitoring for renewable CCS in subseafloor lignite coal layers", Principal Investigator, US\$20,000 (JPN¥2,000,000) in FY2013, 2012-2013, 2012.
7. Grant-in-Aid for Scientific Research from Japan Society for the Promotion of Science (KAKENHI) Kiban (A), "Development of technology for enhanced oil recovery based on NanoGeoscience" (PI: T. Matsuoka), Co-Investigator, US\$3,000 (JPN¥300,000) in FY2013, 2012-2016.
8. Grant-in-Aid for Scientific Research from Japan Society for the Promotion of Science (KAKENHI) Kiban (C), "Analysis of stress heterogeneity for identification of the unrevealed active faults" (PI: Y. Yamada), Co-Investigator, US\$2,000 (JPN¥200,000) in FY2013, 2012-2015.
9. Collaborative research with Shikoku Research Institute. Inc., "Research on subsurface structure of median tectonic line in Shikoku (Core-Log-Seismic integration)", 2012, Principal-Investigator, US\$5,500 (JPN¥550,000).
10. Research grant for IODP co-chief scientist, "Juan de Fuca Ridge-flank hydrogeology: the hydrogeologic architecture of basaltic oceanic crust: compartmentalization, anisotropy, microbiology, and crustal-scale properties on the eastern flank of Juan de Fuca Ridge, eastern Pacific Ocean", 2011-2012, Principal-Investigator, US\$15,000 (JPN¥1,500,000).
11. JOGMEC Development of Innovative Techniques in oil-gas fields, "Development of wireless, multi-channel, multi-component seismometer network for 4D seismological monitoring", (PI: Suncoh consultant), 2012, Co-Investigator, US\$4,000 (JPN ¥400,000).
12. Collaborative research with Shikoku Research Institute. Inc., "Research on subsurface structure of median tectonic line in Shikoku (Core-Log-Seismic integration)", 2011, Principal-Investigator, US\$10,000 (JPN ¥1,000,000).
13. Collaborative research with Shikoku Research Institute. Inc., "Research on subsurface structure of median tectonic line in Shikoku (Common Reflection Stack analysis for seismic reflection data)", 2010, Principal-Investigator, US\$10,000 (JPN¥1,000,000).
14. Grant-in-Aid for Scientific Research on Innovative Areas (MEXT) "Structure of oceanic crust and its properties revealed by seismic reflection method: Insight into subseafloor hydrothermal fluid circulation", 2009-2010, Principal-Investigator, US\$42,000 (JPN¥4,200,000).

15. Grant-in-Aid for Scientific Research from Japan Society for the Promotion of Science Kiban (B), "Characterization of seismic velocity and evolution of rock properties in the plate convergent margin", 2009 – 2011, Co-Investigator, US\$10,000 (JPN¥1,000,000).
16. Collaborative research with Shikoku Research Institute. Inc., "Research on subsurface structure of median tectonic line in Shikoku (Seismic attribute analysis for seismic reflection data)", 2009, Principal-Investigator, US\$20,000 (JPN ¥2,000,000).
17. Global COE, Project for young researcher/student, "Research and education project on active fault evaluation to mitigate earthquake/tsunami disasters at Indonesian mega-cities", 2008-2012, Principal-Investigator, US\$25,000 (JPN¥2,500,000).
18. Grant-in-Aid for Scientific Research from Japan Society for the Promotion of Science Kiban (B), "Reservoir characteristics and evaluation technique of CO<sub>2</sub> in aquifer", 2008-2010, Co-Investigator, US\$8,500 (JPN¥850,000).
19. Grant-in-Aid for scientific research from Japan Society for the Promotion of Science, "Development of a method to estimate underground stress state using rock physics theory", 2008-2009, Principal-Investigator, US\$42,900 (JPN¥4,290,000).

(3) Article citations (*Titles of major publications, and number of citations.*)

(2014)

1. K. Ishitsuka, Y. Fukushima, T. Tsuji, Y. Yamada, T. Matsuoka and P.H. Giao, Natural surface rebound of the Bangkok plain and aquifer characterization by persistent scatterer interferometry, *Geochemistry, Geophysics, Geosystems*, doi: 10.1002/2013GC005154, 2014.
2. R. Kamei, G. Pratt, and T. Tsuji, Misfit function in Laplace-Fourier domain waveform inversion, with application to wide-angle Ocean Bottom Seismograph data, *Geophysical Prospecting*, 2013, in press.
3. A. Miyakawa, S. Saito, Y. Yamada, H. Tomaru, M. Kinoshita, and T. Tsuji, Gas hydrate saturation at Site C0002 of IODP Expeditions 314 and 315 in the Kumano Basin, Nankai Trough, *Island Arc*, 2014, in press.
4. Y. Shigei, T. Tsuji, T. Matsuoka, M. Ikeda, N. Nishizaka, and Y. Ishikawa, Seismic-derived quality factor for lithology classification around the Median Tectonic Line, *JSMS journal*, 63, 250-257, 2014.
5. J. Ishibashi, F. Ikegami, T. Tsuji, and T. Urabe, Hydrothermal activity in the Okinawa Trough back-arc basin - geological background and hydrothermal mineralization -, Subseafloor Biosphere Linked to Global Hydrothermal Systems; TAIGA Concept, *Springer Japan*, 2014, in press.
6. F. Ikegami, T. Tsuji, H. Kumagai, J. Ishibashi and K. Takai, Active rifting structures in Iheya Graben and adjacent area of the mid-Okinawa Trough observed through seismic reflection surveys, Subseafloor Biosphere Linked to Global Hydrothermal Systems; TAIGA Concept, *Springer Japan*, 2014. In press.

(2013)

7. T. Tsuji, K. Kawamura, T. Kanamatsu, T. Kasaya, K. Fujikura, Y. Ito, T. Tsuru, and M. Kinoshita, 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, *Earth and Planetary Science Letters*, 364, 44-58, 2013. (3 citations)
8. T. Ikeda, T. Tsuji, and T. Matsuoka, Window-controlled CMP cross-correlation analysis for surface waves on laterally heterogeneous media, *Geophysics*, 78, EN95-EN105, 2013. (0 citation)
9. Y. Yamada, R. Masui, and T. Tsuji, Characteristics of a tsunamigenic megasplay fault in the Nankai Trough, *Geophysical Research Letters*, 40, 4594-4598, 2013. (0 citation)
10. K. Becker, A.T. Fisher, and T. Tsuji, New Packer Experiments and Borehole Logs in Upper Oceanic Crust: Evidence for Ridge-parallel Continuity in Crustal Hydrogeological Properties, *Geochemistry, Geophysics, Geosystems*, 14, 2013. (1 citation)
11. R. Kamei, G. Pratt, T. Tsuji, On acoustic waveform tomography of wide-angle OBS data - Strategies for preconditioning and inversion, *Geophysical Journal International*, 194, 1250-1280, 2013. (1 citation)
12. S. Minato, T. Matsuoka, T. Tsuji, Singular-value decomposition analysis of source illumination in seismic interferometry by multidimensional deconvolution, *GEOPHYSICS*, 78, Q25-Q34, 2013. (1 citation)
13. M.Y.N. Khakim, T. Tsuji, and T. Matsuoka, Detection of Localized Surface Heave at Oil Sands Field by Differential SAR Interferometry, *IEEE Journal of Selected Topics in Applied Earth Observations and Remote Sensing*, 99, 1-11, 2013. (1 citation)
14. T. Tsuji, S. Kodaria, J. Ashi, and J-O. Park, Widely distributed thrust and strike-slip faults within subducting oceanic crust in the Nankai Trough off the Kii Peninsula, Japan, *Tectonophysics*, 600,



- 52-62, 2013. (1 citation)
15. Y. Hashimoto, N. Doi, and T. Tsuji, Difference in acoustic properties at seismogenic fault along a subduction interface: Application to estimation of effective pressure and fluid pressure ratio, *Tectonophysics*, 600, 134-141, 2013. (0 citation)
  16. K. Ishitsuka, T. Tsuji, and T. Matsuoka, Improved correlation analysis to detect liquefied area using multi-temporal SAR images -Application to the 2011 Tohoku Earthquake and the 2011 Christchurch Earthquake-, *Exploration Geophysics*, 66, 1, 25-33, 2013. (0 citation)
  17. S. Chiyonobu, T. Nakajima, Y. Zhang, T. Tsuji, and Z. Xue, Effect of reservoir heterogeneity of Haizume Formation, Nagaoka Pilot Site, based on high-resolution sedimentological analysis, *Energy Procedia*, 37, 3546-3553, doi: 10.1016/j.egypro.2013.06.247, 2013. (2 citations)
- (2012)
18. G. Kimura, S. Hina, Y. Hamada, J. Kameda, T. Tsuji, M. Kinoshita, and A. Yamaguchi, Runaway slip to the trench due to rupture of highly pressurized megathrust beneath the middle trench slope: The tsunamigenesis of the 2011 Tohoku earthquake off the east coast of northern Japan, *Earth and Planetary Science Letters*, 339-340, 32-45, 2012. (12 citations)
  19. K. Ishitsuka, T. Tsuji, and T. Matsuoka, Detection and mapping of soil liquefaction associated with the 2011 Tohoku earthquake using SAR Interferometry, *Earth Planets and Space*, 64, 1267-1276, 2012. (1 citation)
  20. M.Y.N. Khakim, T. Tsuji, and T. Matsuoka, Geomechanical Modeling for InSAR-derived surface deformation at steam-injection oil sand fields, *Journal of Petroleum Science and Engineering*, 96-97, 152-161, doi:10.1016/j.petrol.2012.08.003, 2012. (0 citation)
  21. Y. Ito, R. Hino, M. Kido, H. Fujimoto, Y. Osada, D. Inazu, Y. Ohta, T. Inuma, M. Ohzono, S. Miura, M. Mishina, K. Suzuki, T. Tsuji, and J. Ashi, Episodic slow slip events in the Japan subduction zone before the 2011 Tohoku-Oki earthquake, *Tectonophysics*, doi:10.1016/j.tecto.2012.08.022, 2012. (14 citations)
  22. S. Minato, T. Tsuji, T. Matsuoka, and K. Obana, 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, Article ID 101545, doi:10.1155/2012/101545, 2012. (2 citations)
  23. T. Ikeda, T. Matsuoka, T. Tsuji, and K. Hayashi, Multi-mode inversion with amplitude response of surface waves in the spatial autocorrelation method, *Geophysical Journal International*, 190, 541-552, 2012. (2 citations)
  24. S. Minato, T. Tsuji, S. Ohmi, and T. Matsuoka, Monitoring seismic velocity change caused by the 2011 Tohoku-oki earthquake using ambient noise records, *Geophysical Research Letters*, 39, L09309, 2012. (7 citations)
  25. A.T. Fisher, T. Tsuji, K. Petronotis, C.G. Wheat, K. Becker, J.F. Clark, J. Cowen, K. Edwards, H. Jannasch, and the IODP Expedition 327 and Atlantis Expedition AT18-07 Shipboard Parties, IODP Expedition 327 and Atlantis Expedition AT 18-07: Observatories and Experiments on the Eastern Flank of the Juan de Fuca Ridge, *Scientific Drilling*, 13, 4-11, ISSN: 1816-8957, 2012. (1 citation)
  26. T. Tsuji, T.A. Johansen, B.O. Ruud, T. Ikeda, and T. Matsuoka, Surface-wave analysis for identifying unfrozen zones in subglacial sediments, *Geophysics*, 77, 3, EN17-EN27, 2012. (3 citations)
  27. K. Ishitsuka, T. Tsuji, T. Matsuoka, T. Mizuno, Surface displacement induced by liquefaction of the 2011 Tohoku-Oki earthquake in Tokyo bay area using INSAR analysis, *JSCE journal*, 68,1,175-182, 2012. (0 citation)
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  29. T. Tsuji, K. Takai, H. Oiwane, Y. Nakamura, Y. Masaki, H. Kumagai, M. Kinoshita, F. Yamamoto, T. Okano, and S. Kuramoto, Hydrothermal fluid flow system around the Iheya North Knoll in the mid-Okinawa Trough based on seismic reflection data, *Journal of Volcanology and Geothermal Research*, 213-214, 41-50, 2012. (5 citations)
  30. R. Kamei, R.G. Pratt, and T. Tsuji, Waveform Tomography Imaging of a Megasplay Fault System in the Seismogenic Nankai Subduction Zone, *Earth and Planetary Science Letters (Elsevier)*, 317-318, 1, 343-353, 2012. (12 citations)
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31. T. Tsuji, R. Hino, Y. Sanada, K. Yamamoto, J.-O. Park, T. No, E. Araki, N. Bangs, R. von Huene, G. Moore, and M. Kinoshita, In situ stress state from walkaround VSP anisotropy in the Kumano basin southeast of the Kii Peninsula, Japan, *Gechem. Geophys. Geosyst.*, 12, Q0AD19,

- doi:10.1029/2011GC003583, 2011. (2 citations)
32. N. Nakata, R. Snieder, T. Tsuji, K. Larner, and T. Matsuoka, Shear-wave imaging from traffic noise using seismic interferometry by cross-coherence, *Geophysics*, 76, SA97-SA106, 2011. (7 citations)
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  34. T. Tsuji, Y. Ito, M. Kido, Y. Osada, H. Fujimoto, J. Ashi, M. Kinoshita, and T. Matsuoka, Potential Tsunamigenic Faults of the 2011 Tohoku Earthquake, *Earth Planets and Space*, 63, 831-834, 2011. (21 citations)
  35. T. Ikeda, T. Matsuoka, T. Tsuji, K. Hayashi, Spatial auto-correlation (SPAC) method for higher modes considering different correlation distance, *Butsuri-tansa*, 64, 127-138, 2011. (0 citation)
  36. T. Tsuji, et al., Vp/Vs ratio and seismic anisotropy in the Nankai Trough seismogenic zone: Insights into effective stress, pore pressure and sediment consolidation, *Geophysics*, 76, No.3, WA71-WA82, 2011. (4 citations)
  37. S. Minato, T. Matsuoka, T. Tsuji, D. Draganov, J. Hunziker, and K. Wapenaar, Seismic interferometry using multidimensional deconvolution and crosscorrelation for crosswell seismic reflection data without borehole sources, *Geophysics*, 76, SA19-SA34. (1st author is my supervised student), 2011. (16 citations)
  38. N. Nakata, T. Tsuji, and T. Matsuoka, Acceleration of computation speed for elastic wave simulation using graphic processing unit, *Exploration Geophysics*, 42, 98-104, 2011. (3 citations)  
(2010)
  39. H. Kumagai, S. Tsukioka, H. Yamamoto, T. Tsuji, K. Shitashima, M. Asada, F. Yamamoto, and M. Kinoshita, Hydrothermal plumes imaged by high-resolution side-scan sonar on a cruising AUV, Urashima, *Geochem. Geophys. Geosyst.*, 11, Q12013, doi:10.1029/2010GC003337, 2010. (8 citations)
  40. T. Tsuji, H. Yamaguchi, T. Ishii, and T. Matsuoka, Mineral Classification from Quantitative X-ray Maps using Neural Network: Application to Volcanic Rocks, *Island Arc*, 19, 105-119, 2010. (3 citations)
  41. A. Miyakawa, T. Tsuji, T. Matsuoka, T. Yamamoto, Self-organizing maps classification of soil properties in levee using different geophysical data, *JSCE journal*, 66, 89-99, 2010. (1 citation)  
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  43. T. Tsuji, J-O. Park, G. Moore, S. Kodaira, Y. Fukao, S. Kuramoto, and N. Bangs, Intraoceanic Thrusts in the Nankai Trough off the Kii Peninsula: Implications for Intraplate Earthquakes, *Geophysical Research Letters*, 36, L06303, doi:10.1029/2008GL036974, 2009. (8 citations)
  44. G. Moore, J-O. Park, N.L. Bangs, S.P. Gulick, H.J. Tobin, Y. Nakamura, S. Sato, T. Tsuji, T. Yoro, H. Tanaka, S. Uraki, Y. Kido, Y. Sanada, S. Kuramoto, and A. Taira, Structural and seismic stratigraphic framework of the NanTroSEIZE Stage 1 transect Proc. IODP, 314-315-316: College Station, TX, doi:10.2204/iodp.proc.314315316.102.2009, 2009. (98 citations)
  45. T. Tsuji, K. Yamamoto, Y. Yamada, T. Matsuoka, and T. Asakura, Damage mechanisms of mountain tunnels in the 2007 Niigata Chuetsu-oki earthquake: Insight from SAR interferometry, *JSCE journal*, Vol. 65, No. 4, pp.989-997, 2009. (1 citation)
  46. S. Minato, T. Tsuji, T. Noguchi, K. Shiraishi, T. Matsuoka, Y. Fukao, and G. Moore, Estimation of detailed temperature distribution of sea water using seismic oceanography, *Butsuri-tansa*, 62, 509-520, 2009. (0 citation)  
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  47. T. Tsuji, H. Tokuyama, P. Costa Pisani, and G. Moore, Effective stress and pore pressure in the Nankai accretionary prism off the Muroto Peninsula, southwestern Japan, *Journal of Geophysical Research – Solid Earth*, 113, B11401, doi:10.1029/2007JB005002, 2008. (27 citations)
  48. T. Tsuji, and G. J. Iurrino, Velocity-porosity relationships of oceanic basalt from eastern flank of the Juan de Fuca ridge: The effect of crack closure on seismic velocity, *Exploration Geophysics*, 39, 41-51, 2008. (8 citations)  
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  49. T. Tsuji, Y. Nakamura, H. Tokuyama, M. F. Coffin, K. Koda, Oceanic crust and Moho of the Pacific Plate in the eastern Ogasawara Plateau region, *Island Arc*, 16, 361-373, 2007. (7 citations)  
(2006)

