World Premier International Research Center Initiative (WPI) FY2014 WPI Project Progress Report (Post-Interim Evaluation)

Host Institution	Kyushu University	Host Institution Head	Chiharu Kubo
Research Center	International Institute for Carbon-Neutral Energy Research (I ² CNER)	Center Director	Petros Sofronis

Common instructions:

Unless otherwise specified, prepare this report from the timeline of 31 March 2015.

* So as to base this fiscal year's follow-up review on the document "Post-interim evaluation revised center project," please prepare this report from the perspective of the revised project. * Use yen (¥) when writing monetary amounts in the report. If an exchange rate is used to calculate the yen amount,

give the rate.

Summary of State of WPI Center Project Progress (write within two pages)

As we embark upon I²CNER's second term, our principal goal is to establish the I²CNER brand worldwide through international, collaboration-driven transformational scientific advances which will lead to a carbon-neutral energy society. I²CNER's success in establishing this pinnacle will be determined by the international community's perception of the degree of I²CNER's success as a test bed for internationalization of scientific research and education in Japan, the U.S., and across the world. To achieve this international acclaim, I²CNER is tackling the key scientific challenges that define the path toward a carbon-neutral energy Japan and the establishment of sustainable energy supplies using limited energy resources. We believe that the requisite foundation and infrastructure for I²CNER to fully realize this global brand has been catalyzed during its first term.

Conducting research of the highest world level: Evidence of I²CNER's growing international stature and relevance can be seen in its 318 journal publications in FY 2014, of which, 28 were published in journals with an impact factor greater than 10. This accomplishment demonstrates a steadily increasing rate of the Center's productivity over the years (53, 150, 263, and 318, respectively in FY 2011, 12, 13, and 14). On a related note, since its inception, 117 of the Institute's publications have been cited 10 or more times, 42 have been cited 20 or more times, 20 have been cited 30 or more times, 10 have been cited 40 or more times, and 4 have been cited 50 or more times. In addition, we filed for 10 patents (7 of which are from the Fuel Cells division via the NEXT-FC center and within the Center-Of-Innovation Program).

In addition to being aligned with the roadmap scenarios for a carbon-neutral energy Japan developed by the Energy Analysis Division (EAD) of I²CNER, each I²CNER research effort has been focused so that it serves the objectives of the corresponding project in the division roadmap, and is aimed at the specific milestones that are identified on the division roadmaps. The roadmaps themselves have been updated to consolidate and focus our research effort as a whole, ensuring that they include ultimate targets and benchmarks, and, wherever possible, that long-term milestones have been converted into mid-term milestones.

The research activities of FY 2014 are as follows: PI Ishihara's group's discovery of a different surface composition of perovskite materials used in electrochemical cells is transforming the way we understand the operating principles of these materials in hydrogen production devices. In collaboration with the Ishihara group, Illinois Prof. X. Li has applied her remarkable MacEtch process for highly anisotropic wet etching of semiconductors to the fabrication of unique nanostructures that can potentially serve as an outstanding material for photo electrochemical cells. In the area of hydrogen compatible materials, PIs Robertson and Sofronis revealed a continuously changing microstructure by hydrogen. This result indicates future directions for development of physically-based model of hydrogen-induced degradation of metals. In addition, the Takaki group demonstrated the hydrogen compatibility of ultra-fine grained stainless steels, a crucial milestone in establishing the technological viability of these steels. This advance holds promise for reducing hydrogen fuel system costs by replacing the current low-strength, high-nickel steels (e.g., SUS316). Through a highly collaborative effort, Illinois Professors Kenis and Gewirth and Kyushu Prof. Nakashima, who is a world expert on stabilizing Pt-based electrocatalysts on carbon nanotubes, managed to electrochemically reduce CO₂ to CO with the lowest potential reported in the literature, and with current densities approaching those required for practical applications. The CO₂ Capture and Utilization division demonstrated that flue gas from a power plant can be used directly as the feed for electroreduction of CO₂ to CO, thus eliminating the energy intensive process of CO₂ separation from the flue gas. In the area of Fuel Cells, advances by the Sasaki group in Fe/N metal-free electrocatalysts have the potential of impacting PEFCs, due to their

remarkable durability and superb performance over 60,000 potential cycles in alkaline solution; the importance of this accomplishment can be better captured if we consider that the recently released Toyota Mirai car uses the expensive Pt/Co for its catalyst. Working with Illinois Professor Cahill, the Takata and Horita groups managed to reduce the thermal conductivity of silicon by a factor of up to 20 using severe material deformation, a significant contribution if one considers that high lattice thermal conductivity prevents the use of silicon as a thermoelectric material. Prof. Takata, advancing the field of adsorbents for next generation cooling systems, developed two new and promising absorbents that exhibit the highest ethanol uptake. The group of PI Akiba is leading the development of hydrogen storage materials by synthesizing new carbon-based materials with potential capacity over 10 wt % by tailoring their microstructure to meet required performance standards. Storing hydrogen as formic acid, PI Ogo and his group have discovered a bio-inspired catalyst that converts formic acid into hydrogen; this has the revolutionary potential to define a process to store hydrogen as a liquid under atmospheric conditions. The group of PI Katsuki, building on previous catalytic aerobic oxidation results with the use of iron or ruthenium complexes, has accomplished the monumental task of developing non-energy requiring aerobic oxidation. PIs Tsuji and Christensen carried out numerical and experimental studies of the role of capillary, viscous, and inertial forces for CO₂ trapping in geologic formations. This concerted effort yielded a transformation in our understanding of pore-scale flow processes, particularly in terms of the inertial effects not captured in pore-scale models currently used in geologic reservoir characterization. This advances our ability to both predict reservoir viability as well as post-injection CO₂ migration.

Advancing fusion: I^2 CNER has undertaken multiple initiatives to advance fusion research, most notably, the I^2 CNER Competitive Funding Program for young I^2 CNER researchers. The specific objective of this program is to foster interdisciplinary research and nurture young faculty and postdocs. The stringent criteria for this program include relevance to the I^2 CNER roadmap and a demonstrated potential for high-impact results. Participation in the program required proposal submission from young faculty and postdocs who have neither collaborated with one another previously, nor published together over the last two years. Winning recipients of I^2 CNER Competitive Funds are required to submit quarterly progress reports. The success of the Competitive Funding Program will be assessed at the end of FY2015.

This year's annual symposium on fuel generation and use brought together 12 prominent international scholars from disparate fields amongst the 141 total participants. Similarly, the nine international workshops run by the each of I²CNER's research divisions specifically focused on the interdisciplinary aspects of their research objectives. A major outcome of the 2015 I²CNER Annual Symposium and individual division workshops is that in FY 2015, I²CNER plans to host a workshop to explore cross-cutting themes for computational science, including catalysis, degradation, and select defect behaviors in order to discern what computational questions/problems I²CNER is best poised address in the future.

Globalization of the Institute: The addition of Prof. Fraser Armstrong of Oxford, Prof. Michael Celia of Princeton, and Mr. Mark Paster, a former energy analyst of the US Department of Energy, to I²CNER's External Advisory Committee is indicative of the international standing of the Institute. As of March 31, 2015, I²CNER has a total of 23 partner institutions in the US, Europe, and Asia, of which, I²CNER has agreements or MOUs with 4. A notable advance in I²CNER's international visibility is the conversations and exchanges of information with the Air Resources Board of the State of California (CARB), and ongoing discussions for an agreement with Helmholtz-Zentrum Geesthacht (HZG) of Germany. In addition, the second I²CNER in Tokyo Symposium was held on December 12, 2014 in order to show how merging Japan and the US academic and research cultures is impacting and transforming multidisciplinary international research and academic infrastructures, and explore what can be done to improve, enhance, and accelerate the transition of our research to impactful energy solutions. The US Ambassador to Japan, Ms. Caroline Kennedy, honored I²CNER by attending and giving remarks at this symposium. The Institute hosted 24 speakers (54% of which were foreign) in 22 seminars as part of the I²CNER Seminar Series.

The researchers of the Institute have also had success at elevating the Institute's visibility on an individual level. By way of example, I²CNER researchers hosted 42 distinguished visitors to Kyushu University from the United States, Canada, Europe, Korea, China, South Africa, Australia, France, Norway, Japan, and the United Kingdom. The Institute's researchers were responsible for organizing or co-organizing 8 international conferences, 6 international conference sessions, and 9 I²CNER international workshops. Similarly, our researchers have given more than 32 keynote, plenary, and invited presentations in international conferences and fora (for a list of the 10 most significant, please see Appendix 1B). In addition, our researchers have joint publications with researchers from 26 institutions around the world. Lastly, Institute researchers are playing leading roles in international networks for advancing hydrogen research and development, e.g. PI Akiba and International Energy Agency (for full details, please see Section 3).

Implementing organizational reforms: In support of the vision of Prof. Chiharu Kubo, KU's new President, the KU Administration has awarded I²CNER 3 tenured positions (2 associate professors and 1 professor) through the University Reform Revitalization Program in FY 2014. Two of these positions must be used to hire foreign faculty into the Institute. In view of the success of Prof. Sofronis' cross-appointment between Kyushu University and the University of Illinois, KU institutionalized a university-wide cross-appointment system in March 2015. Mr. Shunichi Masuda was appointed as the new Administrative Director, with a mandate to execute President Kubo's vision toward the goal of realizing the WPI mission Mr. Masuda's extensive experience working in industry, both in the US and Japan, makes him an within KU. ideal candidate for this position. I²CNER provides an unparalleled opportunity for many permanent Kyushu University employees, especially those who serve in the Institute's Administrative Office, to strengthen their English language skills, which can then be used in subsequent posts at KU. By way of example, a former I²CNER Associate Administrative Director was promoted to the Head of the International Student Exchange Division of the International Affairs Department as of September 1, 2014. These actions as well as the commitment from KU demonstrate the impact of the Institute in guiding institutional reform.

Others In FY 2014, I²CNER took major steps to increase its international visibility. The most notable of these steps may be the strengthening of the relationship between Kyushu University and the University of Illinois at Urbana-Champaign (UIUC). Specific actions to promote interaction between I²CNER and the I²CNER Satellite included a visit by UIUC Chancellor Phyllis Wise to Kyushu University; the signing of an Agreement on Academic Cooperation between the two universities on May 26, 2014; the signing of an Undergraduate Exchange Agreement on October 24, 2014; preliminary negotiations for a Revised Satellite Agreement, which will be finalized by November 2015; the hosting of 6 undergraduate exchange students from Kyushu University's Faculty of Engineering at UIUC from February 23-March 25, 2015; and a coordinated effort between the two universities to submit a joint pre-proposal to the NSF/JSPS Partnerships for International Research and Education (PIRE) program (the full proposal for this effort will be submitted on May 15, 2015).

• Please concisely describe the progress being made by the WPI center project from the viewpoints described below.

- In addressing the below-listed 1-6 criteria, please place emphasis on the following:
 - (1) Whether research is being carried out at a top world-level (including whether research advances are being made by fusing fields).
 - (2) Whether a proactive effort continues to be made to establish itself as a "truly" world premier international research center.
 - (3) Whether a steadfast effort is being made to secure the center's future development over the mid- to long term.

• Please prepare this report within 10-20 pages (excluding the appendices, and including Summary of State of WPI Center Project Progress (within two pages)).

1. Conducting research of the highest world level

* Regarding the criteria used when evaluating the world level of center, please note any updated results using your previous evaluation criteria and methods or any improvements you have made to those criteria and methods.

Evidence of I²CNER's growing international stature and relevance can be seen in its 318 journal publications in FY 2014, of which, 28 were published in journals with an impact factor greater than 10. In fact, the Institute's rate of productivity is steadily increasing (53, 150, 263, and 318 publications in FY 2011, 12, 13, and 14, respectively). On a related note, since its inception, 117 of the Institute's publications have been cited 10 or more times, 42 have been cited 20 or more times, 20 have been cited 30 or more times, 10 have been cited 40 or more times, and 4 have been cited 50 or more times. In addition, in FY 2014, I²CNER researchers received 50 national and international awards (including best poster presentations) from various societies and institutions, including Prof. T Kunitake's 2014 Order of Culture: Prof. Tsuji's award from the Seismological Society of Japan; Dr. A. Nagao's award from the Japan Institute of Invention and Innovation; Dr. H. Téllez-Lozano's award from 11th European SOFC&COE FORUM 2014; and Dr. B. P. Somerday's award from the U. S. Department of Energy. As an Institute, in FY 2014, we realized 4 of the short term milestones in our division roadmaps and made significant progress toward 5 milestones in other projects. We filed for 10 patents (7 of which are from the Fuel Cells division via the NEXT-FC center and within the Center-Of-Innovation Program). We hold agreements with 4 internationally recognized research centers/universities (SINTEF/NTNU, Illinois, CARB, and NFCRC) and ECOSTORE, a consortium based in the European Union.

In FY2014, I²CNER hosted 3 international symposia, and held 16 seminars in the Institute Interest Seminar Series and 22 seminars in the I²CNER Seminar Series. The Institute's researchers were responsible for organizing or co-organizing 8 international conferences, 6 international conference sessions, and 9 I²CNER international workshops. In addition, our researchers have joint publications with researchers from 26 institutions around the world. Our researchers have given more than 59 keynote, plenary and invited presentation in international conferences and fora (for a list of the 10 most significant, please see Appendix 1B).

The relevance of the I²CNER research efforts and objectives to enabling the green innovation initiative of the government of Japan is demonstrated by the large number (49) of collaborative projects in which its researchers are involved with industry (10 of these are within the NEXT-FC center). The following four projects resulted in technology transfer events: i) Prof. Horita's collaboration with Nagano Forging Co. Ltd to build an HPS (High-Pressure Sliding) facility with a maximum capacity of 500 tons, which is an upscaling of his laboratory facility; ii) Innovative surface-wave analysis to estimate localized heterogeneities in the Tomakomai CO₂ injection site has been provided by Prof. Tsuji to Japan CCS Corporation to help with the decisions on the suitability of drilling site locations; iii) Prof. Tsuji provided the Shikoku Research Institute, INC. & Shikoku Electric Power Co. INC. with a new approach to estimate earthquake intensity at their plants using conventional seismic data; and iv) Acting Lead PI of the EAD, Prof. Itaoka, is working on model development for hydrogen refueling stations and supply infrastructure for Toyota Motor Corporation (Geographical allocation in metropolitan areas and business model for refueling stations). Other projects that may result in technology transfer (commercial application) are: i) (Hydrogen Materials Compatibility Division) The development of a weld joint of XM-19 tubes for cost reduction of hydrogen refueling stations, Air Liquide Laboratories-results may lead to commercialization of weld joints and gases for welding; ii) (Hydrogen Materials Compatibility Division)

the inhibition of hydrogen embrittlement of pipeline materials by addition of impurities, Air Liquide Laboratories—results may lead to commercial application of chemical inhibitors; iii) (Hydrogen Storage Division) the development of rare-earth free AB₂ alloys for negative electrode of Ni-MH battery in collaboration with Panasonic Corporation—may result in a technology transfer event; and iv) (Catalytic Materials Transformations) Collaboration with DAIHATSU Motor Co., Ltd., Japan New Chisso Co., Ltd, and MITSUBISHI Chemical Co., Ltd within the framework of Fukuoka Industry-Academia Symphonicity to develop functional Pt-free molecular catalysts and biocatalysts for H₂ activation for low-cost hydrogen fuel cells.