50. Y. Nakamura, T. Noguchi, T. Tsuji, S. Ito, H. Niino, T. Matsuoka, Simultaneous seismic reflection and physical oceanographic observations of oceanic finestructure in the Kuroshio extension front, *Geophysical Research Letters*, 33, L23605, doi:10.1029/2006GL027437 (I analyzed the seismic data), 2006. (40 citations)
51. T. Tsuji, G. Kimura, S. Okamoto, F. Kono, H. Mochinaga, T. Saeki, H. Tokuyama, Modern and ancient seismogenic out-of-sequence thrusts in the Nankai accretionary prism: Comparison of laboratory-derived physical properties and seismic reflection data, *Geophysical Research Letters*, 33, L18309, doi:10.1029/2006GL027025, 2006. (10 citations)  
(2005)
52. T. Tsuji, T. Noguchi, H. Niino, T. Matsuoka, Y. Nakamura, H. Tokuyama, S. Kuramoto, N. Bangs, Two-dimensional mapping of finestructures in the Kuroshio Current using seismic reflection data, *Geophysical Research Letters*, 32, L14609, doi:10.1029/2005GL023095, 2005. (34 citations)
53. T. Tsuji, T. Matsuoka, Y. Yamada, Y. Nakamura, J. Ashi, H. Tokuyama, S. Kuramoto, N. Bangs, Initiation of plate boundary slip in the Nankai Trough off the Muroto peninsula, southwest Japan, *Geophysical Research Letters*, 32, L12306, doi:10.1029/2004GL021861, 2005. (15 citations)

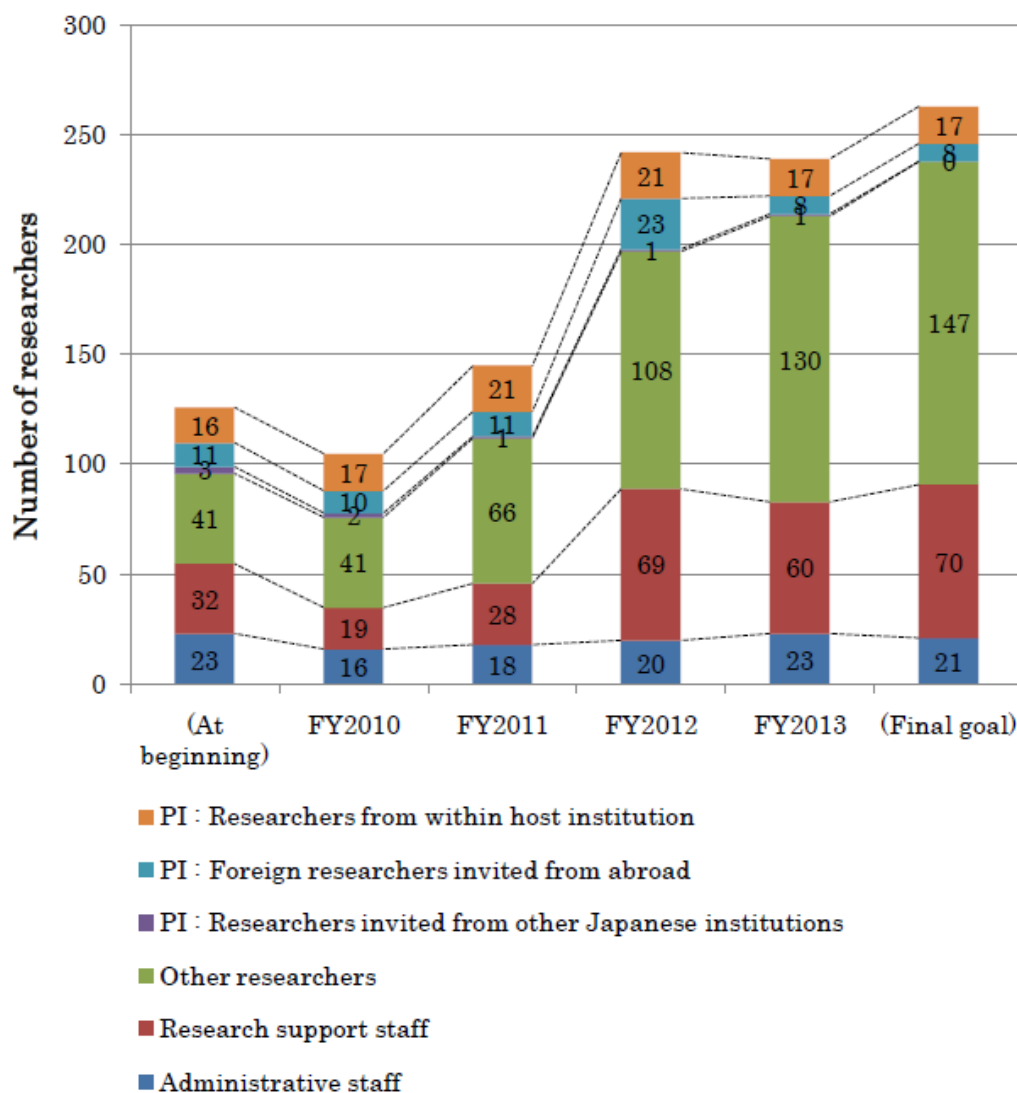
(4) Others (*Other achievements that indicate qualification as a top-caliber researcher, if any.*)

1. Tsuji invited >20 lectures or presentations.
2. Tsuji reviewed many journals including NatureGeoscience as well as NSF research proposal.
3. Tsuji is committee member of evaluation of geological formation for new CO<sub>2</sub> storage sites around Japanese Island, Japan CCS Corporation supported by METI, 2013.
4. Tsuji received four awards from Society of Exploration Geophysics of Japan.

## 2. Number of researchers in the "core" established within the host institution

All members:

\*Make a graph of the annual transition in the number of center personnel since the start of project.



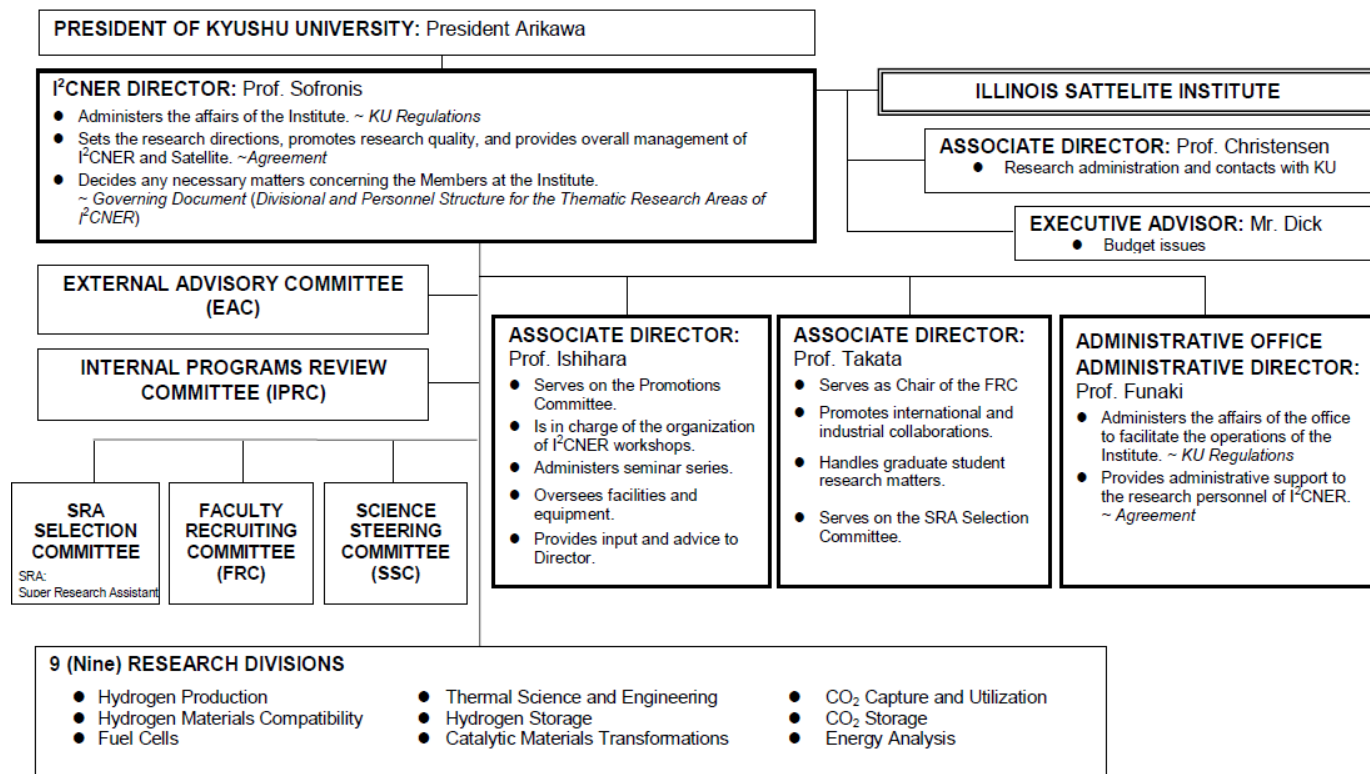
- Enter matters warranting special mention, such as concrete plans for achieving the Center's goals, established schedules for employing main researchers, particularly principal investigators.

- The Institute's Faculty Recruiting Committee (FRC) has conducted an extensive recruiting campaign to hire permanent-staying foreign principal investigator(s), including 1) Advertising in international journals, 2) Accessing faculty candidate files from the Mechanical Science and Engineering Department of the University of Illinois, 3) Contacting the head-hunting agency UIUC uses, 4) Requesting that all divisions nominate potential candidates, and 5) Instituting a "Faculty Fellows Program." The Institute has devoted maximum effort to recruit foreign PIs who would reside at I<sup>2</sup>CNER.
- One post-doc will be newly employed on May 1, 2014.

### 3. Center's Management System

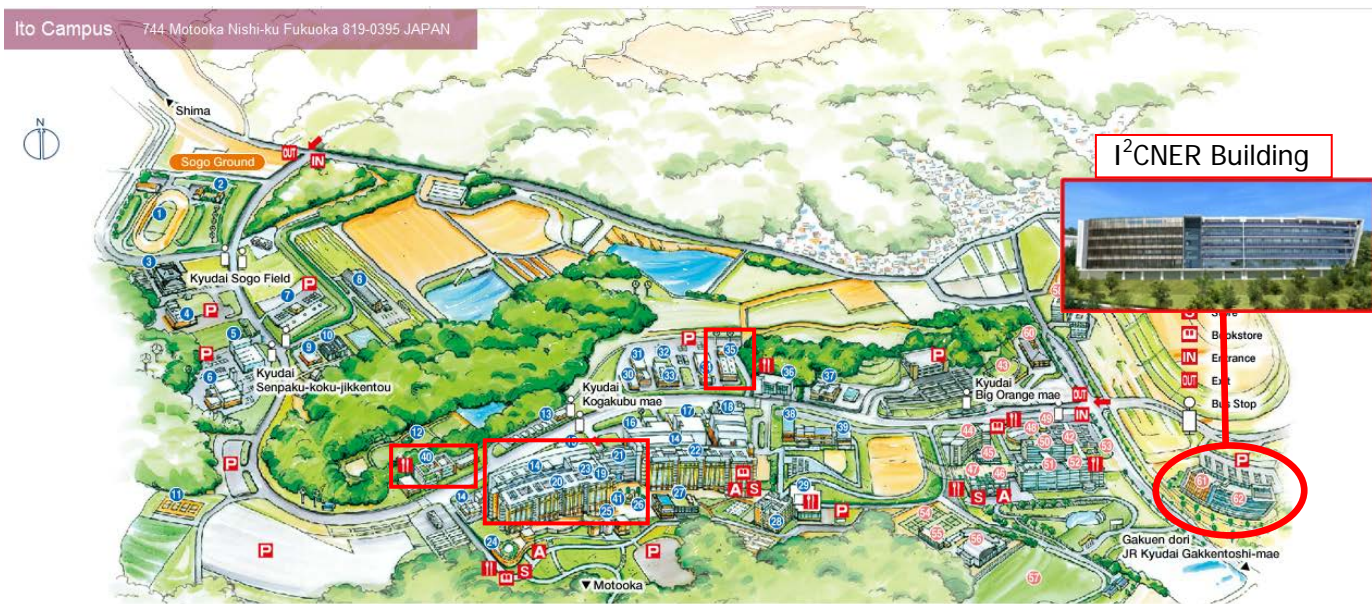
- Please diagram management system in an easily understood manner.

#### I<sup>2</sup>CNER ORGANIZATIONAL STRUCTURE



## 4. Campus Map

- Please draw a simple map of the campus showing where the main office and principle investigator(s) are located.



### West Zone

- |  |  |  |
|--|--|--|
| <ul style="list-style-type: none"> <li>1 Multipurpose Sports Field</li> <li>2 Japanese Archery Range</li> <li>3 Extracurricular Activities Facility II</li> <li>4 Center for Accelerator and Beam Applied Science (CE70)</li> <li>5 Seakeeping and Maneuvering Basin / High Speed Circulating Water Channel (EN80)</li> <li>6 Center for Advanced Aerospace Engineering (EN70)</li> <li>7 Satellite Communications Laboratory (IE20)</li> <li>8 Agri-Bio Research Laboratory</li> <li>9 Exploratory Research Project Laboratory (CE80)</li> <li>10 Demonstration Facility for Future Energies</li> <li>11 Tennis Court</li> <li>12 Biodiversity Conservation Zone</li> <li>13 Academic Lantern</li> <li>14 Engineering Department Experimental Facilities</li> <li>15 <b>Research Center for Steel (EN40)</b></li> </ul> | <ul style="list-style-type: none"> <li>16 Hydrogen Station</li> <li>17 International Research Center for Hydrogen Energy (HY30)</li> <li>18 Research Center for Hydrogen Industrial Use and Storage (HY10)</li> <li>19 Counseling and Health Center, West Zone Office</li> <li>20 <b>West Zone 4</b></li> <li>21 <b>West Zone 3</b></li> <li>22 West Zone 2</li> <li>23 School of Engineering International Relations Office, International Student and Researcher Support Center</li> <li>24 Big Dora - Restaurant &amp; Shops</li> <li>25 Lecture Hall West - Faculty of Engineering</li> <li>26 QIAO - Rock Art</li> <li>27 Open Learning Plaza</li> <li>28 Faculty of Mathematics Institute of Mathematics for Industry</li> </ul> | <ul style="list-style-type: none"> <li>29 Ito Library</li> <li>30 Low Temperature Center (Ito Center) (CE60)</li> <li>31 Research Institute of Superconductor Science and Systems (CE50,51)</li> <li>32 Research Institute of Environment for Sustainability (CE40)</li> <li>33 Research Institute for East Asia Environments (CE40)</li> <li>34 Research Laboratory for High Voltage Electron Microscopy (CE20, 21)</li> <li>35 <b>Institute for Materials Chemistry and Engineering (CE11)</b></li> <li>36 INAMORI Center (INAMORI Frontier Research Center)</li> <li>37 Energy Center</li> <li>38 Student Activity Support Facility</li> <li>39 Eco Center</li> <li>40 <b>Center for Organic Photonics and Electronics Research (OPERA)</b></li> <li>41 CENTENNIAL GALLERY</li> </ul> |
|--|--|--|