The Institute's best accomplishments by division are as follows:

i) <u>Hydrogen Production</u>: Demonstration by the Ishihara group and collaborators of a different surface composition of perovskite materials used in electrochemical cells is changing the way we understand the operating principles of these materials in hydrogen production devices; the Adachi group has synthesized rare-metal free molecules that make light from nearly all current injected into organic light emitting devices for the first time, greatly advancing the methods for making high-efficiency organic light emitting devices.

ii) <u>Hydrogen Materials Compatibility:</u> Current hydrogen-induced degradation models assume an invariant material microstructure, but the Institute's recent results demonstrate a tangible step toward incorporating the observed hydrogen-induced dislocation microstructure evolution in a predictive, physics-informed model; demonstrating the hydrogen compatibility of ultra-fine grained (UFG) stainless steels is a crucial milestone in establishing the technological viability of these steels, which hold promise for reducing hydrogen fuel system costs by replacing the current low-strength, high-nickel steels (e.g., SUS316).

iii) <u>Fuel Cells:</u> Our research results in the chemomechanics of fuel cells provides a novel path forward to design durable oxides for next-generation solid oxide fuel cells, solid oxide electrolysis cells, gas separation membranes, and high temperature sensors, all with long lifetimes; whereas the recently-commercialized Toyota Mirai car uses Pt/Co for a catalyst, our advances in Fe/N metal-free electrocatalysts have the potential of impacting PEFCs, due to their remarkable durability and superb performance over 60,000 potential cycles in alkaline solution.

iv) <u>Thermal Science and Engineering</u>: Our newly synthesized adsorbent, based on spherical phenol resin treated with different mass ratios of KOH, can make waste-heat driven refrigeration systems more efficient, thus contributing drastically to the reduction of CO₂ emissions.

v) <u>Hydrogen Storage:</u> Hydrogen storage capacity over 10 wt % can be achieved by lightweight borohydrides and TiFe can be used to store renewable energy efficiently and cost-effectively.

vi) <u>Catalytic Materials Transformations</u>: Bio-derived [NiFe]Hydrogenase from citrobacter sp. S-77 natural catalyst is more active and potentially far cheaper than platinum as an electrode for H₂ oxidation reaction; Developed a catalyst for burning renewable fuels without generating carbon dioxide, underpinning green power generation technologies.

vii) <u>CO₂ Capture and Utilization</u>: Use of an IrO₂ catalyst instead of the much more costly Pt catalyst as an anode in a CO₂ electrolyzer flow cell improved current densities for CO production to over 250mA/cm² and energetic efficiencies to over 70% (an increase in efficiency of 40% over the use of Pt).

viii) <u>CO₂ Storage:</u> Numerical and experimental studies of the role of capillary, viscous, and inertial forces for CO₂ trapping yielded a transformation in our understanding of pore-scale flow processes, particularly in terms of the inertia effects not captured in pore-scale models currently used in reservoir characterization. This advances our ability to predict both reservoir viability and post-injection CO₂ migration. Detection of localized heterogeneity in the geological formation of the Tomakomai CO₂ capture and storage site advances our ability to characterize candidate storage reservoirs marked by heterogeneous rock formations—a key challenge towards fully realizing accurate characterization of candidate storage reservoirs, as well as monitoring and predicting CO₂ fate at the field scale in heterogeneous rock formations.

ix) <u>Energy Analysis:</u> Cost analysis of the I²CNER scenarios indicates that the overall cost benefits that we gain from the implementation of renewables hinges upon new research and technology for the integration of renewables into the grid.

In the following, the Institute's best accomplishments are described in more detail:

Hydrogen Production (Lead Principal Investigator: Prof. Ishihara)

The research in this division falls under the themes of energy production, conservation, and storage. Energy production is based on the conversion of solar to electric energy, storage is achieved through hydrogen fuel, and conservation is achieved through enhanced lighting efficiency based on high efficiency solid state lighting. Unique aspects are techniques for the analysis of the interface structure of organic dye and inorganic semiconductors, 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. As a complement, organic light emitting devices are being developed for high efficiency lighting for energy conservation. Selected results are:

Novel Surface Compositions of Perovskite Oxide Electrode Fuel Cell Materials

Our work has shown that after exposure to elevated temperatures, the surfaces of solid oxide electrode materials for electrolyzers (SOECs) and fuel cells (SOFCs) universally show a surface dominated by alkaline earth cations, with the transition metal (assumed to be the catalytically active site) absent. Although absent from the very outer layers, the transition metals are, however, enriched in a subsurface layer (see Fig. 1.1). Furthermore, this rearrangement occurs very rapidly and at relatively low temperatures. This improvement in our understanding of the surface composition of solid oxide electrode materials was achieved mainly through the application of a unique surface analytical technique, Low Energy Ion Scattering (LEIS) spectroscopy, which selectively probes the composition of the very outer atomic surface of a material.

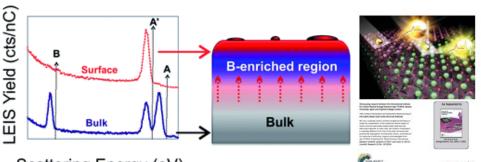
This is a significant accomplishment for I²CNER, because it challenges the prevailing consensus about the surface composition and oxygen exchange properties of solid oxide electrodes – most models assume transition metals are present in the very outer surface, which is disproved by our results. There is currently no model explaining how a surface such as SrO, which we typically observe, can facilitate the oxygen reduction reaction, which is critical to device performance. Our findings are already guiding computational studies both with Profs. Staykov and Ertekin within I²CNER, and groups at other international institutions.

The achievement represents a revolution in our understanding of the surface composition of the materials of interest, and contributes to the short-term milestone of the Hydrogen Production Division Project 1-1 (High Temperature Electrolysis), to improve the energy efficiency of electrolysers working at 500 °C. The understanding of changes in surface composition with time also contributes to the overall target of increasing durability to 0.5% degradation per 1000 hours.

Key Publications for this work

J. Druce, H. Téllez, M. Burriel, M.D. Sharp, L.J. Fawcett, S.N. Cook, D.S. McPhail, T. Ishihara, H.H. Brongersma, J.A. Kilner, Surface Termination and Subsurface Restructuring of Perovskite-Based Solid Oxide Electrode Materials, Energy and Environmental Science, vol. 7, iss. 11, pp. 3593 – 3599, 2014.

H. Téllez, J. Druce, Y.-W. Ju, J. Kilner, T. Ishihara, Surface chemistry evolution in LnBaCo₂O_{5+ δ} double perovskites for oxygen electrodes, International Journal of Hydrogen Energy, vol.39, pp. 20856 – 20863, 2014.



Scattering Energy (eV)

Fig. 1.1. Low energy ion scattering [LEIS] data (left) showing peaks due to Ba (peak A*), Gd (peak A), and Co (peak B) related to the surface and bulk composition of $GdBaCo_2O_{5+\delta}$. The surface of the sample shows only Ba indicating a surface consisting entirely alkali earth cations. The underlying region is enriched in the transition metal (for example Co; middle schematic figure). The right hand figure shows an artists conception of LEIS experiment here featured on the cover of the journal issue.

Design of Metal-free Fluorescent/Phosphorescent Blends for High Efficiency Light Emission

Organic materials exhibiting thermally active delayed fluorescence (TADF) show great promise as emitters in organic light-emitting diodes (OLEDs) for application to highly-efficient and low-cost lighting and displays and have reached internal quantum efficiencies (IQE) of 100% in some cases. By enabling

the conversion of triplets into singlets for emission by fluorescence in a purely organic molecule, TADF emitters overcome some of the limitations of fluorescent materials. The latter are restricted to an IQE of 25% because only one-fourth of electrically-generated excitons are formed as light-emitting singlets. Phosphorescent materials typically require expensive rare-earth metals to utilize the three-fourths of excitons generated as triplets. However, TADF materials still suffer from short operational lifetimes and strong efficiency roll-off at high brightnesses.

One key cause of these issues is the large population of long-lived triplets in OLEDs using TADF emitters. The triplets participate in degradation reactions and exciton annihilation processes. The large triplet population partially results from a relatively slow rate of fluorescence (kf) in most TADF emitters compared to conventionally fluorescent emitters. Although a small energy difference between the triplet and singlet states (Δ EST) enables the triplets in TADF materials to up-convert into singlets by absorbing thermal energy, the low kf allows singlets to down-convert back into triplets before emission, leading to multiple conversion cycles, a higher population of triplets, and a longer exciton lifetime.

To confront these issues, we have pursued two routes in parallel. On the one hand, we have synthesized new blue TADF emitters with increased fluorescent emission, while maintaining a small singlet-to-triplet energy state difference. We have thus achieved a maximum external quantum efficiency (EQE) of 21%. This was accomplished by developing new molecular design guidelines based on relationships between molecular structures and properties. On the other hand, we were able to achieve 100% IQE with improved molecular lifetimes by devising a new system that uses conventional fluorescent materials as emitters and TADF molecules as assistant dopants to convert the non-emitting triplets into singlets before transfer of the energy to the fluorescent emitters.

For the development of new blue emitters, we systematically studied the relationships between computationally modeled and experimentally measured properties for a series of molecules (Fig. 1(a)). The energy separation of the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO), used to minimize the energy difference between the singlet and triplet states, often leads to a small fluorescence emission rate. From this investigation, we found that a small energy difference can be maintained while increasing fluorescence by delocalizing the HOMO and/or LUMO over a larger volume.

Through this study, we developed a new blue TADF emitter with a peak electroluminescence (EL) wavelength of 478 nm and nEQE of 16.8%, which corresponds to an nIQE of 84%. For a material with a greener blue emission (peak EL wavelength of 487 nm), an even higher nEQE of 20.6% was achieved (Figs. 1.2 (b) and (c)). The high efficiencies are attributed in part to the high fluorescence rate in these materials, reducing the number of singlets that go through multiple cycles before emission. This reduces the triplet population. The new molecules are an important step toward efficient blue emitters, which are important for full-color displays but have been difficult to realize with TADF materials. Furthermore, these guidelines for the design of TADF molecules will aid in the development of new materials.

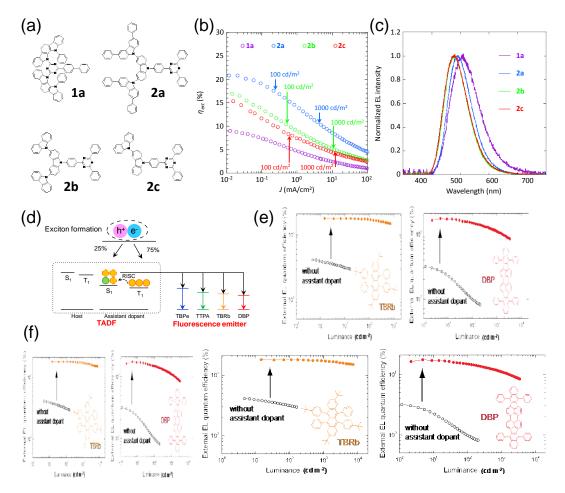


Fig. 1.2. (a) Chemical structures of the studied materials. The degree of HOMO delocalization increases from compound **2c** down to **2a**. (b) External quantum efficiency vs. current density (*J*) characteristics for OLEDs using the TADF materials as emitter. (c) Emission spectra of the OLEDs. (d) Working mechanism of the TAF system. (e) Emission spectra for four different TAF OLEDs using different fluorescent emitters. (f) Output characteristics for three of the TAF OLEDs with (filled shapes) and without (empty shapes) the fluorescent emitter. The assistant dopants for the TBPe, TTPA, TBRb, and DBP devices were ACRSA, ACRXTN, PXZ-TRZ, and Tri-PXZ-TRZ, respectively.

In our second route, we exploited the higher fluorescence rate, better stability, and color purity of conventional fluorescent organic molecules while using our TADF materials to harvest nearly 100% of excitons. In our system, which we call TADF-assisted fluorescence (TAF), excitons are formed and converted into triplets on the TADF materials before being transferred to conventional fluorescent emitters doped into the same film (Fig. 1.2 (d)). The fast nature of singlet energy transfer from TADF to fluorescent materials and the high fluorescence rate of conventional fluorescent materials, which exceeds that of TADF materials, reduces the triplet population by rapid shuttling of the singlets to the fluorescent materials for quick radiative decay before they can convert back into triplets. The use of a conventional fluorescent material also improves the color purity of emission and enables the realization of additional colors using existing materials without the development of new TADF emitters.

To realize this system, we first selected candidate materials from our inventory of developed TADF materials and known fluorescent materials with properties suitable for energy transfer and high emission efficiency. After identifying and optimizing material combinations exhibiting energy transfer based on photoluminescence measurements, we applied the best combinations to devices. We achieved EQE of 13%-18% from blue, green, yellow, and red fluorescent emitters, as shown in Figs. 1.2 (e) and (f). These correspond to maximum power efficiencies of 47 and 58 lm/W for green and yellow emission, respectively, and an IQE approaching 100% for yellow and red emission. Furthermore, comparison of TADF-based and TAF-based OLEDs showed an approximately five-fold increase in half-brightness operational lifetime to 194 h by inclusion of the fluorescent emitter in the yellow device. Although small-area devices (1 mm²) for ease of fabrication and testing were used here, these results are a step toward our short-term milestone of achieving power efficiencies of over 80 lm/W in 5 cm × 5 cm devices (benchmark of 131 lm/W) and long-term goal of half-brightness lifetimes surpassing 10,000 h.

This work can be seen as a progression of our previous work for harvesting triplets for light emission without the use of phosphorescent materials containing heavy metals that started with the development

of TADF emitters. The new blue TADF emitters and design guidelines are the result of a continued deepening of our prior studies on TADF emitters and will advance the design of new TADF materials as both emitters and assistant dopants. The TAF system branches off from our previous work by utilizing the TADF materials for a different role. In addition to improvements in stability and efficiency relative to TADF and conventional fluorescence, respectively, our new route also enables the realization of highly-efficient emission with various colors from a wide-range of existing fluorescent materials using already-developed TADF materials. For these reasons, this accomplishment has great potential for the further development of highly-efficient lighting and displays based on OLEDs.

Publications

S. Hirata, Y. Sakai, K. Masui, H. Tanaka, S.Y. Lee, H. Nomura, N. Nakamura, M. Yasumatsu, H. Nakanotani, Q. Zhang, K. Shizu, H. M., C. Adachi, Highly efficient blue electroluminescence based on thermally activated delayed fluorescence. Nature Materials, vol. 14, pp. 330-336, 2015.

H. Nakanotani, T. Higuchi, T. Furukawa, K. Masui, K. Morimoto, M. Numata, H. Tanaka, Y. Sagara, T. Yasuda, C. Adachi, High-efficiency organic light-emitting diodes with fluorescent emitters, Nature Communications, vol. 5, no. 4016, 2014.

Hydrogen Materials Compatibility (Lead Principal Investigator: Dr. Somerday)

The goal of this division is to provide the basic science that will enable 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:

Effect of hydrogen-induced microstructure evolution on the mechanisms of fracture.

The integrated scientific achievements described below represent progress toward the milestone of identifying mechanisms for hydrogen-induced fracture mode transitions in ferritic and austenitic alloys, considering the role of hydrogen-induced microstructure evolution. This short-term milestone is featured in the division Project 1: Physical Descriptions of Hydrogen-Materials Interactions.