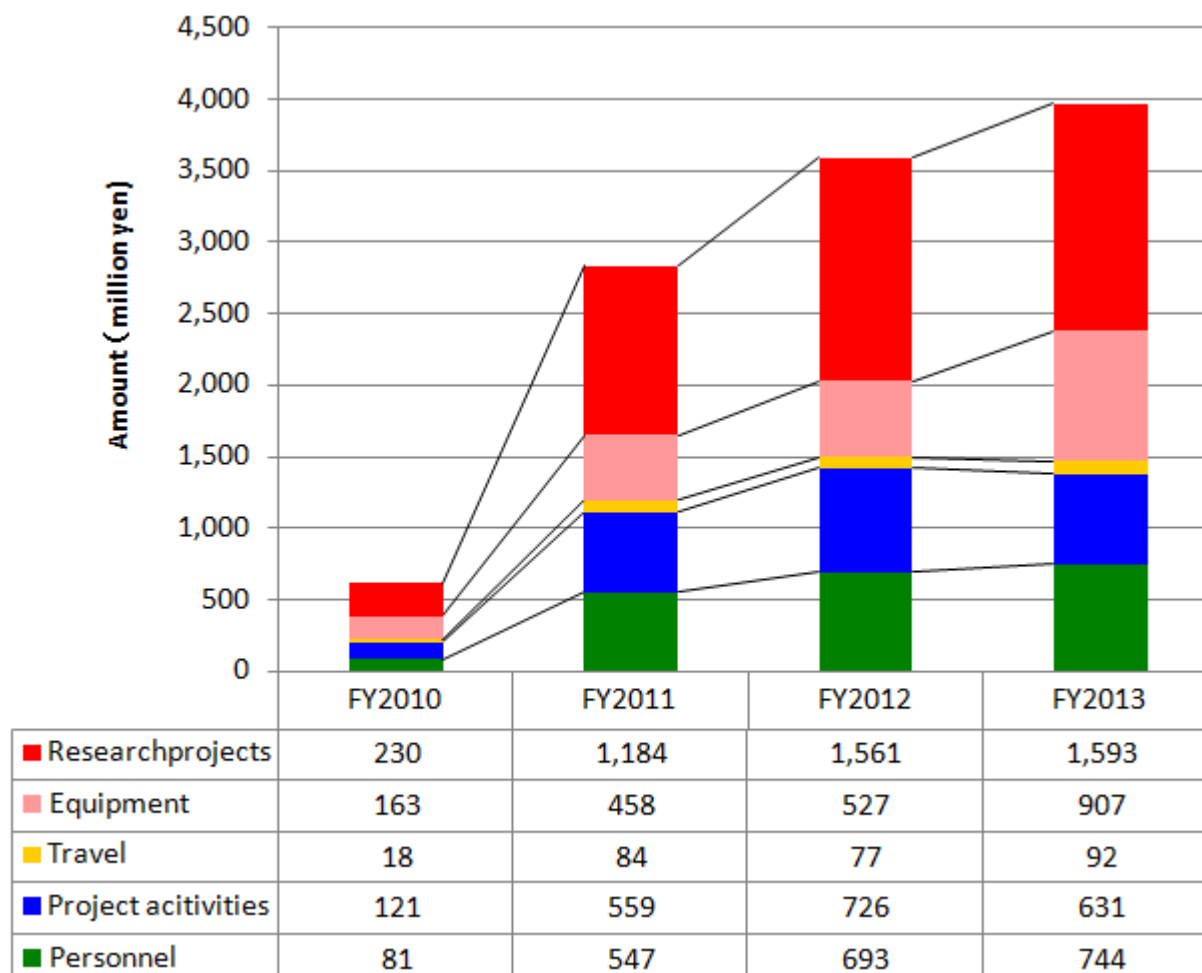
### Center Zone

- |  |   |
|--|---|
| <ul style="list-style-type: none"> <li>42 International Student and Researcher Support Center</li> <li>43 Water Supply Center</li> <li>44 Faculty of Social and Cultural Studies, Faculty of Languages and Cultures</li> <li>45 Administrative Office, Social and Cultural Studies, Languages and Cultures and Mathematics</li> <li>46 Counseling and Health Center, Center Zone Office</li> <li>47 Big Sand - Restaurant &amp; Shops</li> <li>48 Big Orange - Information Center</li> <li>49 Security Office</li> <li>50 Center Zone 1</li> <li>51 Center Zone 2</li> <li>52 Learning &amp; Community Space "Q-Commons"</li> <li>53 Bronze Bust of the First President Kenjiro Yamakawa</li> <li>54 Tennis Court</li> </ul> | <ul style="list-style-type: none"> <li>55 Extracurricular Activities Facility I</li> <li>56 Gymnasium</li> <li>57 Multipurpose Sports Field</li> <li>58 Dormitory 1 (Student residence)</li> <li>59 Dormitory 2 (Student residence)</li> <li>60 Ito Guest House</li> <li>61 <b>International Institute for Carbon-Neutral Energy Research (I²CNER)</b></li> <li>62 Next-Generation Fuel Cell Research Center (NEXT-FC)</li> </ul> |
|--|---|

## 5. Project funding

## 5-1. Annual transition in the amounts of project funding

\*Make a graph of the transition in the number of overall project funding.



-To date, what has the Center's thinking been about spending project funding, and how has the Funding been spent?

I<sup>2</sup>CNER strives for the project funds to be spent on increasing the numbers of postdocs and faculty in the institute and purchasing of large equipment for common use that is difficult to acquire through individual research grants. Funds are spent on project activities and travel to the extent that they advance I<sup>2</sup>CNER' s research objectives and international visibility.

i) Overall project funding

1 million yen

Cost Items	Details	Costs (1 million yen)
Personnel	Center director and Administrative director	18
	Principal investigators (no. of persons):16	205
	Other researchers (no. of persons):74	368
	Research support staffs (no. of persons):28	57
	Administrative staffs (no. of persons):25	96
	Total	744
Project activities	Gratuities and honoraria paid to invited principal investigators (no. of persons):51	9
	Cost of dispatching scientists (no. of persons):0	0
	Research startup cost (no. of persons):34	46
	Cost of satellite organizations (no. of satellite organizations):1	201
	Cost of international symposiums (no. of symposiums):3	4
	Rental fees for facilities	265
	Cost of consumables	38
	Cost of utilities	17
	Other costs	51
	Total	631
Travel	Domestic travel costs	17
	Overseas travel costs	46
	Travel and accommodations cost for invited scientists (no. of domestic scientists):21 (no. of overseas scientists):40	26
	Travel cost for scientists on secondment (no. of domestic scientists):1 (no. of overseas scientists):6	3
	Total	92
	Equipment	Depreciation of buildings
Depreciation of equipment		906
Total		907
Other research projects	Projects supported by other government subsidies, etc.	136
	Commissioned research projects, etc.	634
	Grants-in-Aid for Scientific Research, etc.	823
	Total	1,593
Total		3,967

WPI grant

1,334

Costs of establishing and maintaining facilities

1

Establishing new facilities  
(Number of facilities: , 0m<sup>2</sup>)

Costs paid: 0

Repairing facilities  
(Number of facilities: , 0m<sup>2</sup>)

Costs paid: 0

Others

1

Cost of equipment procured

1,583

Name of equipment: Nuclear magnetic resonance spectroscopy system

Number of units: 1

Costs paid: 90

Name of equipment: Server

Number of units: 2

Costs paid: 19

Others

1,474

ii) Costs of Satellites and Partner institutions

Cost Items	Details	Costs (1 million yen)
Personnel	Principal investigators (no. of persons):2	/
	Other researchers (no. of persons):13	
	Research support staffs (no. of persons):20	
	Administrative staffs (no. of persons):4	
	Total	
Project activities		38
Travel		18
Equipment		22
Other research projects		0
Total		201



## World Premier International Research Center Initiative (WPI)

### List of papers underscoring each research achievement

- List papers underscoring each research achievement listed in the item 2-1 "Research results to date" (up to 40 papers) and provide a description of the significance of each (within 10 lines).
- For each, write the author name(s); year of publication; journal name, volume, page(s), and article title. Any listing order may be used as long as format is the same. If a paper has many authors, underline those affiliated with the Center.
- If a paper has many authors (say, more than 10), all of their names do not need to be listed.

#### [1] Photocatalytic water splitting

1. Lee, S., Apgar, B. A. and Martin, L. W. (2013), Strong visible-light absorption and hot-carrier injection in TiO<sub>2</sub>/SrRuO<sub>3</sub> heterostructures, *Advanced Energy Materials*, 3 (8), 1084-1090.

First observation of strong visible light absorption in correlated electron oxide and subsequent coupling to TiO<sub>2</sub> for production of high-performance photocatalyst that uses a large portion of the solar spectrum to complete catalytic reactions. Devices operate by hot-carrier injection which is not limited by traditional efficiency limitations.

*The article combines the disciplines of epitaxial thin film material science, solid state physics, and photoelectrochemistry.*

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84882242626&partnerID=40&md5=384d3a9b5be3a6fa84d853f250c45149>

2. Apgar, B. A., Lee, S., Schroeder, L.E. and Martin, L. W. (2013), Enhanced photoelectrochemical activity in All-oxide heterojunction devices based on correlated "metallic" oxides, *Advanced Materials*, 25 (43), 6201-6206.

Identification of wide variety of materials – including earth abundant and low-cost oxide materials – with strong visible light absorption across the solar spectrum, long-term stability in solution and under illumination, and electronic compatibility with high-performance solar photocatalysts. This work served as the impetus for a now filed patent

*The article combines the disciplines of electronic condensed matter physics, solar photochemistry, and materials science.*

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84888009876&partnerID=40&md5=c874e562865edd96d787cd7f780a0199>

3. Ida, S., Takashiba, A., Koga, S., Hagiwara, H. and Ishihara, T. (2014), Potential gradient and photocatalytic activity of an ultrathin p-n junction surface prepared with two-dimensional semiconducting nanocrystals, *Journal of the American Chemical Society*, 136 (5), 1872-1878.

The synthesis and characterization of p-n (NiO/Ca<sub>2</sub>Nb<sub>3</sub>O<sub>10</sub>) and n-p junction (NiO/Ca<sub>2</sub>Nb<sub>3</sub>O<sub>10</sub>) nanosheets, in which Kelvin probe microscopy established that the higher activity from the n-p architecture arises from a potential gradient on the surface that allows spatial separation of the oxidation and reduction reactions.

*The article involves synthesis and atomic-scale characterization.*

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84893718775&partnerID=40&md5=3e0960d08f82283db0bd03fd6597c7db>

#### [2] Organic light emitting devices (OLEDs)

4. Zhang, Q., Li, B., Huang, S., Nomura, H., Tanaka, H., and Adachi, C. (2014), Efficient blue organic light-emitting diodes employing thermally activated delayed fluorescence, *Nature Photonics*, 8 (4), 326-332.

The first demonstration of metal-free organic blue light-emitting diodes of comparable in quantum efficiency to the best phosphorescent OLEDs used today. The high efficiencies arise from thermally-activated delayed fluorescence (TADF), a novel approach that enables all excited carriers, rather than some, to produce light.

*The article involves computational modeling and design, synthesis, and characterization.*

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84897148279&partnerID=40&md5=58798adf95b21f9b5df87f066a2591c0>

5. 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.

A new class of designer metal-free organic electroluminescent molecules that allow highly efficient conversion from the non-radiative triplet to radiative singlet states, resulting in the harnessing of both singlet and triplet excitons for light emission and intrinsic efficiencies of > 90%.

*The article involves computational modeling and design, synthesis, and characterization.*

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84871027786&partnerID=40&md5=2d2b356d17025d976b00c822254b7310>

**[3] On board hydrogen storage materials for fuel cell vehicles and stationary storage and a new pathway for hydrogen storage using High Pressure Torsion (HPT)**

6. Matsuda, J. and Akiba, E. (2013), Lattice defects in V-Ti BCC alloys before and after hydrogenation, *Journal of Alloys and Compounds*, 581, 369-372.

With the use of transmission electron microscopy (TEM) this work elucidated the effects of Ti/V ratio on the microstructure and hydrogenation/dehydrogenation properties of Ti-V binary BCC. It was found that the effective hydrogen capacity decreases and the density of twin boundaries increases with increasing Ti content. This indicates that twin boundaries formed upon hydrogenation act as hydrogen traps, thus increasing the desorption resistance of these alloys.

*The article combines materials science, microstructural characterization, and crystallography.*

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84881180517&partnerID=40&md5=79d7887cb5952ff507a1638c61e118d4>

7. He, L., Li, H.-W., Hwang, S.-J. and Akiba, E. (2014), Facile Solvent-Free Synthesis of Anhydrous Alkali Metal Dodecaborate  $M_2B_{12}H_{12}$  ( $M = Li, Na, K$ ), *The Journal of Physical Chemistry C*, 118 (12), 6084-6089.

Metal borohydrides, e.g.  $M(BH_4)_n$ , have hydrogen capacity of over 10 wt %, but reaction speed and hydrogen release temperature are serious roadblocks at present. To study and improve the thermodynamic and kinetic properties of this system, the division developed a novel solvent-free synthesis process that can be applied to the synthesis of various kinds of dehydrogenation intermediates (e.g.  $[B_3H_8]^-$ ,  $[B_5H_9]^{2-}$ ), which are extremely important to the clarification of the de- and re-hydrogenation mechanisms of metal borohydrides.

*The article combines materials synthesis, materials chemistry, and thermodynamics.*

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84897462763&partnerID=40&md5=a4dd50bfd5e0ddf1de79de39cb91118b>

8. Edalati, K., Matsuda, J., Iwaoka, H., Toh, S., Akiba, E. and Horita, Z. (2013), High-pressure torsion of TiFe intermetallics for activation of hydrogen storage at room temperature with heterogeneous nanostructure, *International Journal of Hydrogen Energy*, 38 (11), 4622-4627.

TiFe after the High Pressure torsion (HPT) treatment readily absorbs hydrogen without activation at high temperature and high pressure as is required without HPT treatment. In addition, even though Ti and Fe are easily oxidized, TiFe exposed to air for a few months after several cycles of hydrogenation/dehydrogenation still readily reacts with hydrogen without activation.

*The article combines materials science, mechanical engineering, and metallurgy.*

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84875365667&partnerID=40&md5=c12318e3c69d62237f20bcd8a421a3d4>

9. Edalati, K., Matsuda, J., Arita, M., Daio, T., Akiba, E. and Horita, Z. (2013), Mechanism of activation of TiFe intermetallics for hydrogen storage by severe plastic deformation using high-pressure torsion, *Applied Physics Letters*, 103 (14), 143902.

Fe-rich islands forming by HPT are suggested to act as catalysts for hydrogen dissociation, the microcracks and nanograin boundaries act as pathways for hydrogen transport, and probably dislocations for the sites of hydride formation.

*The article combines material synthesis, materials science, mechanical engineering, surface science, and characterization techniques to explore the activation mechanisms.*

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84885648001&partnerID=40&md5=3b33eddc6dfef3e2f7384330e560773>

#### [4] Alternative Electrocatalysts

10. Fujigaya, T. and Nakashima, N. (2013), Fuel Cell Electrocatalyst Using Polybenzimidazole-Modified Carbon Nanotubes As Support Materials, *Advanced Materials*, 25 (12), 1666-1681.

An invited review article in which the team's recent advances on the fuel cell electrocatalysts using polybenzimidazole-modified carbon nanotubes are summarized.

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84875145062&partnerID=40&md5=579329e8cccd1037531ef29862b53bd8>

11. Fujigaya, T., Okamoto, M., Matsumoto, K., Kaneko, K. and Nakashima, N. (2013), Interfacial engineering of platinum catalyst for fuel cells: Methanol oxidation is dramatically improved by polymer coating on a platinum catalyst, *ChemCatChem*, 5 (7), 1701-1704.

In this paper, the following discovery is reported: pyridine-containing polybenzimidazole (PyPBI)-coating on the platinum catalyst nanoparticles on the MWNTs wrapped by the PyPBIs dramatically improves the methanol oxidation activity of the Pt.

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84879708611&partnerID=40&md5=4d8660fb0c33156f385205fa659100f4>

12. Berber, M. R., Fujigaya, T. and Nakashima, N. (2014), High-Temperature Polymer Electrolyte Fuel Cell Using Poly(vinylphosphonic acid) as an Electrolyte Shows a Remarkable Durability, *ChemCatChem*, 6 (2), 567-571.

The design and fabrication of an electrocatalyst based on carbon black (CB), polybenzimidazole (PBI) doped with poly(vinylphosphonic acid) (PVPA) and platinum nanoparticles (Pt) respectively as an electron-conducting support material, electrolyte, and metal catalyst are described. It was revealed that the use of PVPA is crucial for the high performance of the MEA because it prevents the leaching of the acid molecules from the MEA, leading to remarkably high durability in comparison to the phosphoric acid-doped MEAs.

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84893320110&partnerID=40&md5=5687a8c162ca7b371dc1c74dd5e922b9>

13. Fujigaya, T., Hirata, S. and Nakashima, N. (2014), A Highly-Durable Fuel Cell Electrocatalyst Based on Polybenzimidazole-coated Stacked Graphene, *Journal of Materials Chemistry A*, 2 (11), 3888-3893.

Graphene has emerged as a promising candidate for a wide range of applications due to its outstanding properties, such as high electron conductivity, high surface area, mechanical toughness, unique optical properties, etc. In this paper, it is described, for the first time, the design and fabrication of a highly-durable fuel cell electrocatalyst for fuel cells. This catalyst is composed of polybenzimidazole (PBI)-covered graphene and Pt-nanoparticles.

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84894432385&partnerID=40&md5=a67a1bc1fd8ffd87498b393c43e5a952>

14. Fujigaya, T., Kim, C., Matsumoto, K. and Nakashima, N. (2014), Palladium-based Anion-exchange Membrane Fuel Cell using KOH-doped Polybenzimidazole as the Electrolyte, *ChemPlusChem*, 79 (3), 400-405.

A polymer electrolyte fuel cell (PEFC) using an anion-exchange membrane (AEM) operating under alkaline conditions has recently emerged as an alternative technology of conventional PEFC using a proton-exchange membrane (PEM) due to the fact that various lower cost metals can be used instead of Pt for the oxygen reduction reaction (ORR) in the cathode. In this work, we used Pd in place of Pt, and described the preparation and characterization of Palladium (Pd)-based anion-exchange membrane fuel cell using KOH-doped polybenzimidazole as the electrolyte, in which multi-walled carbon nanotubes (MWNTs) were used as the electron conducting carbon support material. We found that Pd-based electrocatalyst was employed in the cathode of the AEMFC and was found to show a remarkably high power density (241 mW/cm<sup>2</sup>).

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84896367096&partnerID=40&md5=ebbad1161d456ae953de3aa1cd86d62b>

15. Berber, M. R., Fujigaya, T., Sasaki, K. and Nakashima, N. (2013), Remarkably Durable High Temperature Polymer Electrolyte Fuel Cell Based on Poly(vinylphosphonic acid)-doped Polybenzimidazole, *Scientific Reports*, 3, 1764.

In this paper, we reported that our designed and fabricated novel PEFC free from acid leaching shows remarkably high durability (single cell test: >400,000 cycling) together with a high power density (252 mW/cm<sup>2</sup>) at high temperature (120°C) under a non-humidified condition. This was achieved by using a poly(vinylphosphonic acid)-doped polybenzimidazole-wrapped carbon nanotubes. Such a high performance PEFC opens the door for the next-generation PEFC for "real world" use.

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84878642649&partnerID=40&md5=881c8fdf33b3b3be6eb14eafe338f2c5>

16. Fujigaya, T., Kim, C., Matsumoto, K. and Nakashima, N. (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.

It was found that the sulfonated poly(arylene thioethersulfone) and sulfonated polyimide performed well as effective polymeric anchors for CNTs to immobilize Pt nanoparticles. It was revealed that the hydrophobic thioethersulfone unit functioned as a CNT anchor and the sulfonate moiety functioned as a Pt anchor for sulfonated poly(arylene thioethersulfone).

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84874599521&partnerID=40&md5=a435cc0c4606e091851ec6cddb8009d3>

17. Liu, J., Takeshi, D., Orejon, D., Sasaki, K. and Lyth, S. M. (2014), Defective Nitrogen-Doped Graphene Foam: A Metal-Free, Non-Precious Electrocatalyst for the Oxygen Reduction Reaction in Acid, *Journal of the Electrochemical Society*, 161 (4), F544-F550.

There is a major research effort worldwide to develop Pt-free, non-precious catalysts for the oxygen reduction reaction at PEFC cathodes. In this work, nitrogen-doped graphene foam with large surface area (> 700 m<sup>2</sup>/g) was synthesized as model metal-free non-precious electrocatalysts for the oxygen reduction reaction (ORR) in PEFCs. The purpose is to clarify the ORR in Fe/N/C-based electrocatalysts catalysts, which are still poorly understood. The results demonstrate the highest activity in acid for such Fe-free catalysts; that majority 4-electron ORR can occur in the absence of Fe; and the first double-Tafel slope, indicating Pt-like ORR. These catalysts are currently being explored at high temperature (> 120°C).

*The article combines materials synthesis, organic chemistry, nanotechnology, advanced characterization techniques, and electrochemistry.*

[http://apps.webofknowledge.com/full\\_record.do?product=UA&search\\_mode=GeneralSearch&qid=1&SID=U1vBU4jc4mqGWfmlsdi&page=1&doc=1](http://apps.webofknowledge.com/full_record.do?product=UA&search_mode=GeneralSearch&qid=1&SID=U1vBU4jc4mqGWfmlsdi&page=1&doc=1)

**[5] Understanding the origin of chemical expansion in SOFCs and developing new materials with reduced chemical expansion**

18. 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.

The origin of detrimental chemical expansion in oxides commonly used in fuel cells is uncovered for the first time with insight from atomistic level computational studies tied to experimental evidence. The article lays the groundwork to mitigate chemical expansion with expected improvements in fuel cell mechanical durability and lifetime.

*The article combines the disciplines of materials science thermodynamics, ceramic mechanical deformation, crystallography, and computational materials science. It also strongly couples experiment and theory.*

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84860711946&partnerID=40&md5=614ce74dc908f4b1414145b7bfe0727d>

19. Marrocchelli, D., Bishop, S. R. and Kilner J. A. (2013), Chemical expansion and its dependence on the host cation radius, *Journal of Materials Chemistry A*, 1 (26), 7673-7680.

The first computational finding that chemical expansion in fluorite structured oxides for fuel cell applications is coupled to the host cation size. A new method for reducing chemical expansion was hypothesized and experimentally validated in the following publication.

*The article combines the disciplines of materials science thermodynamics, ceramic mechanical deformation, crystallography, and computational materials science.*

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84880061122&partnerID=40&md5=8db048e864a85b0be51aa79c691c0066>

20. Bishop, S. R., Marrocchelli, D., Fang, W., Amezawa, K., Yashiro, K. and Watson, G. W. (2013), Reducing the chemical expansion coefficient in ceria by addition of zirconia, *Energy and Environmental Science*, 6 (4), 1142-1146.

First demonstration that the oxygen vacancy size can be tuned by isovalent doping, leading to both control and reduction in detrimental chemical expansion. Results will aid in improving mechanical durability of fuel cells with corresponding increases in lifetime.

*The article combines the disciplines of materials science thermodynamics, ceramic mechanical deformation, and computational materials science.*

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84875659290&partnerID=40&md5=2b48088a6a6260463a01801a45b91eac>

21. Bishop, S. R., Marrocchelli, D., Chatzichristodoulou, C., Perry, N. H., Mogensen, M. B., Tuller, H. L. and Wachsman, E. D., Chemical Expansion: Implications for Electrochemical Energy Storage and Conversion Devices, *Annual Review of Materials Research*, Accepted for Publication/Online.

This is the first comprehensive review of chemical expansion in energy related materials. It covers chemo-mechanical coupling across several energy-related technology areas.

<http://www.annualreviews.org/doi/pdf/10.1146/annurev-matsci-070813-113329>  
(Abstract only)

**[6] Interaction between evaporation and dynamic wetting**

22. Fukuda, S., Kohno, M., Tagashira, K., Ishihara, N., Hidaka, S. and Takata, Y. (2014) Behavior of small droplet impinging on a hot surface, *Heat Transfer Engineering*, 35 (2) 204-211.

Collision of small water droplet on a hot surface is a fundamental process of phase change in heat transfer involved in various industrial processes. However, parameters such as impinging velocity

and diameter of the sprayed droplet cannot be resolved through conventional experimental systems due to lack of control capabilities amongst the parameters. This work describes the development of a unique experimental system that enables independent control of parameters, e.g. impinging velocity, droplet size, and flow rate, thus obtaining the heat transfer characteristics from a hot surface to an individual droplet.

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84884640028&partnerID=40&md5=564952b183f46d20929a2a9c6cc086e0>

23. Deendarlianto, Takata, Y., Hidaka, S., Indarto, Widyaparaga, A., Kamal, S., Purnomo and Kohno, M. (2014), Effect of static contact angle on the droplet dynamics during the evaporation of a water droplet on the hot walls, *International Journal of Heat and Mass Transfer*, 71, 691-705.

In this article, the effect of surface wettability on the wetting limit temperature was examined. Through the use of TiO<sub>2</sub>, we succeeded in changing the surface wettability only by on-and-off of UV illumination. It was found that wettability elevates the wetting limit temperature and the wetting diameter of the droplet on the hot surface.

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84893177376&partnerID=40&md5=6377ff7881e62d660716480b2bb6f8d2>

24. Sefiane, K., Fukatani, Y., Takata, Y. and Kim, J. (2013), Thermal Patters and Hydrothermal Waves (HTWs) in Volatile Drops, *Langmuir*, 29 (31), 9750-9760.

Using high-speed infrared camera, we elucidated the evaporation process of volatile liquid on a hot substrate and observed the Hydrothermal Wave (HTW) inside the droplet. The method developed for this measurement can be applied to various phase change processes to understand the mechanism and distribution of heat transfer.

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84881444255&partnerID=40&md5=deb4e040a452ec61419608a175675e53>

**[7] Biology's ways with hydrogen: The first synthetic analog of the active site of the [NiFe] hydrogenase that oxidizes hydrogen**

25. Ogo, S., Ichikawa, K., Kishima, T., Matsumoto, T., Nakai, H., Kusaka, K. and Ohhara, T. (2013), A Functional [NiFe]Hydrogenase Mimic That Catalyzes Electron and Hydride Transfer from H<sub>2</sub>, *Science*, 339 (6120), 682-684.

This paper reports a functional [NiFe]-based model of [NiFe]hydrogenase enzymes, which can heterolytically activate hydrogen to form a hydride complex.

*The article combines Bioinorganic Chemistry, Biochemistry, Coordination chemistry.*

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84873509989&partnerID=40&md5=d789830de1c6bd2751fe28e504d63c2c>

26. Inoki, D., Matsumoto, T., Nakai, H. and Ogo, S. (2013), Isolation and Crystal Structure of the Proposed Low-Valent Active Species in the H<sub>2</sub> Activation Catalytic Cycle, *European Journal of Inorganic Chemistry*, 2013 (22-23), 3978-3986.

This report provides the confirmation of our proposed design principles for a H<sub>2</sub> activation catalytic cycle by constructing a new catalyst.

*The article combines Bioinorganic Chemistry, Coordination chemistry, Biochemistry.*

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84886530957&partnerID=40&md5=f53e4479839ffb9d3155f729daa60ce8>

27. Matsumoto, T., Nagahama, T., Cho, J., Hizume, T., Suzuki, M. and Ogo, S. (2011), Preparation and Reactivity of a Nickel Dihydride Complex, *Angewandte Chemie - International Edition*, 50 (45), 10578-10580.

A dinuclear octahedral bis( $\mu$ -hydrido)dinickel(II) complex acts as an electron donor to reduce electron

acceptors such as methyl viologen. The complex is proposed as a functional model for the dihydride intermediate of an NiRu hydrogenase mimic and, by extension, of [NiFe]hydrogenase itself.

*The article combines Bioinorganic Chemistry, Biochemistry, Coordination Chemistry.*

<http://www.scopus.com/inward/record.url?eid=2-s2.0-80155214281&partnerID=40&md5=6dc89d3a0e0e02f052d19bd991bc881c>

28. Matsumoto, T., Kim, K. and Ogo, S. (2011), Molecular Catalysis in a Fuel Cell, *Angewandte Chemie - International Edition*, 50 (47), 11202-11205.

The first molecular fuel cell based on a single molecular catalyst using a [NiFe]hydrogenase mimic was constructed that can function both in solid and solution phases, allowing precise observation of the mechanism of H<sub>2</sub> oxidation catalysis, while also exhibiting activity for the oxygen reduction reaction.

*The article combines Bioinorganic Chemistry, Coordination Chemistry, Electrochemistry.*

<http://www.scopus.com/inward/record.url?eid=2-s2.0-81255179172&partnerID=40&md5=c7c2072e2d27761e4b088ce8772fff65>

**[8] Elucidating the variables affecting accelerated fatigue crack growth in hydrogen gas with low oxygen concentrations**

29. Somerday, B. P., Sofronis, P., Nibur, K.A., San Marchi, C. and Kirchheim, R. (2013), Elucidating the Variables Affecting Accelerated Fatigue Crack Growth of Steels in Hydrogen Gas with Low Oxygen Concentrations, *Acta Materialia*, 61 (16), 6153-6170.

It is for the first time that fatigue crack growth rate experiments were performed on a structural alloy in hydrogen gas in which oxygen concentration, load-cycle frequency, and mean stress, were identified and systematically varied. An analytical model was developed which accurately quantifies how these variables affect the onset of accelerated crack growth for X52 steel in hydrogen gas containing trace oxygen concentrations. The model is the only predictive capability for quantifying the effects of oxygen on hydrogen-accelerated fatigue crack growth.

*The article combines the disciplines of material science, materials physics, and solid mechanics.*

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84882816876&partnerID=40&md5=af58abae5cf99750b5e03db5a485c37b>

30. Staykov, A., Yamabe, J. and Somerday, B. P. (2014), Effect of Hydrogen Gas Impurities on the Hydrogen Dissociation on Iron Surface, *International Journal of Quantum Chemistry*, 114 (10), 626-635.

This is a first-principles study that identified the basic mechanisms for oxygen inhibition of hydrogen uptake into steel. It was discovered that 1) oxygen can out-compete hydrogen for surface adsorption sites since the gas molecule-iron surface attractive force is stronger for oxygen compared to hydrogen, and 2) adsorbed oxygen on iron surfaces increases the activation barrier for molecular hydrogen dissociation on this surface, since the highly electronegative oxygen concentrates electron density in its vicinity. Although the poisoning effect of oxygen on hydrogen dissociation has been recognized for catalysts, the association of this phenomenon with oxygen inhibition of hydrogen uptake into materials was not previously demonstrated

*The article combines computational and experimental materials science.*

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84897572950&partnerID=40&md5=0fe642e9be988ed00ea5160dbcd0d8b4>

**[9] Free-standing and nanometer-thick membrane for gas separation and elucidation of the mechanism of preferential CO<sub>2</sub> permeation**

31. Taniguchi, I., Duan, S., Kai, T., Kazama, S. and Jinnai, H. (2013), Effect of phase-separated structure on CO<sub>2</sub> separation performance of poly(amidoamine) dendrimer immobilized in a poly(ethylene glycol) network, *Journal of Materials Chemistry A*, 1 (46), 14514-14523.

3D tomographic electron microscopy reveals that a phase-separated structure of poly (amidoamine)

dendrimer (PAMAM) is formed in a membrane matrix of poly(ethylene glycol). The phase of PAMAM forms a continuous network of channels and pores across the membrane and can act as a path for CO<sub>2</sub> permeation through the membrane to show preferential transport of CO<sub>2</sub>.

*The article combines the disciplines of polymer material science, chemical engineering and advanced electron microscopy.*

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84887218342&partnerID=40&md5=6f4d7b34b83e220aa9cd7196f42360a2>

32. Taniguchi, I., Urai, H., Kai, T., Duan, S. and Kazama, S. (2013), A CO<sub>2</sub>-selective molecular gate of Poly(amidoamine) dendrimer immobilized in a poly(ethylene glycol) network, *Journal of Membrane Science*, 444, 96-100.

A polymeric membrane composed of poly(amidoamine) (PAMAM) dendrimer immobilized in a poly(ethylene glycol) (PEG) network exhibits excellent selectivity of CO<sub>2</sub> transport over transport of the much smaller H<sub>2</sub>. NMR measurements helped to elucidate the mechanism of preferential CO<sub>2</sub> separation.

*The article combines the disciplines of polymer material science, analytical chemistry and chemical engineering.*

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84878830450&partnerID=40&md5=d62c9b0cc052d43d7b98e5f34dd9ba15>

#### **[10] Simulation of injected and trapping of CO<sub>2</sub> and estimation of CO<sub>2</sub> stored volume from seismic velocity**

33. Jiang, F., Tsuji, T. and Hu, C., Elucidating the role of interfacial tension for hydrological properties of two-phase flow in natural sandstone by an improved lattice Boltzmann method, *Transport in Porous Media*, doi: 10.1007/s11242-014-0329-0, Accepted for publication.

Largest-scale LBM simulation to date of multi-phase and reactive flow in heterogeneous geologic formations illustrating the dominant influence of interfacial tension on relative permeability, and thus on residual trapping of CO<sub>2</sub>. Such observations are critical for informing models of residual trapping that underly reservoir-scale simulations of large-scale CO<sub>2</sub> fate.

*The article combines the disciplines of fluid mechanics, geology and computational sciences.*

34. Jiang, F. and Tsuji, T., Evolution of Pore-geometry and Relative Permeability due to Carbonate Precipitation in Porous Media, *Physical Review E*, Reviewed and a moderate revision has been requested.

Ground-breaking LBM simulations combining multiphase and reactive flow with a model for carbonate precipitation in heterogeneous geologic formations. These simulations revealed that pore-space evolution due to mineral precipitation (mineralization trapping) impacts the dynamics of the non-wetting phase (injected CO<sub>2</sub>) more than the wetting phase (resident brine).

*The article combines the disciplines of fluid mechanics, geology and computational sciences.*

35. Kitamura, K., Xue, Z., Kogure, T. and Nishizawa, O. (2014), The potential of Vs and Vp-Vs relation for the monitoring of the change of CO<sub>2</sub>-saturation in porous sandstone, *International Journal of Greenhouse Gas Control*, 25, 54-61.

Identified hysteresis in the relationship between the P-wave seismic velocity and CO<sub>2</sub> saturation within reservoirs calling into question the standard use of P-wave velocity signals for monitoring CO<sub>2</sub> saturation in reservoirs. Proposed a more robust and reliable detection method using both P- and S-wave velocities to overcome this hysteric effect.

*The article combines the disciplines of geology, seismology and fluid mechanics.*

[http://ac.els-cdn.com/S1750583614000814/1-s2.0-S1750583614000814-main.pdf?\\_tid=7e973a3a-db41-11e3-b8aa-00000aab0f01&acdnat=1400056192\\_dc664a0ab72fb17d469730c66ca01876](http://ac.els-cdn.com/S1750583614000814/1-s2.0-S1750583614000814-main.pdf?_tid=7e973a3a-db41-11e3-b8aa-00000aab0f01&acdnat=1400056192_dc664a0ab72fb17d469730c66ca01876)

36. Kamei, R., Pratt, G. and Tsuji, T. (2013), On acoustic waveform tomography of wide-angle OBS data - Strategies for preconditioning and inversion, *Geophysical Journal International*, 194 (2), 1250-1280,



Develop a new advanced method of waveform tomography to estimate high-resolution seismic velocity of deep subsurface reservoir. By developing this method, the resolution of seismic velocity obtained by our method is ~5 times higher than the conventional methods (i.e., traveltime tomography). This is ground-breaking method for accurate reservoir characterization.

*The article combines the disciplines of geophysics, mathematics and computational sciences.*

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84880283984&partnerID=40&md5=e26bd24f8b9601f88c847f42b287bc44>

## World Premier International Research Center Initiative (WPI)

### List of the cooperative research agreements in and outside Japan

#### 1. Counterpart of the Agreement :

- The UK QICS Project Consortium which consists of Plymouth Marine Laboratory, the British Geological Survey, Heriot Watt University, the National Oceanography Centre, the Scottish Association for Marine Sciences, the University of Edinburgh, and the University of Southampton
- Central Research Institute of Electric Power Industry, Japan
- Japan NUS CO., LTD., Japan
- National Institute of Advanced Industrial Science and Technology, Japan
- Research Institute of Innovative Technology for the Earth, Japan
- The University of Tokyo, Japan

#### Name of the Agreement :

- Memorandum of Understanding on UK-Japan Collaboration in the QICS Project

#### Date of the Agreement :

- April 27, 2012

#### Summary of the Agreement :

- The Parties are to collaborate with one another by synergising UK planned tasks and Japan's complementary tasks in the UK-funded Project entitled "Quantifying and Monitoring Potential Ecosystem Impacts of Geological Carbon Storage" in short "QICS," for improving our understanding of the potential impacts of a leak from offshore CO<sub>2</sub> storage on the marine ecosystems.

#### 2. Counterpart of the Agreement :

- The Norwegian University of Science and Technology (NTNU)

#### Name of the Agreement :

- Memorandum of Understanding between International Institute for Carbon-Neutral Energy Research, Kyushu University (I<sup>2</sup>CNER) and the Norwegian University of Science and Technology (NTNU)

#### Date of the Agreement :

- March 17, 2014

#### Summary of the Agreement :

- The MOU's objective is to facilitate further cooperation in research and education, including exchange of students and faculty, joint research activities and publications, participation in seminars and academic meetings, exchange of academic materials and academic publications, and special short-term academic programs.