In previous accomplishments, hydrogen-affected deformation was implicated as a contributing factor to hydrogen-induced degradation of structural metals. For example, it was suggested that hydrogen-induced cracking at grain boundaries in nickel was promoted in part by hydrogen-affected deformation. One objective for Project 1 is to explore a potential link between hydrogen-affected deformation and hydrogen-induced degradation across material classes and to identify specific mechanistic roles for hydrogen-affected deformation in promoting material damage.

In conventional austenitic stainless steels currently specified for hydrogen containment components, the mechanism for reduced ductility or higher fatigue crack growth rate in the presence of hydrogen has not been well understood. In a study led by Dr. Akihide Nagao (WPI Visiting Scholar), two commercial austenitic stainless steels with different alloy compositions were examined: 316L and 304. Non-charged (4 mass ppm of H) and hydrogen-charged (104 mass ppm of H) specimens were subjected to slow strain rate and fatigue-crack growth tests. In the slow strain rate tests, hydrogen-charged 316L does not show any reduction in ductility compared with the non-charged material, whereas 304 shows a 74% decrease in ductility in the hydrogen-charged state. A ductile dimpled morphology was observed on fracture surfaces for both non-charged and hydrogen-charged 316L. In contrast for 304, the fracture surface in the non-charged state was dominated by ductile dimples, whereas in the hydrogen-charged state it has a mixed morphology of "flat" and "quasi-cleavage" features. The mechanism for the reduction in ductility of 304 is being pursued by mainly revealing the microstructure immediately beneath the hydrogen-induced fracture surface using a FIB-TEM technique. This FIB-TEM technique was featured in previous accomplishments and represents a state-of-the-art method for evaluating a potential link between hydrogen-affected deformation and material damage.

In a complementary study led by Prof. Reiner Kirchheim (WPI PI), experiments on the effect of hydrogen on the formation of dislocations during plastic deformation of metals were conducted and interpreted in a general model of solute defect interaction. Palladium was chosen as a model face-centered cubic (FCC) material for studying the development of dislocations during slow strain rate and fatigue testing of hydrogen-exposed alloys. In this study, it was shown that during cold rolling of palladium more dislocations were produced in the presence of dissolved hydrogen when compared with hydrogen-free palladium. The increased dislocation density was determined by X-ray diffraction, transmission electron microscopy (Fig. 1.3), and using hydrogen as a probe. This experimental evidence

provides compelling support for a general model on solute-defect interaction developed by Prof. Kirchheim. These results obtained for the Pd-H system suggest that the effect of hydrogen on dislocation microstructure evolution has general validity in FCC alloys, i.e., such hydrogen-dislocation interactions likely apply to the 316L and 304 stainless steels described above. It is possible that this effect of hydrogen on dislocation microstructure evolution may be linked to material damage.

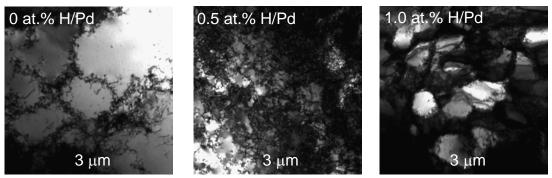


Fig. 1.3. Transmission electron microscopy (TEM) micrographs of cold-rolled palladium with various amounts of dissolved hydrogen. In H-free Pd (left) the dislocations are arranged in walls around dislocation free cells. With 0.5 at.% H significantly more dislocations have been generated and the cells become smaller (middle). With 1 at.% H the contrast between adjacent cells is pronounced due to a very high dislocation density in the walls and a corresponding misorientation between cells.

The results on hydrogen-induced dislocation formation in the Pd-H system suggest that the dislocation microstructure and hydrogen transported by mobile dislocations may play important roles in establishing the local conditions that promote failure. For example, hydrogen transport by mobile dislocations may allow excess hydrogen concentrations at the levels required for decohesion events to initiate, e.g. at grain boundaries. In a study led by Prof. Petros Sofronis (WPI PI) and Prof. Ian Robertson (WPI PI), this effect was quantified by developing a revised model for hydrogen transport that accounts for hydrogen carried by dislocations along with stress driven diffusion and trapping at other microstructural defects. This revised model represents an advancement in predicting local hydrogen concentrations, since the classical hydrogen transport model accounts for hydrostatic drift and trapping of hydrogen at defects but neglects the effect of hydrogen transport by moving dislocations. The impact of this additional transport mechanism was explored for cracked specimens under small scale yielding and plane strain conditions, assuming the material is hydrogen-exposed austenitic stainless steel, i.e., Nitronics 40. This modeling indicates that dislocation transport can contribute to elevated local hydrogen concentrations ahead of the crack tip to levels above those predicted by the classical diffusion model. This is the first step toward capturing the experimentally observed effect of hydrogen on dislocation microstructure evolution in a predictive model for hydrogen-induced material degradation. Such models must accurately quantify the hydrogen populations ahead of a crack tip to inform the failure criterion.

Publications

K.E. Nygren, A. Nagao, M. Dadfarnia, P. Sofronis, I.M. Robertson, Effect of hydrogen on fatigue-crack growth behavior of types 316L and 304 austenitic stainless steels, CAMP-ISIJ, vol. 28, p. 301, 2015.

M. Deutges, H.P. Barth, Y. Chen, C. Borchers, R. Kirchheim, Hydrogen diffusivities as a measure of relative dislocation densities in palladium and increase of the density by plastic deformation in the presence of dissolved hydrogen, Acta Materialia, vol. 82, pp. 266–274, 2015.

R. Kirchheim, A. Pundt, Hydrogen in Metals. In: D.E. Laughlin, K. Hono (Eds.), Physical Metallurgy, pp. 2597–2705, 2014.

Y.Z. Chen, X.Y. Ma, X.H. Shi, T. Suo, C. Borchers, K.H. Zhang, F. Liu, R. Kirchheim, Hardening effects in plastically deformed Pd with the addition of H, Scripta Materialia, vol. 98, pp. 48-51, 2015.

M. Dadfarnia, M.L. Martin, A. Nagao, P. Sofronis, I.M. Robertson, Modeling hydrogen transport by dislocations, Journal of the Mechanics and Physics of Solids, 2015, in press. (DOI: 10.1016/j.jmps.2015.03.002).

Ultra-fine grained materials for hydrogen compatibility: technology impact.

The scientific achievements described below represent progress toward the milestones of develop hydrogen-compatible, lower-cost austenitic stainless steels having 400 MPa yield strength and quantify fatigue limit in hydrogen gas for austenitic stainless steel with 400 MPa yield strength. These short-term milestones are featured in the division's Project 2: High-Strength, Low-Cost Stainless Steels for H_2 Service.

Prof. Setsuo Takaki (WPI PI) has pioneered the process of ultra-grain refinement in austenitic stainless steels. Such grain refinement significantly increases the strength of austenitic steels while retaining acceptable ductility. Based on physical descriptions of hydrogen-materials interactions reported in the literature (i.e., studies related to Project 1), it was expected that ultra-grain refinement of austenitic steels could also improve resistance to hydrogen-induced degradation. Previous research results in Project 2 confirmed this trend from slow strain rate testing of hydrogen-exposed ultra-fine grained (UFG) stainless steels. As demonstrated from the stress vs. strain curves in Fig. 1.4, the tensile ductility of the metastable Fe-16Cr-10Ni austenitic stainless steel with grain sizes of 1µm and 6µm is not degraded by hydrogen (24.5 mass ppm concentration). Since the UFG steel with 1µm grain size has a yield strength of 585 MPa, these results represent progress toward the short-term milestone of developing a hydrogen compatibile austenitic stainless steel having 400 MPa yield strength. However, evaluating hydrogen compatibility with slow strain rate testing on hydrogen-exposed stainless steels. Results from fatigue testing are more relevant for establishing hydrogen compatibility of structural materials for hydrogen fuel technology applications.

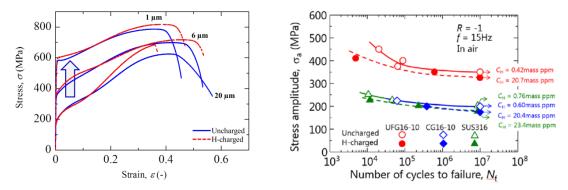


Fig. 1.4. The stress vs. strain curves measured for Fe-16Cr-10Ni stainless steel show that hydrogen does not degrade tensile ductility for materials with 1 μ m and 6 μ m grain sizes (left). The stress amplitude vs. cycles to failure relationships measured for Fe-16Cr-10Ni stainless steel with 1 μ m grain size (UFG16-10) and 20 μ m grain size (CG16-10) demonstrate that the UFG material has a higher fatigue limit that is not degraded by hydrogen (right).

The need for technology-relevant hydrogen compatibility data was addressed by performing fatigue tests on the hydrogen-exposed UFG stainless steel. As shown in Fig. 1.4, the number of cycles to failure was measured for several stainless steels as a function of the cyclic stress amplitude. These stainless steels included the UFG material, a coarse-grained (CG) material with the same alloy composition, and a commercial stainless steel (SUS316). The stress amplitude vs. cycles to failure relationship was determined for the stainless steels in the hydrogen-charged (20 to 23 mass ppm concentration) and non-charged conditions. Two notable results are revealed from the data in Figure 1.4. First, the fatigue limit (e.g., stress amplitude at 10⁷ cycles) is significantly higher for the UFG material compared to the CG and commercial stainless steels. In addition, this relatively high fatigue limit is not degraded by hydrogen. This result demonstrates that hydrogen containment components designed according to the fatigue limit can be fabricated with UFG stainless steel and be considered as hydrogen compatible.

The results presented above represent a significant advancement toward the collective milestones of develop hydrogen-compatible, lower-cost austenitic stainless steels having 400 MPa yield strength and quantify fatigue limit in hydrogen gas for austenitic stainless steel with 400 MPa yield strength. The remaining effort to complete this milestone may be to measure the fatigue limit of the UFG stainless steel with higher hydrogen concentrations. The UFG stainless steel could tangibly benefit hydrogen fuel technology by reducing the cost of components without compromising hydrogen compatibility. By applying the UFG material processing, high-strength type 304 stainless steel could replace low-strength type 316 stainless steel in hydrogen fuel systems, which would significantly decrease system cost while retaining resistance to hydrogen-induced degradation.

Publications

A. Macadre, K. Tsuboi, N. Nakada, T. Tsuchiyama, S. Takaki, Ultra-grain refinement effect on tensile and phase transformation behaviour in a metastable austenitic steel charged in hydrogen gas, Procedia Materials Science, vol. 3, pp. 350-356, 2014.

K. Mori, M. Kubota, A. Macadre, Fatigue properties of ultra-fine grain austenitic stainless steel and effect of hydrogen, Proceedings of the third Japan-China Joint Symposium on Fatigue of Engineering Materials and Structures, Takayama, Japan, pp. 82-85, 2014.

Fuel Cells (Lead Principal Investigator: Prof. Sasaki)

The objective of this division is to develop more durable and efficient, lower cost fuel cells, such as polymer electrolyte fuel cells (PEFCs) and solid oxide fuel cells (SOFCs). In PEFCs, efforts are directed at a) the development of higher temperature (> 100°C) hydrogen PEM fuel cells with durable catalyst support, b) finding and evaluating high temperature electrolytes with emphasis on a polybenzimidazole (PBI)-based ionomer in combination with carbon nanotubes, including additional materials, such as graphene. 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 the Integrated Gasification Fuel Cell Combined Cycle (IGFC) and the Natural Gas Triple Combined Cycle. Selected representative results are:

Chemo-Mechanics of Fuel Cell Oxides

One goal of the fuel cell division is to enhance the durability of solid oxide fuel cells with a target of 90,000 h stable operation. Currently, the operating lifetime is limited, in part, by thermo-chemical expansion-induced stresses within the brittle oxide components (Fig. 1.5), exceeding their strength and leading to mechanical failure, such as cracking and delamination of the electrolyte and electrodes. Chemical expansion is one causative process, whereby the oxides expand in an amount proportional to the loss of oxygen from their lattice; the proportionality is described by the chemical expansion coefficient. In order to minimize these strains and thereby enhance durability, it is necessary to understand the chemical expansion process at a fundamental level so that materials with low chemical expansion coefficients can be rationally designed.

Therefore, in our work we combine both *in situ* macroscopic and crystal-level experimental studies with atomistic computational simulations of model systems, to investigate the chemical expansion of fuel cell oxides in detail. Building on the work of previous years, in FY2014 this approach led to several key achievements: 1) In response to the emergence of this new field of chemo-mechanics of oxides, we published an invited review paper in collaboration with experts around the world defining chemical expansion and its implications for energy conversion devices; 2) We identified four key factors impacting chemical expansion in the technologically important perovskite structure – charge localization, crystal symmetry, temperature, and oxygen vacancy size – leading to development of design principles for low chemical expansion coefficients in perovskites; and 3) We developed a comprehensive empirical model that relates perovskite chemical expansion to the size of the constituent ions, enabling determination of the effective size of an oxygen vacancy in a variety of perovskite oxides, a key parameter controlling chemical expansion.

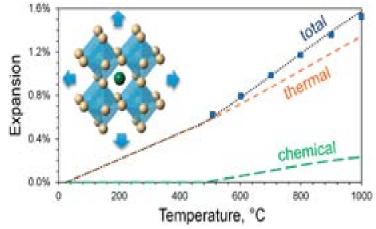


Fig. 1. 5. Relative contributions of thermal and chemical processes to the expansion of a perovskite. *J. Mater. Chem. A* 3, 3602-3611, (2015)

These achievements are expected to have widespread impact. First, our review paper increases awareness of the significance of chemo-mechanical coupling in energy devices and describes tools to investigate it to a wide audience, potentially leading to a broader international effort to design durable energy device materials. Second, we have demonstrated for the first time, by theory and experiment, certain controllable variables that correlate to smaller chemical expansion coefficients (and therefore greater durability) of perovskites. These variables provide a novel path forward to design durable oxides for next-generation solid oxide fuel cells, solid oxide electrolysis cells, gas separation membranes, and high temperature sensors, with long lifetimes.

This work is a significant accomplishment toward the long term durability milestone against all major degradation mechanisms, especially impurity poisoning of SOFCs, in Project 2 in the Division's Roadmap.

Publications

S.R. Bishop, D. Marrocchelli, C. Chatzichristodoulou, M. Mogensen, N.H. Perry, H.L. Tuller, E.D. Wachsman (Invited review), Chemical Expansion: Implications for Electrochemical Energy Storage and Conversion Devices, Annual Review of Materials Research, vol. 44, pp. 205-239, 2014.

N.H. Perry, S.R. Bishop, H.L. Tuller, Tailoring Chemical Expansion by Controlling Charge Localization: In Situ X-ray Diffraction and Dilatometric Study of $(La,Sr)(Ga,Ni)O_{3-\delta}$ Perovskite, Journal of Materials Chemistry A, vol. 2, pp. 18906-18916, 2014.

N.H. Perry, J.J. Kim, S.R. Bishop, H.L. Tuller, Strongly Coupled Thermal and Chemical Expansion in the Perovskite Oxide System Sr(Ti,Fe)O_{3-a}, Journal of Materials Chemistry A, vol. 3, pp. 3602-3611, 2015. D. Marrocchelli, N.H. Perry, S.R. Bishop, Understanding Chemical Expansion in Perovskite-Structured Oxides, Physical Chemistry Chemical Physics, vol. 17, pp. 10028-10039, 2015.