#### 3. Counterpart of the Agreement :

- ECOSTORE Beneficiaries such as Helmholtz-Zentrum Geesthacht Zentrum für Material- und Küstenforschung GmbH (HZG), Institutt for Energiteknikk (IFE), Aarhus Universitet (AU), Università Degli Studi di Torino (UNITO), Centre National de la Recherche Scientifique (CNRS), the University of Birmingham (UoB), Université de Genève (UNIGE), Westfälische Wilhelms-Universität Münster (WWU), National Centre for Scientific Research Demokritos (NCSR), Zoz GmbH (ZOZ), SAFT SAS (SAFT) and Rockwood Lithium GmbH (ROLI)
- Tohoku University

#### Name of the Agreement :

- Consortium agreement for the FP7 Initial Training Network ECOSTORE "Novel complex metal hydrides for efficient and compact storage of renewable energy as hydrogen and electricity"

Date of the Agreement :

- October 1, 2013

Summary of the Agreement:

- The purpose of this Consortium Agreement is to specify with respect to the Project the relationship among the Parties, in particular concerning the organisation of the work between the Parties, the management of the Project and the rights and obligations of the Parties concerning inter alia liability, Access Rights, and dispute resolution relating to the Project entitled "Novel complex metal hydrides for efficient and compact storage of renewable energy as hydrogen and electricity," in short "ECOSTORE."

4. Counterpart of the Agreement :

- National Fuel Cell Research Center, University of California Irvine, USA

Name of the Agreement :

- Agreement for Academic Exchange and Cooperation between National Fuel Cell Research Center, University of California Irvine, U.S.A. and International Institute for Carbon-Neutral Energy Research, Kyushu University, Japan

Date of the Agreement :

- December 31, 2013

Summary of the Agreement :

- This agreement aims at bridging science to practical application, wherein I<sup>2</sup>CNER focuses on the science and NFCRC focuses on the bridging of science to practical application. In this fashion, NFCRC will be able to complement/support the mission of I<sup>2</sup>CNER by making the "connection" to practical application. The specific roles of NFCRC are to provide direct support to the Energy Analysis efforts of I<sup>2</sup>CNER, to provide direct support through analyses of "Fuel Cell Systems" and "Energy Systems," and to provide direct support in planning methodologies associated with H<sub>2</sub> fueling infrastructure deployment. The general goal is to facilitate a sustained and enduring dialog, fundamental and practical research, and educational cooperation between the two parties.

5. Counterpart of the Agreement :

- Air Resources Board of the State of California (CARB), USA

Name of the Agreement :

- Letter of Understanding

Date of the Agreement :

- Pending

Summary of the Agreement :

- This agreement aims at creating a mutual awareness between I<sup>2</sup>CNER and CARB of the activities/goals/policies of each party. Moreover, the plan is to identify a "contact person" for each party in order to facilitate communication. I<sup>2</sup>CNER is expected to provide its master roadmap to CARB, with the goal being to have CARB identify the I<sup>2</sup>CNER activities that they believe to be especially relevant to the goals of the State of California. It has already been suggested by CARB that I<sup>2</sup>CNER adopt 2035 as its goal for "viable" technology and 2050 as its goal for "dream" technology. Through this activity, (1) CARB will become familiar with the investment of Japan in advanced technology research and the types of technologies under consideration, and (2) I<sup>2</sup>CNER will become familiar with the types of policy and regulation that California is implementing as a world leader to address and accelerate the deployment of advanced technology, energy efficiency, and conservation measures.

6. Counterpart of the Agreement :

- The University of Illinois at Urbana-Champaign, USA

Name of the Agreement :

- Agreement on Academic Cooperation between Kyushu University, Japan and the University of Illinois at Urbana-Champaign, USA

Date of the Agreement :

- Pending

Summary of the Agreement :

- The purpose of this agreement is to develop scientific, academic, and educational cooperation on the basis of equity and reciprocity, and to promote relations and mutual understanding between Kyushu University and the University of Illinois.

## World Premier International Research Center Initiative (WPI)

### Major Awards, Invited Lectures, Plenary Addresses (etc.)

#### 1. Major Awards

- List main internationally-acclaimed awards received/unofficially announced in order from the most recent.
- For each, write the recipient's name, name of award, and year issued.
- In case of multiple recipients, underline those affiliated with the center.

1. Michihisa Koyama, The Young Scientists' Prize, The Commendation for Science and Technology by the Minister of Education, Culture, Sports, Science and Technology, 2014
2. Robert O. Ritchie, David Turnbull Award, Materials Research Society, 2013
3. Naoya Sakoda, Young Scientist Award, The 10th Asian Thermophysical Properties Conference, 2013
4. Takeshi Tsuji, The Incentive Award, Society of Exploration Geophysicists of Japan (SEGJ), 2013
5. Kazuto Tsuda, Keisuke Adaniya, Naoya Kobayashi, Kousuke Shinto, Takahiro Takaki, Youhei Nagamatsu, Masaru Takada, Yasuhiro Toyofuku, Liana Christiani, Shingo Baba, Kota Miyoshi, Kyouhei Hirata, "Development of A Hydrogen Production and Fueling Infrastructure in the Northeastern United States." Grand Prize, 2012-2013 Hydrogen Student Design Contest, Hydrogen Education Foundation, 2013
6. Atsushi Takahara, The Society of Rheology, Japan Award, 2013
7. Seiji Ogo, Prize for Science and Technology, The Commendation for Science and Technology by the Minister of Education, Culture, Sports, Science and Technology, 2013
8. Zenji Horita, The Japan Institute of Metals Distinguished Contribution Award, 2013
9. Chihaya Adachi, Outstanding achievement award from Japan Society of Organic Electroluminescence, 2013
10. Seiji Ogo, The 30th Chemical Society of Japan Award, 2013
11. Harry L. Tuller, Helmholtz International Fellow Award from the Helmholtz Association of German Research Centers, 2013
12. John A. Kilner, Institute of Materials, Minerals and Mining Platinum Award for "Outstanding contributions to materials science", 2012
13. Tatsumi Ishihara, John A. Kilner and Harry L. Tuller, Somiya Award, 2012
14. Sean R. Bishop, Young Scientist Gold Award for an oral presentation at the International Union of Materials Research Societies - International Conference on Electronic Materials, Yokohama, Japan, 2012
15. Atsushi Takahara, METI Minister Award in the 9th Industry-Academia-Government Collaboration Contribution Award, 2011
16. Ian Robertson, Petros Sofronis, US Department of Energy Hydrogen and Fuel Cells Program Research and Development Award, "in recognition of outstanding contributions to the understanding of hydrogen embrittlement," 2011
17. Zenji Horita, Prize for Science and Technology, The Commendation for Science and Technology by the Minister of Education, Culture, Sports, Science and Technology, 2011

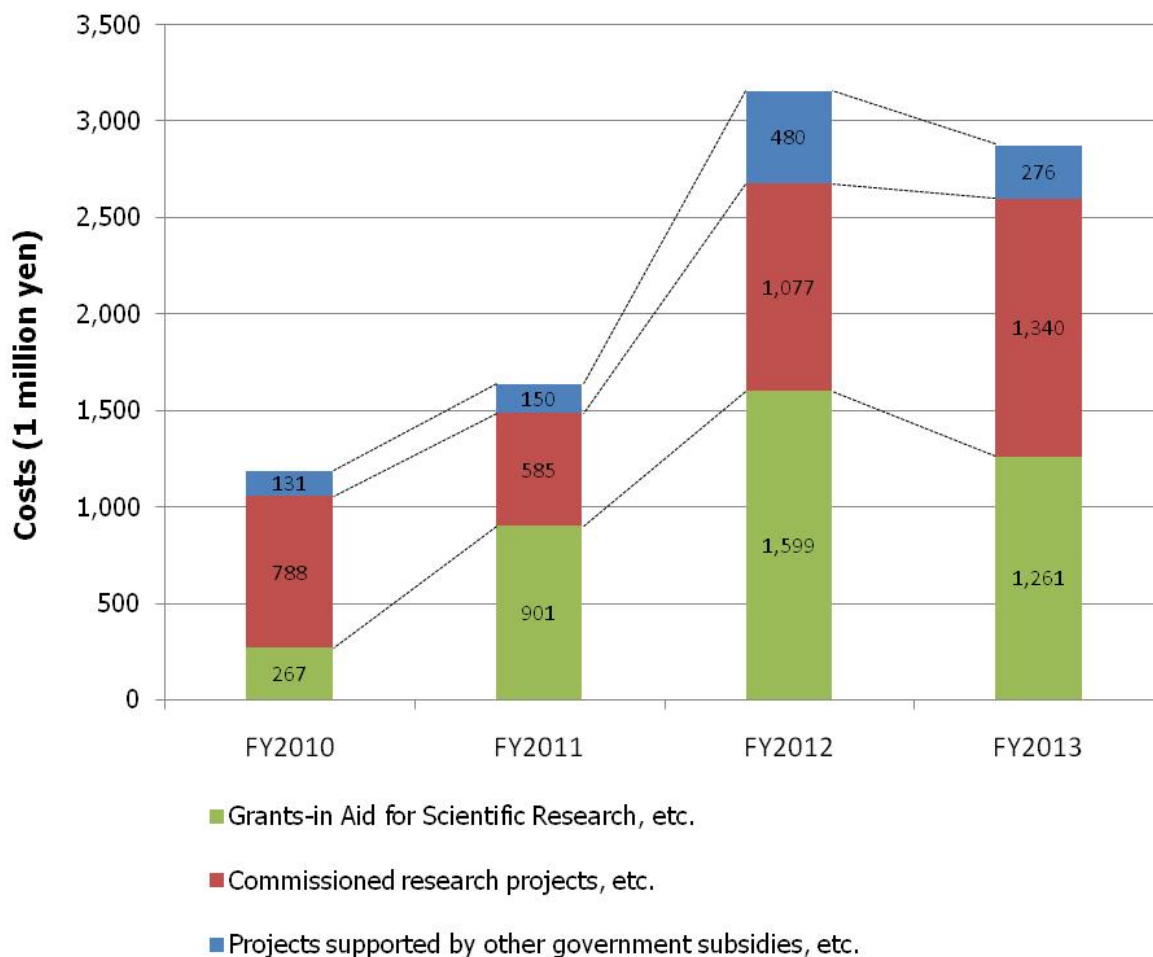
## 2. Invited Lectures, Plenary Addresses (etc.) at International Conferences and International Research Meetings

- List up to 10 main presentations in order from most recent.
  - For each, write the lecturer/presenter's name, presentation title, conference name and date(s)
1. Zenji Horita, (2014) Application of High-Pressure Torsion to TiFe Hydrogen Storage Material: No Requirement for Activation, TMS 2014 Annual Meeting and Exhibition Ultrafine-Grained Materials: Eight International Symposium (UFG-VIII), Feb. 17.
  2. Harry L. Tuller, (2013) Electro-Chemo-Mechanics – Applications to Solid State Ionic Materials, International Conference of Solid State Ionics, Jun. 5.
  3. Yasuyuki Takata, (2013) Wettability Effects in Boiling Heat Transfer, The 8th International Conference on Multiphase Flow (ICMF2013), May 29.
  4. Naotoshi Nakashima, (2013) Thermodynamics on Soluble Carbon Nanotubes: How Do Molecules Replace Surfactants On Carbon Nanotubes?, The 223rd ECS Meeting, May 13.
  5. Seiji Ogo, (2013) A significant contribution to the fundamentals and applications of chemistry: Catalytic electron and hydride transfer from H<sub>2</sub> by functional hydrogenase mimic, The 30th Chemical Society of Japan (CSJ) Award, Mar. 24.
  6. Petros Sofronis, (2013) Climate Change and National Security Speaker Series, Sandia National Laboratories, Jan. 16.
  7. Kiminori Shitashima, (2012) Strategies for detection and monitoring of CO<sub>2</sub> leakage in sub-seabed CCS, 11th International Conference on Greenhouse Gas Control Technologies (GHGT-11), Nov. 18-22.
  8. Tatsumi Ishihara, (2012) High Power Density Solid Oxide Fuel Cells Using LaGaO<sub>3</sub> Perovskite Oxide Thin Film Prepared by PLD Method, The 13th Asian Conference on Solid State Ionics IONICS for Sustainable World, Jul. 18.
  9. Andrew A. Gewirth, (2012) Cu-Containing Oxygen Reduction Catalysts, The 221st ECS meeting, May 6-10.
  10. Junko Matsuda, (2011) Direct imaging of hydrogen in metal hydride, Gordon Research Conference on Hydrogen-Metal Systems, Jul. 20.
  11. Miho Yamauchi, (2011) Hydrogen Induced Phenomena in Nanometals and Nanoalloys, Gordon Research Conference on Hydrogen-Metals Systems, Stonehill College, Easton, MA, Jul. 17.

## World Premier International Research Center Initiative (WPI)

### Non-WPI project funding (grants)

\*Make a graph of the annual transition in non-WPI project funding (grants).



- Describe external funding warranting special mention. Include the name and total amount of each grant.

#### FY2010

- Name: Funding Program for World-Leading Innovative R&D on Science and Technology (from JSPS)  
Total Amount: 648,397,800 JPY (acquired by Chihaya Adachi)

#### FY2011

- Name: Funding Program for World-Leading Innovative R&D on Science and Technology (from JSPS)  
Total Amount: 654,296,000 JPY (acquired by Chihaya Adachi)
- Name: Fundamental Research Project on Advanced Hydrogen Science (from NEDO)  
Total Amount: 265,454,000 JPY (acquired by Saburo Matsuoka)

FY2012

- Name: Funding Program for World-Leading Innovative R&D on Science and Technology (from JSPS)  
Total Amount: 761,772,570 JPY (acquired by Chihaya Adachi)
- Name: Fundamental Research Project on Advanced Hydrogen Science (from NEDO)  
Total Amount: 381,004,000 JPY (acquired by Saburo Matsuoka)
- Name: Installation Project for Base as a Mediator of Technology (from METI)  
Total Amount: 717,659,000 JPY (Including KU budget of 239,220,000 JPY) (acquired by Kazunari Sasaki)

FY2013

- Name: Funding Program for World-Leading Innovative R&D on Science and Technology (from JSPS)  
Total Amount: 112,273,000 JPY (acquired by Chihaya Adachi)
- Name: Installation Project for International Scientific Innovative Base (from MEXT)  
Total Amount: 704,958,503 JPY (acquired by Chihaya Adachi)
- Name: R&D Project on Useful Technology of Hydrogen (from NEDO)  
Total Amount: 382,612,000 JPY (acquired by Joichi Sugimura)



## World Premier International Research Center Initiative (WPI)

### Center's achievements and outcomes in basic research that contribute to the transition to a low-carbon society

- List up to 20 papers underscoring research activity that contribute to the transition to a low-carbon society and give brief accounts (within 10 lines).
- For each, write the author name(s); year of publication; journal name, volume, page(s), and article title. Any listing order may be used as long as format is the same. (The names of the center researchers do not need to be underlined.)  
If a paper has many authors, underline those affiliated with the Center.
- If a paper has many authors (say, more than 10), all of their names do not need to be listed.

1. 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.

*Here we report a class of metal-free organic electroluminescent molecules in which the energy gap between the singlet and triplet excited states is minimized by design. In other words, these molecules harness both singlet and triplet excitons for light emission through fluorescence decay channels, leading to an intrinsic fluorescence efficiency in excess of 90 per cent and a very high external electroluminescence efficiency, of more than 19 per cent, which is comparable to that achieved in high-efficiency phosphorescence-based. A switch to solid state lighting will substantially reduce the use of electricity.*

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84871027786&partnerID=40&md5=2d2b356d17025d976b00c822254b7310>

2. Goushi, K., Yoshida, K., Sato, K. and Adachi, C. (2012), Organic light-emitting diodes employing efficient reverse intersystem crossing for triplet-to-singlet state conversion, *Nature Photonics*, 6 (4) 253-258.

*Organic light-emitting diodes made using m-MTDATA as the donor material and 3TPYMB as the acceptor material demonstrate that external quantum efficiencies as high as 5.4% can be achieved, and we believe that the approach will offer even higher values in the future as a result of careful material selection. A switch to solid state lighting will substantially reduce the use of electricity.*

<http://www.scopus.com/record/display.url?eid=2-s2.0-84862790099&origin=inward&txGid=A699E56669944C1>

3. Lee, S., Apgar, B. A. and Martin, L. W. (2013), Strong visible-light absorption and hot-carrier injection in TiO<sub>2</sub>/SrRuO<sub>3</sub> heterostructures, *Advanced Energy Materials*, 3 (8) 1084-1090.

*A low-carbon society will require clean energy production methods and clean energy sources. The work on all oxide high-performance photocatalysts provides for both of these by leveraging widely-abundant materials that can efficiently utilize solar energy to potentially produce clean burning fuels thereby reducing carbon production at all stages of the process. Current solar photocatalysts suffer from two critical problems: 1) those with band gaps that provide for ample light absorption are often not stable in solution and under illumination and 2) those that are stable, often possess band gaps that are too large for the efficient utilization of solar radiation. Our research addresses these challenges directly by applying lessons from condensed matter and semiconductor physics to develop a new class of strongly light-absorbing, stable materials.*

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84882242626&partnerID=40&md5=384d3a9b5be3a6fa84d853f250c45149>

4. Okamoto, Y., Ida, S., Hyodo, J., Hagiwara, H. and Ishihara, T. (2011), Synthesis and photocatalytic activity of rhodium-doped calcium niobate nanosheets for hydrogen production from a water/methanol system without cocatalyst loading, *Journal of the American Chemical Society*, 133 (45) 18034-18037.