Metal-free Electrocatalysts for the Oxygen Reduction Reaction

Pt/Co/C is the state-of-the-art catalyst for the oxygen reduction reaction (ORR) in PEFCs. However this material is expensive and degrades during potential cycling. Fe/N/C-based catalysts are the most promising alternative ORR catalysts to date, but their durability is still problematic due to significant H_2O_2 production and the presence of Fe which leaches during operation. Fundamental understanding of these electrocatalysts is necessary to make further improvements.

We take a unique approach of studying *metal-free* nitrogen-doped graphene as a model electrocatalyst system. Previous studies generally struggle to remove the influence of Fe contamination. We observe high current densities for the ORR in acid, with some 4-electron transfer contribution. *This challenges the current paradigm that Fe-free sites only catalyze 2-electron ORR.* We show that metal-free tertiary N sites may catalyze the 4-electron ORR in acid. Additionally we have demonstrated remarkable durability of this catalyst, far out-performing Pt over 60,000 potential cycles in alkaline solution.

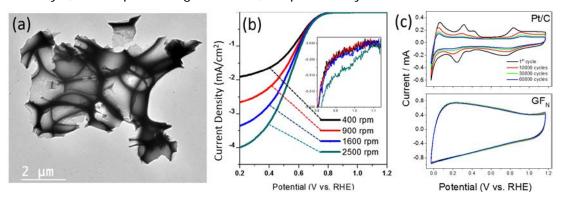


Fig. 1. 6. (a) TEM of nitrogen-doped graphene foam. (b) ORR current density in acid solution. (c) Comparison of the durability of Pt/C and nitrogen-doped graphene foam in alkaline solution, over 60,000 cycles (FCCJ protocol).

This work is a major accomplishment against the short term milestone to meet NEDO/FCCJ & DOE durability targets and the ultimate target of achieving durability for longer than 15 years in Project 1 in the division roadmap.

Publications

J. Liu, T. Daio, D. Orejon, K. Sasaki, S.M. Lyth, Defective Nitrogen-Doped Graphene Foam: A Metal-Free, Non-Precious Electrocatalyst for the Oxygen Reduction Reaction in Acid, Journal of the Electrochemical Society, vol. 161, iss. 4, pp. F544-F550, 2014.

J. Liu, T. Daio, B. Cunning, K. Sasaki, S.M. Lyth, Nitrogen-Doped Graphene Foam as a Highly Durable Metal-Free Electrocatalyst for the Oxygen Reduction Reaction in Alkaline Solution, Journal of Materials Chemistry A (Under Revision, 2015).

Thermal Science and Engineering (Lead Principal Investigator: Prof. Takata)

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 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 efficiency and

reduced CO₂ emissions. Selected representative results are:

Near-vacuum generation by hydrogen permeation

Hydrogen permeation through metals and alloys is of great concern in hydrogen containment systems. In this study, hydrogen contained in seamless coiled tube vessels made of SUS316L and Inconel 625 permeated the vessel walls at temperatures from 573 K to 773 K, and the decreasing interior pressure of the vessels was monitored for an extended period of time to characterize the behavior of the pressure change. It was found that the pressure in the vessels became lower than the surrounding atmospheric pressure, and the vessels reached nearly vacuum conditions, (exactly, the partial pressure of impurities). Hydrogen permeabilities through SUS316L and Inconel 625 were determined from the pressure drop measurements. The pressure drop behavior was compared to, and found to be consistent with, theoretical calculations performed using the obtained permeabilities based on Fick's law of diffusion.

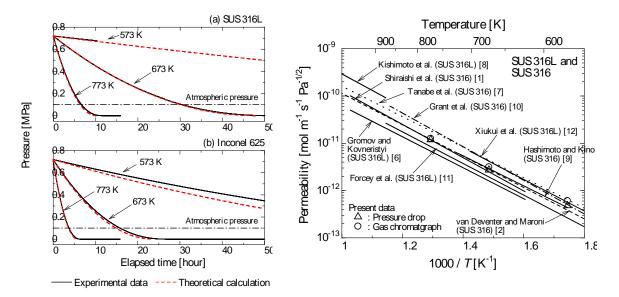


Fig. 1. 7. (Left) Pressure drop due to permeation of hydrogen in seamless coiled tube vessels made of (a) SUS316L and (b) Inconel 625. (Right) Temperature dependence of the hydrogen permeability through SUS316L and SUS316. References quoted inside brackets are from the references section of the publication below.

This work satisfies the short term milestone of the establishment of a prediction method for hydrogen permeation through a metal wall in Thermophysical Properties Project 1 (TP-1) in the division roadmap.

Publication:

N. Sakoda, R. Kumagai, R. Ishida, K. Shinzato, M. Kohno, Y. Takata, Vacuum generation by hydrogen permeation to atmosphere through austenitic and nickel-basealloy vessel walls at temperatures from 573 K to 773 K, International Journal of Hydrogen Energy, vol. 39, pp. 11316-11320, 2014.

Adsorbents for next generation cooling systems

Adsorption characteristics of ethanol onto two promising adsorbents have been investigated for developing high performance adsorption chillers. These new adsorbents are based on spherical phenol resin treated with different mass ratios of KOH named as KOH4-PR and KOH6-PR. Experimental adsorption isotherm measurements show that the adsorption capacity of KOH4-PR/ethanol is as high as 1.43 kg kg⁻¹ while one kg of KOH6-PR is able to adsorb nearly about 2 kg of ethanol. To the best of our knowledge, the studied adsorbents possess the highest ethanol uptake. Moreover, we found that the KOH4-PR/ethanol pair has notably high adsorption kinetics at the lower range of adsorption temperatures. Experimental measurements of adsorption uptake and adsorption uptake rate of the studied pairs have been analyzed and isosteric heats of adsorption have also been extracted.

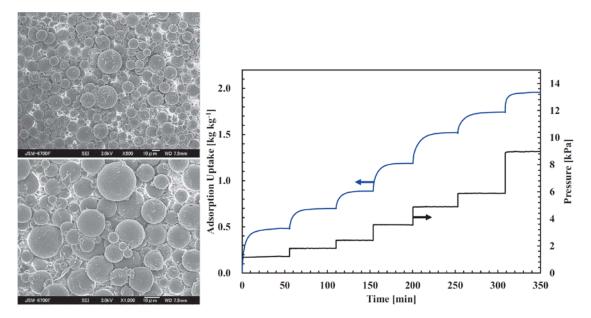


Fig. 1.8. (Left) SEM pictures of KOH4-PR adsorbent samples. (Right) Profiles of adsorption uptake and pressure for KOH6-PR/ethanol pair at adsorption temperature 30°C.

This work satisfies the short- and mid-term milestones of developing a clear understanding of adsorption/desorption processes of activated carbon in HMT Project 2 in the division roadmap.

Publication:

1.1. El-Sharkawy, K. Uddin, T. Miyazaki, B.B. Saha, S. Koyama, H.-S. Kil, S.-H. Yoon, J. Miyawaki, Adsorption of ethanol onto phenol resin based adsorbents for developing next generation cooling systems, International Journal of Heat and Mass Transfer, vol. 81, pp. 171–178, 2015.

Hydrogen Storage (Lead Principal Investigator: Prof. Akiba)

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. Selected representative results are:

Influence of grain boundaries on activation of TiFe

TiFe samples were processed by four different routes (annealing, groove rolling, high-pressure torsion (HPT) and ball milling) to produce different microstructural features. It was found that there is a strong relationship between the grain size (fraction of grain boundaries) and activation pressure for hydrogen absorption: the hydrogen pressure for activation decreases with decreasing grain size as shown in Fig. 1.9.

The generation of grain boundaries (as well as stacking faults) also appears to be effective for activation of other hydrogen storage materials such as Mg₂Ni.