*One possible way to achieve a low carbon society is by using sunlight to split water and generate*

hydrogen fuel which then can be consumed in a device such as a fuel cell. No carbon need be involved in this scheme. In this paper, the authors develop a new water splitting catalyst based on niobium and rhodium and show that this system has promise for high efficiency water splitting.

<http://www.scopus.com/inward/record.url?eid=2-s2.0-80755123421&partnerID=40&md5=a93a5e9d4ada288327f97c3e8d72784c>

5. Somerday, B.P., Sofronis, P., Nibur, K.A., San Marchi, C. and Kirchheim, R. (2013), Elucidating the variables affecting accelerated fatigue crack growth of steels in hydrogen gas with low oxygen concentrations, *Acta Materialia*, 61 (16) 6153-6170.

*Fatigue is a degradation mechanism demonstrated by crack propagation when materials are subjected to cyclic loading. In the presence of gaseous hydrogen, this crack propagation is accelerated for reasons we still do not understand. In this work it was found out that by adding a few molecules of oxygen in the hydrogen gas, hydrogen induced acceleration of fatigue can be suppressed. Most importantly a compact formula governing the mitigation of the hydrogen effect in terms of the material, environmental, and loading parameters has been devised. It is for the first time that engineers are given a single formula that describes the hydrogen effect on fatigue acceleration in terms of all parameters that govern this complex phenomenon of fatigue crack growth.*

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84882816876&partnerID=40&md5=af58abae5cf99750b5e03db5a485c37b>

6. Matsuoka, Y., Iwasaki, T., Nakada, N., Tsuchiyama, T. and Takaki, S. (2013), Effect of grain size on thermal and mechanical stability of austenite in metastable austenitic stainless steel, *ISIJ International*, 53 (7) 1224-1230.

*Ultra-fine-grained austenitic steels fabricated at the laboratory scale exhibit both high strength and hydrogen compatibility. Whereas this material requires further characterization, it is a promising candidate to satisfy the milestone of developing H<sub>2</sub>-compatible, lower-cost austenitic stainless steels having 600 MPa yield strength. Assuming this material emerges from demonstration and proceeds to the commercialization path, one factor that must be considered is the equipment in high-volume industrial steel production. However, Nippon Steel & Sumitomo Metal Corporation (NSSMC) have just launched the first mass-produced ultra-fine-grained 304 stainless steel in 2013 ([www.nssmc.com/news/20131203\\_100.html](http://www.nssmc.com/news/20131203_100.html)). This indicates that ultra-fine-grain processing routes developed in the laboratory by the Prof. Takaki group can be scaled up to industrial production.*

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84883216716&partnerID=40&md5=02f1b06451b85cb582ea97e4186f20b4>

7. Shiratori, Y., Quang-Tuyen, T. and Sasaki, K. (2013), Performance enhancement of biodiesel fueled SOFC using paper-structured catalyst, *International Journal of Hydrogen Energy*, 38 (23) 9856-9866.

*Solid oxide fuel cells (SOFC) provide a way to achieve high efficiency usage of a fuel, exhibiting efficiencies much greater than that found with a Carnot cycle device (like a turbine or internal combustion engine). Robust SOFCs could provide a way of generating electricity from almost any fuel, the high efficiency producing less carbon relative to other methods of electricity generation. One issue with SOFCs is that they are subject to poisoning (coking) by carbon deposits coming from the fuel. In this paper, the authors develop a method to inhibit this coking issue by structuring the catalyst layer in the fuel cell in a particular way. This may allow the sofc to operate in more demanding environments.*

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84880180583&partnerID=40&md5=91347a67c45e74378c5c2c4c6981485a>

8. Berber, M. R., Fujigaya, T., Sasaki, K. and Nakashima, N. (2013), Remarkably durable high temperature polymer electrolyte fuel cell based on poly(vinylphosphonic acid)-doped polybenzimidazole, *Scientific Reports*, 3, 1764.

*Low durability of polymer electrolyte fuel cell (PEFC) is a major drawback that should be solved. Recent studies have revealed that leaching of liquid phosphoric acid (PA) from both polymer electrolyte membrane and catalyst layers causes inhomogeneous PA distribution that results in*

*deterioration of PEFC performance during long-term operation. Here we describe the finding that a novel PEFC free from acid leaching shows remarkable high durability (single cell test: >400,000 cycling) together with a high power density at 120 °C under a non-humidified conditions. This is achieved by using a membrane electrode assembly (MEA) with Pt on poly(vinylphosphonic acid)-doped polybenzimidazole wrapped on carbon nanotube and poly(vinylphosphonic acid)-doped polybenzimidazole for the electrocatalst and electrolyte membrane, respectively. Such a high performance PEFC opens the door for the next-generation PEFC for "real world" use.*

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84878642649&partnerID=40&md5=881c8fdf33b3b3be6eb14eafe338f2c5>

9. 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.

*The origin of detrimental chemical expansion in oxides commonly used in fuel cells is uncovered for the first time with insight from atomistic level computational studies tied to experimental evidence. This work lays the groundwork to mitigate chemical expansion through using appropriate material microstructures that are expected to improve fuel cell mechanical durability and lifetime.*

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84860711946&partnerID=40&md5=614ce74dc908f4b1414145b7bfe0727d>

10. Erickson, E. M., Thorum, M. S., Vasic, R., Marinkovic, N. S., Frenkel, A. I., Gewirth A. A. and Nuzzo R. G. (2012), In situ electrochemical X-ray absorption spectroscopy of oxygen reduction electrocatalysis with high oxygen flux, *Journal of the American Chemical Society*, 134 (1) 197-200.

*We are interrogating the oxygen reduction reaction (ORR), the crucial reaction for both low and high temperature fuel cells. To date, this reaction operates with high overpotentials, and we are using synchrotron methods to understand why which will then allow us to develop new materials that work better. Low carbon society will rely on more efficient ways to generate electricity, especially portable electricity, and fuel cells are a leading candidate.*

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84855658133&partnerID=40&md5=a629650e85c211eb883e9ed7f8d3ab70>

11. Sefiane, K., Fukatani, Y., Takata, Y. and Kim, J. (2013), Thermal patterns and hydrothermal waves (HTWs) in volatile drops, *Langmuir*, 29 (31) 9750-9760.

*The evaporation and interaction of liquids with solid materials have direct consequences on technologies such as power generation, heat pump, refrigeration systems, and thermal control. Using high-speed infrared camera, we elucidated the evaporation process of volatile liquid on a hot substrate and observed the Hydrothermal Wave (HTW) inside the droplet. The method developed for this measurement can be applied to various phase change processes to understand the mechanism and distribution of heat transfer.*

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84881444255&partnerID=40&md5=deb4e040a452ec61419608a175675e53>

12. Moroe, S., Woodfield, P. L., Kimura, K., Kohno, M., Fukai, J., Fujii, M., Shinzato, K. and Takata, Y. (2011), Measurements of hydrogen thermal conductivity at high pressure and high temperature, *International Journal of Thermophysics*, 32 (9) 1887-1917.

*The thermal conductivity for normal hydrogen gas was measured in the range of temperatures from 323 K to 773 K at pressures up to 99 MPa using the transient short hot-wire method. The experimental uncertainty in the thermal-conductivity measurements was estimated to be 2.2 % ( $k = 2$ ). An existing thermal-conductivity equation of state was modified to include the expanded range of conditions covered in the present study. The new correlation is applicable from 78 K to 773 K with pressures to 100 MPa.*

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84855432080&partnerID=40&md5=f0f6f1517360deba86d484ff8a1a3660>

13. Miao, T., Ma, W., Zhang, X., Wei, J. and Sun, J. (2013), Significantly enhanced thermoelectric properties of ultralong double-walled carbon nanotube bundle, *Applied Physics Letters*, 102 (5) 053105.

*A T-type method is developed to comprehensively evaluate the thermoelectric properties of materials. The thermoelectric properties, including thermal conductivity, thermopower, and electrical conductivity of an ultralong double-walled carbon nanotube bundle are studied from 240 K to 340 K by applying the T-type method. The determined figure of merit achieves  $10^3$  which is significantly larger than that reported for carbon nanotubes samples. The bundle consists of thousands of nanotubes aligned along the long axis with low levels of impurities, and the thermal conductivity is significantly reduced compared to that of individual double-walled nanotube, while the electrical conductivity is superior to most of the carbon nanotubes samples.*

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84874100472&partnerID=40&md5=da26441fb3b60bc885249253d0370a20>

14. Edalati, K., Matsuda, J., Iwaoka, H., Toh, S., Akiba, E. and Horita, Z. (2013), High-pressure torsion of TiFe intermetallics for activation of hydrogen storage at room temperature with heterogeneous nanostructure, *International Journal of Hydrogen Energy*, 38 (11) 4622-4627.

*TiFe is a potential candidate for the stationary hydrogen storage systems, but it requires initial activation to absorb hydrogen. This study shows that TiFe processed by high-pressure torsion (HPT) absorbs and desorbs 1.7 wt.% hydrogen at room temperature without activation. The absorption pressure decreases from 2 MPa in the first hydrogenation cycle to 0.7 MPa in the latter cycles. The HPT-processed TiFe exhibits heterogeneous microstructures composed of nanograins, coarse-grains, amorphous-like phases and disordered phases with a high hardness of  $\sim 1050$  Hv.*

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84875365667&partnerID=40&md5=c12318e3c69d62237f20bcd8a421a3d4>

15. Yatabe, T., Kikkawa, M., Matsumoto, T., Nakai, H., Kaneko, K. and Ogo S. (2014), A model for the water-oxidation and recovery systems of the oxygen-evolving complex, *Dalton Transactions*, 43 (8) 3063-3071.

*A model is proposed for the water-oxidation and recovery systems of the oxygen-evolving complex (OEC) of the photosystem II (PSII) enzyme. Extraction of electrons from water by PSII is extremely important process to convert solar energy into chemical energy, which is used to assimilate CO<sub>2</sub> to make carbohydrates (fuels, hydrocarbon). However, the PSII can be easily degraded after brief light exposure. Understanding the reactivation and recovery mechanisms of PSII is very important to the development of robust artificial photosynthetic catalysts to make hydrocarbons from water and CO<sub>2</sub>, which will directly contribute towards the realization of low-carbon society.*

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84893226228&partnerID=40&md5=326006a89dda0156352de56d021f6d6b>

16. Ogo, S., Ichikawa, K., Kishima, T., Matsumoto, T., Nakai, H., Kusaka, K. and Ohhara, T. (2013), A functional [NiFe]hydrogenase mimic that catalyzes electron and hydride transfer from H<sub>2</sub>, *Science*, 339 (6120) 682-684.

*Hydrogen is a clean energy carrier, highly expected to contribute to the realization of a future low carbon society. However, precious platinum is used as H<sub>2</sub> activation catalyst, which is a big roadblock in the fuel cell technology. We have developed the biomimetic [NiFe]hydrogenase inspired by nature enzymes and we have firstly elucidated the H<sub>2</sub>-activation mechanism using the catalyst in aqua at ambient conditions. Even though the catalyst has low catalytic ability, however, this is an important step to building the next robustly active catalyst for industrial applications.*

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84873509989&partnerID=40&md5=d789830de1c6bd2751fe28e504d63c2c>

17. Sadakiyo, M., Kasai, H., Kato, K., Takata, M. and Yamauchi, M. (2014), Design and synthesis of hydroxide ion-conductive metal-organic frameworks based on salt inclusion, *Journal of the American Chemical Society*, 136 (5) 1702-1705.

*This very recent work proposes a rational approach to constructing novel hydroxide ion-conductive solids. Hydroxide ion-conductive solid is necessary to construct high performance alkaline fuel cells, which does not need expensive platinum catalyst. The basic concept described in this paper will contribute to realization of the cheaper fuel cell system for low carbon society.*

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84893750990&partnerID=40&md5=33c268675f4d8185f8d8a01256789246>

18. Taniguchi, I., Urai, H., Kai, T., Duan, S. and Kazama, S. (2013), A CO<sub>2</sub>-selective molecular gate of poly(amidoamine) dendrimer immobilized in a poly(ethylene glycol) network, *Journal of the Membrane Science*, 444, 96-100.

*Development of CO<sub>2</sub> separation membranes with high selectivity and flux is a promising means to control release of CO<sub>2</sub> emissions to the atmosphere and re-use the CO<sub>2</sub> as a carbon source. In this work, it has been discovered that a polymeric membrane composed of poly(amidoamine) (PAMAM) dendrimer immobilized in a poly(ethylene glycol) (PEG) network exhibits excellent selectivity of CO<sub>2</sub> separation over H<sub>2</sub>. Efficient CO<sub>2</sub> separation from CO<sub>2</sub>/H<sub>2</sub> mixture enables the use of these gases separately in CO<sub>2</sub> utilization technologies and green energy applications, respectively.*

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84878830450&partnerID=40&md5=d62c9b0cc052d43d7b98e5f34dd9ba15>

19. Taniguchi, I., Duan, S., Kai, T., Kazama, S. and Jinnai, H. (2013), Effect of the phase-separated structure on CO<sub>2</sub> separation performance of the poly(amidoamine) dendrimer immobilized in a poly(ethylene glycol) network, *Journal of Materials Chemistry A*, 1 (46) 14514-14523.

*In this article, the mechanism of separation described in article 18 above has been identified and described. This achievement contributes to the design and further development of CO<sub>2</sub> separation membranes with much better selectivity and flux.*

<http://www.scopus.com/record/display.url?eid=2-s2.0-84887218342&origin=inward&txGid=A699E56669944C1>

20. Jhong, H.-R. M., Brushett, F. R. and Kenis, P. J. A. (2013), The effects of catalyst layer deposition methodology on electrode performance, *Advanced Energy Materials*, 3 (5) 589-599.

*Capture of CO<sub>2</sub> produced, for example, by fossil fuel power plants, followed by electrochemical conversion of the CO<sub>2</sub> into chemical building blocks such as CO, which in turn can be used for the synthesis of products such as polymers, fine chemicals, or hydrocarbon fuels. Overall this process reduces greenhouse gas emissions, while at the same time reducing society's dependency on fossil fuels. For electrochemical conversion of CO<sub>2</sub> to become practical for being performed at industrial scale, advances were needed on catalysts and on electrodes. This paper drastically improved the quality (catalyst layer uniformity) and performance (higher throughput and higher energy efficiency) of electrodes for this process, while at the same time reducing the loading of the catalyst (thus reducing cost).*

*More specifically, using an automated setup for airbrush-based deposition of catalyst inks on the micro-porous layer of a gas diffusion electrode, we were able to create very thin, crack free, uniform catalyst layers, for example comprised of Ag nanoparticles. This is significant because these electrodes performed significantly better in CO<sub>2</sub> conversion (>50% improvement in current density) than electrodes prepared by hand painting, while at the same time the catalyst loading was reduced 10-fold.*

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84877706212&partnerID=40&md5=c542eb8912acb29043694c33c4acb95>

21. Tornow, C. E., Thorson, M. R., Ma, S., Gewirth A. A. and Kenis P. J. A. (2012), Nitrogen-based catalysts for the electrochemical reduction of CO<sub>2</sub> to CO, *Journal of the American Chemical Society*, 134 (48) 19520-19523.

*We are developing methods to remediate CO<sub>2</sub>. This remediation may contribute to a low carbon society in a number of ways, the most direct being conversion of CO<sub>2</sub> to more useful products, such as hydrocarbons. The first and hardest step in this process is to convert CO<sub>2</sub> into CO. In*

*this paper we develop a new series of catalysts for this process which work better than that previously utilized.*

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84870702915&partnerID=40&md5=f12dbefe09aeb6a6bdc8a94c984044de>

22. 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.

*To investigate the safety and reliability of CO<sub>2</sub> storage in the sub-seafloor, development of techniques to detect and monitor CO<sub>2</sub> leaked from the seafloor is vital. Seafloor-based acoustic tomography is a technique that can be used to observe emissions of liquid CO<sub>2</sub> or CO<sub>2</sub> gas bubbles from the seafloor. In situ pH/p CO<sub>2</sub> sensor can take rapid and high-precision measurements in seawater, and is, therefore, able to detect pH and pCO<sub>2</sub> changes due to the leaked CO<sub>2</sub>. Thus, by installing the sensor onto an AUV, an automated observation technology is realized that can detect and monitor CO<sub>2</sub> leakage from the seafloor. Furthermore, by towing TMLMS (containing a number of the sensors and transponders) behind the AUV, the dispersion of leaked CO<sub>2</sub> in a CCS area can also be observed. Finally, an automatic elevator can observe the time-series dispersion of leaked CO<sub>2</sub>. This is the world's first paper addressing monitoring of CO<sub>2</sub> leakage in sub-seabed CCS.*

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84875402443&partnerID=40&md5=fb133d54fecce0d32db1c8ff3233ddab>

## World Premier International Research Center Initiative (WPI)

### FY 2013 List of Project's Media Coverage

- Select main items of coverage, and list them within these 2 pages.

No.	Date	Type media (e.g., newspaper, television)	Description
1	25 Apr. 2013	Newspaper	<b>Itoshima Shimbun</b> Newspaper article introducing the partial use of organic electroluminescent devices based on TADF materials, Professor Chihaya Adachi, Hydrogen Production Research Division, I <sup>2</sup> CNER.
2	4 May 2013	Newspaper	<b>The Nikkei Shimbun</b> <b>The Yomiuri Shimbun</b> <b>The Nishinippon Shimbun</b> <b>The Nikkan Kogyo Shimbun</b> <b>Kyodo Tsushin (online)</b> <b>The Shikoku Shimbun (online)</b> <b>The Shizuoka Shimbun (online)</b> Newspaper article introducing remarkably durable high temperature polymer electrolyte fuel cell based on poly(vinylphosphonic acid)-doped polybenzimidazole, Professor Naotoshi Nakashima, Associate Professor Tsuyohiko Fujigaya, Fuel Cells Research Division, I <sup>2</sup> CNER.
3	27 May 2013	Magazine	<b>Nikkei Business</b> Magazine article introducing the groundbreaking organic materials, Professor Chihaya Adachi, Hydrogen Production Research Division, I <sup>2</sup> CNER.
4	16 Aug. 2013	Newspaper	<b>Nikkan Kogyo Shimbun</b> Newspaper article introducing news editions of SPring-8 (FSBL) that Professor Atsushi Takahara (Hydrogen Production Research Division, I <sup>2</sup> CNER) takes on the position of steering committee chairman.
5	29 Aug. 2013	Webpage	<b>Helmholtz Zentrum Berlin</b> <b>Massachusetts Institute of Technology/Materials Processing Center (24 Sept.)</b> Interview of Professor Harry Tuller, Fuel Cells Research Division, I <sup>2</sup> CNER.
6	7 Sep. 2013	Newspaper	<b>The Mid-Japan Economist</b> Newspaper article introducing the successful development without rare metals, Professor Chihaya Adachi, Hydrogen Production Research Division, I <sup>2</sup> CNER.

7	18 Sep. 2013	Newspaper	<b>Nikkan Kogyo Shimbun</b> Newspaper article introducing making things learned from nature 6 - biomimetic technology in Japan, Professor Atsushi Takahara, Hydrogen Production Research Division, I <sup>2</sup> CNER.
8	2 Oct. 2013	Newspaper	<b>The Nikkei Business Daily</b> Newspaper article introducing that fuel cell is expected to be downsized. Solid oxide fuel cell could be operated at 300°C, Professor Tatsumi Ishihara, Hydrogen Production Research Division, I <sup>2</sup> CNER.
9	16 Oct. 2013	Webpage	<b>Nanoinfo.jp</b> <b>Research-er.jp (17 Oct. 2013)</b> <b>Mynavi News (17 Oct. 2013)</b> Web article introducing empirical prediction of electronic potentials of single-walled carbon nanotubes with a specific chirality, Professor Naotoshi Nakashima, Fuel Cells Research Division, I <sup>2</sup> CNER.
10	17 Oct. 2013	Newspaper	<b>Kagaku kogyo nippo</b> Newspaper article introducing the invention of synthetic method for preparation of nanoscale Fe-group alloys, Assoc. Prof. Miho Yamauchi, Catalytic Materials Transformations Research Division, I <sup>2</sup> CNER.
11	21 Nov. 2014	Webpage	<b>Helmholtz-Zentrum Geesthacht</b> Web article introducing international ECOSTORE project, Professor Etsuo Akiba, Hydrogen Storage Research Division, I <sup>2</sup> CNER.
12	15 Jan. 2014	Television	<b>NHK (Ohayou Nippon)</b> Short interview of Assistant Professor Stephen Lyth, Fuel Cells Research Division, I <sup>2</sup> CNER.
13	23 Jan. 2014	Newspaper	<b>The Nishinippon Shimbun</b> Newspaper article, "New era between Japan and South Korea for conciliatory with cars. Take a step forward for contact, competition, and co-prosperity", Professor Tatsumi Ishihara, Hydrogen Production Research Division, I <sup>2</sup> CNER.
14	17 Feb. 2014	Journal	<b>The Bynkyo News</b> Article outline the I <sup>2</sup> CNER & ACT-C Joint Symposium held on Jan. 30 2014.
15	March 2014	Webpage	<b>JST Breakthrough Report</b> Web article introducing Prof. Seiji Ogo's research outcome. (Catalytic Materials Transformations Research Division, I <sup>2</sup> CNER)



## World Premier International Research Center Initiative (WPI)

### List of papers of representative of interdisciplinary research activities

- List up to 10 papers that underscoring each interdisciplinary research activity and give brief accounts (within 10 lines).
- For each, write the author name(s); year of publication; journal name, volume, page(s), and article title. Any listing order may be used as long as format is the same.  
If a paper has many authors, underline those affiliated with the Center.
- If a paper has many authors (say, more than 10), all of their names do not need to be listed.

- 1) Tornow, C. E., Thorson, M. R., Ma, S., Gewirth, A. A. and Kenis, P. J. A. (2012), Nitrogen based Catalysts for the Electrochemical Reduction of CO<sub>2</sub> to CO, *Journal of the American Chemical Society*, 134 (48), 19520-19523.

Synthesis and application of carbon-supported, nitrogen-based organometallic silver catalysts for the reduction of CO. Their performance toward the selective formation of CO is similar to the performance achieved when using Ag as the catalyst, but comparatively at much lower silver loading. Faradaic efficiencies of the organometallic catalyst are higher than 90%, which are comparable to those of Ag. Furthermore, with the addition of an amine ligand to Ag/C, the partial current density for CO increases significantly, suggesting a possible co-catalyst mechanism.

*The paper combines inorganic photochemistry and materials science*

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84870702915&partnerID=40&md5=f12dbefe09aeb6a6bdc8a94c984044de>

- 2) Lyth, S. M., Shao, H., Liu, J., Sasaki, K. and Akiba, K. (2014), Hydrogen adsorption on graphene foam synthesized by combustion of sodium ethoxide, *International Journal of Hydrogen Energy*, 39 (1), 376-380.

Expertise in electrocatalyst synthesis was used to create graphene foam with large surface area (>1500m<sup>2</sup>/g) as a hydrogen storage material, in collaboration between the Fuel Cell and the Hydrogen Storage divisions. A reversible hydrogen adsorption capacity of 2.6 wt.% was achieved; the highest value yet reported for pure graphene materials. In ongoing work the surface area is currently improved and the graphene foam is doped with heteroatoms to further improve the capacity.

*The article combines materials synthesis, organic chemistry, nanotechnology, and surface science.*

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84890441224&partnerID=40&md5=f82e318d876695b1b9410c0a4217db9b>

- 3) Liu, J., Takeshi, D., Orejon, D., Sasaki, K. and Lyth, S. M. (2014), Defective Nitrogen-Doped Graphene Foam: A Metal-Free, Non-Precious Electrocatalyst for the Oxygen Reduction Reaction in Acid, *Journal of the Electrochemical Society*, 161 (4), F544-F550

There is a major research effort worldwide to develop Pt-free, non-precious catalysts for the oxygen reduction reaction at PEFC cathodes. In this work, nitrogen-doped graphene foam with large surface area (> 700 m<sup>2</sup>/g) was synthesized as model metal-free non-precious electrocatalysts for the oxygen reduction reaction (ORR) in PEFCs. The purpose is to clarify the ORR in Fe/N/C-based electrocatalysts catalysts, which are still poorly understood. The results demonstrate the highest activity in acid for such Fe-free catalysts; that majority 4-electron ORR can occur in the absence of Fe; and the first double-Tafel slope, indicating Pt-like ORR. These catalysts are currently being explored at high temperature (> 120°C).

*The article combines materials synthesis, organic chemistry, nanotechnology, advanced characterization techniques, and electrochemistry.*

[http://apps.webofknowledge.com/full\\_record.do?product=UA&search\\_mode=GeneralSearch&qid=1&SID=S1bzly4cUUFzBf8WVR7&page=1&doc=1](http://apps.webofknowledge.com/full_record.do?product=UA&search_mode=GeneralSearch&qid=1&SID=S1bzly4cUUFzBf8WVR7&page=1&doc=1)

- 4) 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.

The origin of detrimental chemical expansion in oxides commonly used in fuel cells is uncovered for the first time with insight from atomistic level computational studies tied to experimental evidence. The article lays the groundwork to mitigate chemical expansion with expected improvements in fuel cell mechanical durability and lifetime.

*The article combines the disciplines of materials science thermodynamics, ceramic mechanical deformation, crystallography, and computational materials science. It also strongly couples experiment and theory.*

<http://www.scopus.com/record/display.url?eid=2-s2.0-84860711946&origin=inward&txGid=42369414EC9D8E3E08DF2702CA3E32EF.Vdktg6RVtMfaQJ4pNTCQ%3a1>

- 5) Bishop, S. R., Marrocchelli, D., Chatzichristodoulou, C., Perry, N. H., Mogensen, M. B., Tuller, H. L. and Wachsman, E. D. Chemical Expansion: Implications for Electrochemical Energy Storage and Conversion Devices, *Annual Review of Materials Research*, Accepted for Publication/Online.

This is the first comprehensive review of chemical expansion in energy related materials.

*It covers chemo-mechanical coupling across several energy-related technology areas.*

<http://www.annualreviews.org/doi/pdf/10.1146/annurev-matsci-070813-113329>  
(abstract only)

- 6) Edalati, K., Matsuda, J., Arita, M., Daio, T., Akiba, E. and Horita, Z. (2013), Mechanism of activation of TiFe intermetallics for hydrogen storage by severe plastic deformation using high-pressure torsion, *Applied Physics Letters*, 103 (14), 143902

Identification of the activation mechanisms in TiFe intermetallics by High Pressure Torsion

*The paper combines material synthesis, materials science, mechanical engineering, surface science, and characterization techniques to explore the activation mechanisms.*

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84885648001&partnerID=40&md5=3b33eddc6dfefb3e2f7384330e560773>

- 7) Inoki, D., Matsumoto, T., Nakai, H. and Ogo, S. (2013), Isolation and Crystal Structure of the Proposed Low-Valent Active Species in the H<sub>2</sub> Activation Catalytic Cycle, *European Journal of Inorganic Chemistry*, 2013 (22-23), 3978-3986.

This report provides the confirmation of our proposed design principles for a H<sub>2</sub> activation catalytic cycle by constructing a new catalyst.

*The paper combines Bioinorganic Chemistry, Coordination chemistry, Biochemistry.*

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84886530957&partnerID=40&md5=f53e4479839ffb9d3155f729daa60ce8>

- 8) Ogo, S., Ichikawa, K., Kishima, T., Matsumoto, T., Nakai, H., Kusaka, K. and Ohhara, T. (2013), A Functional [NiFe]Hydrogenase Mimic That Catalyzes Electron and Hydride Transfer from H<sub>2</sub>, *Science*, 339 (6120), 682-684.

This paper reports a functional [NiFe]-based model of [NiFe]hydrogenase enzymes, which can heterolytically activate hydrogen to form a hydride complex.

*The paper combines Bioinorganic Chemistry, Biochemistry, Coordination chemistry.*

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84873509989&partnerID=40&md5=d789830de1c6bd2751fe28e504d63c2c>

- 9) Matsumoto, T., Kim, K. and Ogo, S. (2011), Molecular Catalysis in a Fuel Cell, *Angewandte Chemie - International Edition*, 50 (47), 11202-11205.

The first molecular fuel cell based on a single molecular catalyst using a [NiFe]hydrogenase mimic was constructed that can function both in solid and solution phases, allowing precise observation of the mechanism of H<sub>2</sub> oxidation catalysis, while also exhibiting activity for the oxygen reduction reaction.

*The paper combines Bioinorganic Chemistry, Coordination Chemistry, Electrochemistry.*

<http://www.scopus.com/inward/record.url?eid=2-s2.0-81255179172&partnerID=40&md5=c7c2072e2d27761e4b088ce8772fff65>

- 10) Staykov, A., Yamabe, J. and Somerday, B. P. (2014), Effect of Hydrogen Gas Impurities on the Hydrogen Dissociation on Iron Surface, *International Journal of Quantum Chemistry*, 114 (10), 626-635

Basic mechanisms for trace oxygen inhibition of hydrogen uptake into steels using density functional theory (DFT) modeling.

*The paper combines materials science, computational chemistry.*

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84897572950&partnerID=40&md5=0fe642e9be988ed00ea5160dbcd0d8b4>

## World Premier International Research Center Initiative (WPI)

### Status of Collaboration with the Illinois Satellite Institute

#### 1. Coauthored Papers

- List the refereed papers that were coauthored between the center's researcher(s) in domestic institution(s) and the satellite in the University of Illinois.
- Provide data in same format as in Appendix 2-1. Italicize the names of authors affiliated with the satellite.
- If a paper has many authors (say, more than 10), all of their names do not need to be listed.

1. *Pacquette, A. L., Hagiwara, H., Ishihara, T. and Gewirth, A.A.* (2014), Fabrication of an oxysulfide of bismuth  $\text{Bi}_2\text{O}_2\text{S}$  and its photocatalytic activity in a  $\text{Bi}_2\text{O}_2\text{S}/\text{In}_2\text{O}_3$  composite, *Journal of Photochemistry and Photobiology A: Chemistry*, 277, 27-36.

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84891811951&partnerID=40&md5=031bc3d65ad90bff88a73afbf6c41f6b>

2. *Murakami, Y., Kanazaki, T., and Sofronis, P.* (2012), 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.

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84874346382&partnerID=40&md5=fda43d7d8a787b9f34e6a11811939236>

3. *Somerday, B. P., Sofronis, P., Nibur, K. A., San Marchi, C., and Kirchheim, R.* (2013) Elucidating the variables affecting accelerated fatigue crack growth of steels in hydrogen gas with low oxygen concentrations, *Acta Materialia*, 61 (16), 6153-6170.

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84882816876&partnerID=40&md5=af58abae5cf99750b5e03db5a485c37b>

4. *Martin, M. L., Sofronis, P., Robertson, I. M., Awane, T., and Murakami, Y.* (2013) A microstructural based understanding of hydrogen-enhanced fatigue of stainless steels, *International Journal of Fatigue*, 57, 28-36.

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84885960355&partnerID=40&md5=bea5e35b6d01580c1deef68da44b9bb3>

5. *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.

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84871955233&partnerID=40&md5=e2b56c1e1df9792076d901e10f9ec85c>

6. *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.

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84859109646&partnerID=40&md5=a36b5ba9044573c97b20909b31706156>

7. *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.

<http://www.scopus.com/inward/record.url?eid=2-s2.0-84864065508&partnerID=40&md5=2169bea8e4a27ee308b9637f73456523>

8. Tellez, H., Druce, J., Liao, D., Hall, A., Ishihara, T., Kilner, J., and Rockett, A., Low Energy Ion Scattering: Surface Preparation and Analysis of Cu(In,Ga)Se<sub>2</sub> for Photovoltaic Applications, submitted, *Progress in Photovoltaics*.
9. Tabara, M., Harish, S., Ikoma, Y., Horita, Z., Takata, Y., Cahill, D. G., and Kohno, M., Reduction in Thermal Conductivity of Crystalline Silicon Processed by High-Pressure Torsion, submitted, *Nanoscale Research Letters*.
10. Staykov, A., Jain, C. A., and Ertekin, E., A hybrid molecular switch for photocatalytic charge separation, planned for submission in June 2014.
11. Kitamura, K., Jiang, F., Valocchi, A.J., Chiyonobu, S., Tsuji, T., and Christensen, K. T., The Study of Heterogeneous Two-Phase Flow around Small-Scale Heterogeneity in Porous Sandstone by Measured Elastic Wave Velocities and LBM Simulation, submitted, *Journal of Geophysical Research—Solid Earth*.
12. Jhong, H.-R. M., Kenis, P. J. A., and Lyth, S. M., Nitrogen-doped Carbon Catalyst for Electrochemical CO<sub>2</sub> Conversion to CO, submitted, *Journal of the American Chemical Society*.

## 2. Status of Researcher Exchanges

- Using the below tables, indicate the number and length of researcher exchanges. Enter by fiscal year, and length of exchange.
- Write the number of principal investigator visits in the top of each space and the number of other researchers in the bottom.

&lt;To satellite&gt;

	Under 1 week	From 1 week to 1 month	From 1 month to 3 months	Over 3 months	Total
FY2010-2011	15 16	1 0	0 1	0 0	16 17
FY2012	0 3	0 0	0 1	0 1	0 5
FY2013	6 10	1 4	0 2	0 0	7 16
Total	21 29	2 4	0 4	0 1	23 38

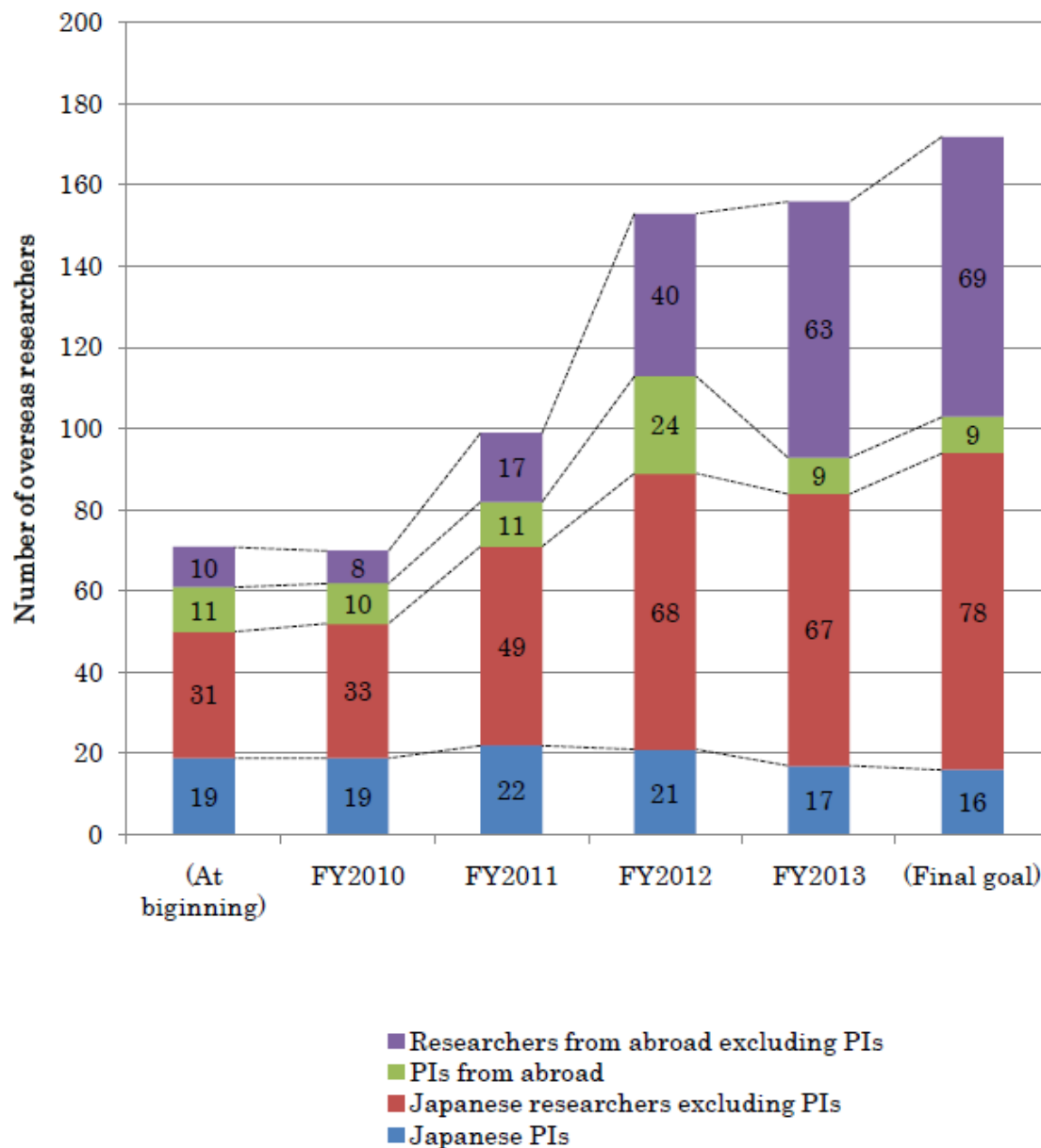
&lt;From satellite&gt;

	Under 1 week	From 1 week to 1 month	From 1 month to 3 months	Over 3 months	Total
FY2010-2011	12 6	4 1	0 0	0 0	16 7
FY2012	20 3	0 0	0 0	0 0	20 3
FY2013	3 16	0 3	0 0	0 0	3 19
Total	35 25	4 4	0 0	0 0	39 29

## World Premier International Research Center Initiative (WPI)

### 1. Number of overseas researchers and annual transition

\*Make a graph of the transition in the number of overseas researchers since the application.



## World Premier International Research Center Initiative (WPI)

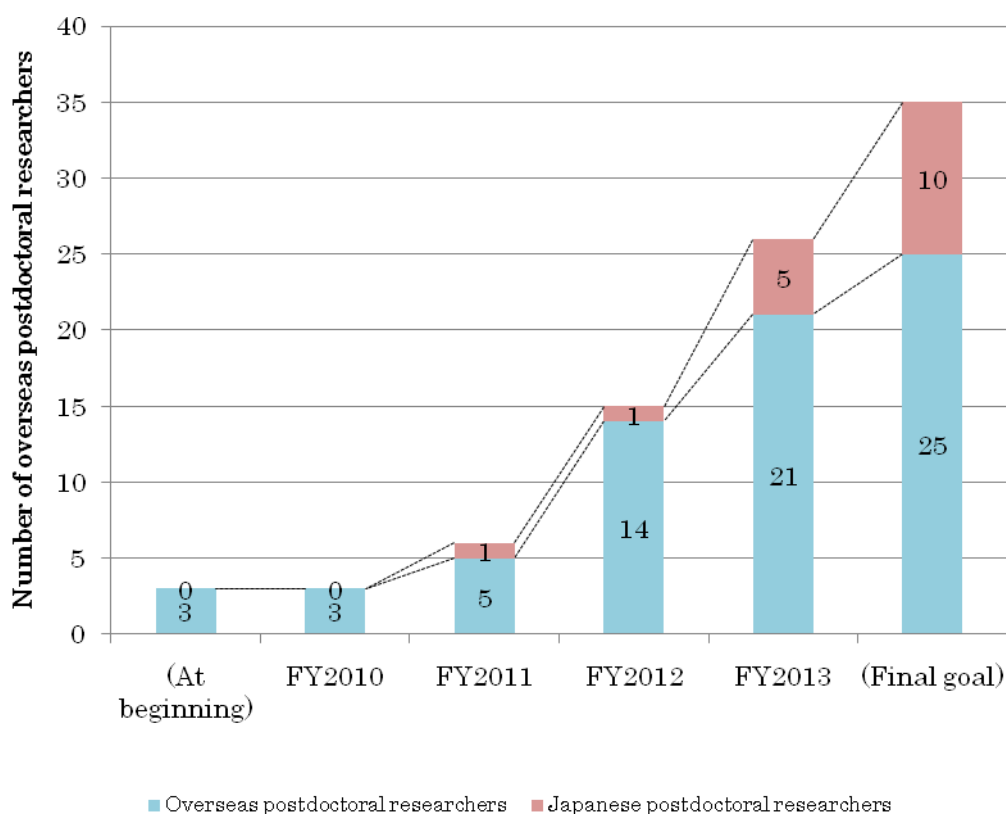
### 1. Postdoctoral positions through open international solicitations

- In the "number of applications" and "number of selection" columns, put the number and percentage of overseas researchers in the < > brackets.

FY	number of applications	number of selection
FY2010	75 <71, 95%>	1 < 0, 0%>
FY2011	62 <62, 100%>	2 < 2, 100%>
FY2012	13 < 12, 92%>	3 < 2, 67%>
FY2013	12 < 11, 92%>	2 < 1, 50%>

### 2. Number of overseas postdoctoral researchers and annual transition

\*Make a graph of the transition in the number of overseas postdoctoral researchers since the project application was submitted.





## 3. Status of postdoctoral researchers employment at institutions

- List each researcher in 1 line. If the list exceeds this form, please add extra pages.

Period of project participation	Previous Affiliation (organization, *country)	Next Affiliation (Position title, organization, *country)
Apr. 1, 2011 ~May. 31, 2012	Kyoto University, Japan	Assistant Professor, Nagoya University, Japan
Jan. 16, 2012 ~Present	Imperial College London, UK	
Apr. 1, 2012 ~Present	Kyushu University, Japan	
Sep. 1, 2012 ~Present	Northwestern University, USA	
Oct. 1, 2012 ~Present	Kyushu University, Japan	
Dec. 1, 2012 ~Present	Tohoku University, Japan	
Dec. 1, 2012 ~Present	Kyushu University, Japan	
Apr. 1, 2013 ~Jan. 31, 2014	Tokyo Institute of Technology, Japan	Postdoc, Eindhoven University of Technology (TU/e), Holland
Apr. 1, 2013 ~Nov. 30, 2014	JST(ERATO), Japan	Postdoc Researcher, Singapore University of Technology and Design, Singapore
Apr. 1, 2013 ~Present	Yale University, USA	
Apr. 1, 2013 ~Present	Kyushu University, Japan	
Apr. 1, 2013 ~Present	Kyushu University, Japan	
Apr. 1, 2013 ~Present	Kyushu University, Japan	
Apr. 1, 2013 ~Present	Kyushu University, Japan	
Apr. 1, 2013 ~Mar. 31, 2014	Hokkaido University, Japan	Assistant Professor, Chuo University, Japan
Apr. 1, 2013 ~Mar. 31, 2014	Kyushu University, Japan	Associate, The Matsushita Institute of Government and Management, Japan
Apr. 16, 2013 ~Present	ICMPE, CNRS-UMR 7182, France	
May. 1, 2013 ~Mar. 31, 2014	Kyushu University, Japan	Researcher, Iwate University, Japan
Oct. 1, 2013 ~Present	University of Edinburgh, UK	
Oct. 1, 2013 ~Present	JSPS(Postdoctoral Fellowship for Foreign Researchers), Japan	
Nov. 1, 2013 ~Dec. 30, 2013	Kyoto University, Japan	Researcher, Sriwijaya University, Indonesia
Jan. 1, 2013 ~Present	University of Kitakyushu, Japan	
Feb. 1, 2013 ~Present	Hokkaido University, Japan	
Feb. 1, 2013 ~Present	Kyushu University, Japan	

Apr. 1,2014 ~Present	Kyushu University, Japan	
Apr. 1,2014 ~Present	Kyushu University, Japan	
Apr. 1,2014 ~Present	Kyushu University, Japan	
Apr. 1,2014 ~Present	Kinki University, Japan	
Apr. 1,2014 ~Present	Toyota Central R&D Labs., inc, Japan	
Apr. 1,2014 ~Present	Kyoto University, Japan	

\*The country in which the organization is physically located.

## World Premier International Research Center Initiative (WPI)

### Holding International Research Meetings

For each fiscal year, indicate the number of international research conferences or symposiums held and give up to two examples of the most representative ones using the table below.

FY 2010-2011: 5 meetings

Major examples (meeting title and place held)	Number of participants
Kick-Off Symposium Kyushu University, Japan	From domestic institutions: 128 From overseas institutions: 26
I <sup>2</sup> CNER Satellite Kick-Off Symposium University of Illinois at Urbana-Champaign, U.S.	From domestic institutions: 70 From overseas institutions: 30

FY 2012: 3 meetings

Major examples (meeting title and place held)	Number of participants
I <sup>2</sup> CNER Tokyo Symposium Tokyo, Japan	From domestic institutions: 130 From overseas institutions: 20
I <sup>2</sup> CNER Annual Symposium Kyushu University, Japan	From domestic institutions: 159 From overseas institutions: 66

FY 2013: 4 meetings

Major examples (meeting title and place held)	Number of participants
Catalytic Concepts for Energy University of Illinois at Urbana-Champaign, U.S.	From domestic institutions: 50 From overseas institutions: 10
I <sup>2</sup> CNER & ACT-C Joint Symposium Kyushu University, Japan	From domestic institutions: 119 From overseas institutions: 58

## World Premier International Research Center Initiative (WPI)

### Host institution's commitment

#### 1. In-kind contributions from host institution (personnel, laboratory space, etc.)

##### **Tenured Positions**

- In addition to 5 tenured positions for associate professors, which were given in FY 2011 and 2012 by Kyushu University, I<sup>2</sup>CNER was successful at winning 1 tenured full professor position in the University Reform Revitalization Program in FY 2013 (I<sup>2</sup>CNER has secured a total of 6 positions as of April 1, 2014), as mentioned in Sections 6-4 and 7-2 of the report.

##### **Transfer of 9 PIs from the Faculty of Engineering**

- As of April 1, 2013, 9 I<sup>2</sup>CNER PIs have transferred to I<sup>2</sup>CNER from the Faculty of Engineering under the Intra-University Faculty Transfer System, which was initiated and administered by the KU President. The transfer of all 9 of them will continue for FY 2014, and is to be extended on an annual basis, as mentioned in Section 6-3 of the report.

##### **Temporary Loan of Laboratory and Office Space**

- As a solution to shortage of space for research activities conducted in the existing I<sup>2</sup>CNER Building 1, Kyushu University has made special arrangements for I<sup>2</sup>CNER to be able to use 4 laboratories and 1 office within the university until the opening of the second building.

##### **Allocation of an additional KU Staff Member**

- As of April 1, 2013, KU allocated one additional experienced Kyushu University staff member to the Administrative Office.

#### 2. System under which the center's director is able to make substantive personnel and budget allocation decisions

##### **Authority of the Director**

- Under the rule of Kyushu University, the Institute is positioned as a permanent international research institute. Governing documents have been developed to enable the Institute Director to make decisions on research plans, research frameworks, budget implementation, and other issues related to Institute management, in consultation with the Science Steering Committee, etc.

##### **Faculty Recruiting**

- New faculty recruitment is carried out through open international calls. The Director has been given the authority to recruit new faculty through open international calls. The Director makes the final hiring decisions in consideration of recommendations from the Faculty Recruiting Committee based on application screening and interviews, as mentioned in Sections 5-1-4 and 9 of the report.

##### **Merit-based Salary System**

- The Institute follows a special salary system (made possible by a special agreement between I<sup>2</sup>CNER and Kyushu University entitled "Regulations on Special Measures on the Hiring of National University Corporation Kyushu University International Institute for Carbon-Neutral Energy Research Employees") which deviates from the established salary ranges. Individual faculty and researcher salaries are determined based on individual accomplishments and contributions to the interests of the Institute, as decided by the Director, in consultation with the two Associate Directors, as mentioned in Section 6-3 of the report.

3. Support for the center director in coordinating with other departments at host institution when recruiting researchers, while giving reasonable regard to the educational and research activities of those departments

#### **Support of Cooperation of KU Researchers**

- Active support is provided to Kyushu University researchers to facilitate their engagement in the Institute's activities in coordination with the parent departments, such as requests for cooperation and arrangements with the head of his/her department.

#### **Intra-University Transfer System**

- In order to enable flexibility in allocating faculty within the University while further improving the standards of education and research conducted at Kyushu University, KU new established rules on the Intra-University Transfer system, which went into effect December 1, 2012. These rules enable researchers to safely and easily transfer their affiliations from their home departments to I<sup>2</sup>CNER. As mentioned above "1. In-kind contributions from host institution," 9 faculty members have transferred to I<sup>2</sup>CNER from the Faculty of Engineering. This process has improved the relationship between I<sup>2</sup>CNER and the Faculty of Engineering, which is an advantage for securing tenure-track positions jointly with the Faculty of Engineering. Most importantly, this relationship between I<sup>2</sup>CNER and the Faculty of Engineering has positively impacted PI mindset, as mentioned in Section 6-3 of the report.

4. Revamping host institution's internal systems to allow introducing of new management methods (e.g., English-language environment, merit-based pay, cross appointment, top-down decision making unfettered by conventional modes of operation)

#### **KU Internationalization Efforts**

- The President of Kyushu University has initiated plans to internationalize research and education within the university. As a part of this plan, efforts have been made to prepare internal documents, and to develop an English version of the university webpage. International Student and Researcher Support Centers have been established at every campus. Additionally, other matters will be changed by establishing new and revising current rules and regulations.

#### **TRIAD System**

- In an effort to improve the efficiency of storing and releasing the University's Japanese-English translated information, Kyushu University launched an online system, "Translated Information Archiving Database (TRIAD)," on March 27, 2014.

#### **Merit-based Salary System**

- As mentioned in 2. Above and Section 6-3 of the report, the Institute follows a special salary system (made possible by a special agreement between I<sup>2</sup>CNER and Kyushu University entitled "Regulations on Special Measures on the Hiring of National University Corporation Kyushu University International Institute for Carbon-Neutral Energy Research Employees") which deviates from the established salary ranges. Individual faculty and researcher salaries are determined based on individual accomplishments and contributions to the interests of the Institute, as decided by the Director, in consultation with the two Associate Directors.

#### **Cross Appointment of Director Sofronis**

- In consultation with the administration of the University of Illinois, it was decided that Prof. Sofronis be employed by Kyushu University as of June 1, 2012. This is KU's first case of cross appointment, as mentioned in Section 6-3 of the report.

5. Accommodation of center's requirements for infrastructural support (facilities, e.g., laboratory space; equipment; land, etc.)

#### **I<sup>2</sup>CNER Building 1**

- In order to continue developing a research environment befitting a top world-level research institute, I<sup>2</sup>CNER building 1 (approximately 4,873 m<sup>2</sup>) was completed at the end of November, 2012. The Institute's members moved into I<sup>2</sup>CNER building 1 in January 2013. A spacious lounge with a high ceiling and electronic black boards was designed in the lobby on the first floor in order to encourage impromptu meetings and exchanges of scientific views among I<sup>2</sup>CNER members. Facility equipment such as fume hoods and pneumatic piping has been installed in I<sup>2</sup>CNER Building 1, as mentioned in Section 2-5 of the report.

#### **Space Sharing with NEXT-FC**

- In January 2013, an additional 7 labs, 15 researcher's offices, and a server room have been secured for I<sup>2</sup>CNER's fuel cell researchers out of the space allocated to the Next-Generation Fuel Cell Research Center (NEXT-FC) within the I<sup>2</sup>CNER building. We also have secured labs for researchers of MIT and Imperial College London in order to promote exchange of researchers between KU and renowned foreign institutions, as mentioned in Section 2-5 of the report.

#### **I<sup>2</sup>CNER Building 2**

- A second I<sup>2</sup>CNER building which has 4 stories and a total floor space of 5,000 m<sup>2</sup> is currently being built. Floor plans for the building include 8 large-scale labs, 2 open offices, and 1 administrative office, with the majority of rooms being designed as open, common experimental spaces in order to promote interdisciplinary research. This building is funded by the FY 2012 supplementary budget from the Japanese government. Completion of I<sup>2</sup>CNER building 2 is planned for the end of February 2015, as mentioned in Section 2-5 of the report.

6. Support for other types of assistance

#### **Associate Directors**

- The two Associate Directors, Professors Ishihara and Takata work in tandem with and on behalf of the Director to meet the objectives of the Institute, as well as coordinating with related departments of the university. When the Director is in Illinois or traveling, Professors Ishihara and Takata maintain daily communication with him in order to relay and implement the Director's plans.

## World Premier International Research Center Initiative (WPI)

### Female researchers

\*Enter the number and percentage of female researchers in the top of each space and the total number of all the researchers in the bottom.

	FY2010	FY2011	FY2012	FY2013	Final goal
Researchers	3, 4%	7, 7%	14, 9%	18, 12%	29, 17%
	70	99	153	156	172
Principal investigators	1, 3%	2, 6%	3, 7%	1, 4%	1, 4%
	29	33	45	26	25
Other researchers	2, 5%	5, 8%	11, 10%	17, 13%	28, 19%
	41	66	108	130	147