This study provides important finding for the milestone of "Start commercialization of HPT-processed TiFe for stationary application and HPT-processed Mg alloys for on board application " in the Project 3 of the Division.

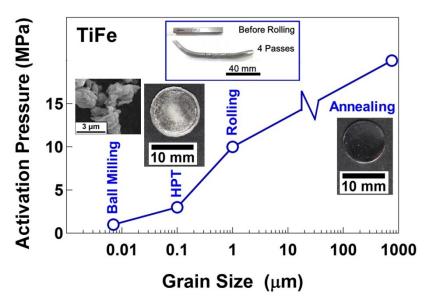


Fig. 1.9. Decreasing activation pressure of TiFe by decreasing grain size.

Publications

K. Edalati, J. Matsuda, A. Yanagida, E. Akiba, Z. Horita, Activation of TiFe for hydrogen storage by plastic deformation using groove rolling and high-pressure torsion: Similarities and differences, International Journal of Hydrogen Energy, vol. 39, pp. 15589-15594, 2014.

H. Emami, K. Edalati, J. Matsuda, E. Akiba, Z. Horita, Hydrogen storage performance of TiFe after processing by ball milling, Acta Materialia, vol. 88, pp. 190-195, 2015.

T. Hongo, K. Edalati, M. Arita, J. Matsuda, E. Akiba, Z. Horita, Significance of grain boundaries and stacking faults on hydrogen storage properties of Mg₂Ni intermetallics processed by high-pressure torsion, Acta Materialia, vol. 92, pp. 46-54, 2015.

*Complex hydride LiBH*₄ as a lightweight hydrogen storage material

The complex hydride LiBH₄, with a hydrogen density of 18.5 mass%, has been attracting significant interest as a lightweight hydrogen storage material. However, it has a high dehydrogenation and rehydrogenation temperature because of the formation of Li₂B₁₂H₁₂ as a dehydrogenated intermediate. Introduction of Ni is expected to reduce the dehydrogenation enthalpy, and suppress the formation of Li₂B₁₂H₁₂ by nickel boride like Ni₄B₃, Ni₂B or Ni₃B.

In this study, we systematically investigated the effect of nanosized Ni on the dehydrogenation and rehydrogenation reactions of LiBH₄ using thermogravimetry, quadrupole mass spectrometry and pressure-composition-isotherm analyses. Nanosized Ni particles were homogeneously dispersed on the surface of LiBH₄ after ball milling. The dehydrogenation peak temperature of LiBH₄ was reduced from 743 K to 696 K with addition of 25 mass% Ni. First, LiBH₄ tended to react with Ni to form Ni₄B₃, which suggests the thermodynamic destabilization effect of Ni. Then, the in-situ formed Ni₄B₃ was suggested to play a catalytic role on the dehydrogenation of the unreacted LiBH₄. Moreover, the rehydrogenation content of LiBH₄ was improved from 4.3 mass% to 10.8 mass% by addition of 25 mass% Ni, suggesting the significant improvement effect of Ni₄B₃ on the rehydrogenation.

This study provides important finding for the milestone of "Define relationship between formation of intermediates and de-/re-hydrogenation of borohydrides" in the Project 2 of the Division.

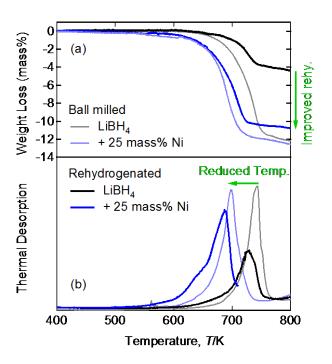


Fig. 1.10 (a) Thermogravimetry (TG) and (b) quadrupole mass spectrometer (QMS) measurement results of ball milled LiBH₄ and LiBH₄—Ni as well as the samples after rehydrogenation under a hydrogen pressure of 35.0 MPa at 823 K for 24 h.

Publications

H.-W. Li, Y. Yan, E. Akiba, S.-i. Orimo, Improved Dehydrogenation and Rehydrogenation Properties of LiBH₄ by Nanosized Ni Addition, Materials Transactions, vol. 55, pp. 1134-1137, 2014.

Catalytic Materials Transformations (Lead Principal Investigator: Prof. Ogo)

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. The 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_2 emissions in energy, power, or industrial production processes. Projects in the division address the development of: (i) novel biological and biomimetic catalysts for H_2 , CO_2 , and H_2O activation based on naturally occurring enzymes; (ii) materials development toward the realization of a carbon-neutral power generation cycle. Selected representative results based on biology's ways with hydrogen are:

[NiFe]Hydrogenase from Citrobacter sp. S-77 Surpasses Platinum as an Electrode for H_2 Oxidation Reaction.

In a paper that combines biochemistry, bioinorganic chemistry, and electrochemistry, we reported an electrode for H₂ oxidation, based on [NiFe]Hydrogenase from our isolated new bacterium *Citrobacter* sp. S-77, that has 637 times higher mass activity than platinum at 50 mV in a hydrogen half-cell. The hydrogenase electrode is also stable in air and, unlike Pt, can be recovered 100% after poisoning by carbon monoxide. Following characterization of the [NiFe]Hydrogenase electrode, we demonstrate the construction of a fuel cell comprising [NiFe]Hydrogenase anode and Pt cathode with a higher power density than that achievable by Pt.

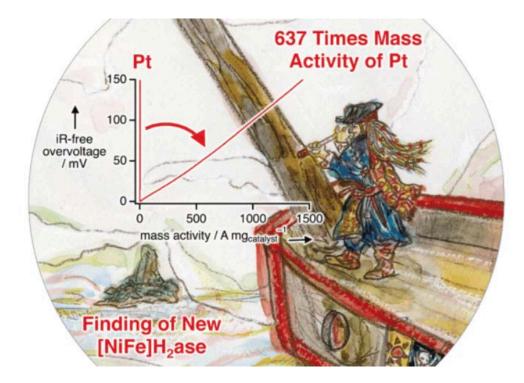


Fig. 1.11 Image of finding of H₂ase S–77. Selected for the cover picture of *Angewandte Chemie International Edition* (ACIE)

Together with the previous studies of biomimetic [NiFe]hydrogenase published in Science 2013, we have satisfactorily realized the short-term milestone on " H_2 -activation: Isolation of new hydrogenase and its model complex" in the division's roadmap for Project 1. In fact this is the best result achieved worldwide (Prof. Ogo's benchmark).

Publication

T. Matsumoto, S. Eguchi, H. Nakai, T. Hibino, K.S. Yoon, S. Ogo, [NiFe]Hydrogenase from Citrobacter sp. S-77 Surpasses Platinum as an Electrode for H_2 Oxidation Reaction, Angew. Chem. Int. Ed., vol. 53, iss. 34, pp. 8895–8898, 2014.

[Cover Picture] [Press Release] [NHK and RKB Mainichi Broadcasting Corporation] [NHK Radio] [Nikkankogyo Shimbun, Nikkei Shimbun, Nishinippon Shimbun, Mainichi Shimbun, Sankei Shimbunand Yomiuri Shimbun] [Wiley Science Cafe] [Science Portal]

*CO*₂-Free Power Generation on an Iron Group Nanoalloy Catalyst via Selective Oxidation of Ethylene Glycol to Oxalic Acid in Alkaline Media

We are developing catalysts which enable electric power generation without CO_2 emission by selective oxidations of fuels as a target in the first period of our road map. In this year, we succeeded in the preparation of nanoalloy (NA) catalysts composed of iron-group elements. An Fe group ternary nanoalloy catalyst exhibits selective electrocatalysis towards CO_2 -free power generation from highly deliverable ethylene glycol (EG). We examined the distribution of oxidised species, including CO_2 , produced on the FeCoNi nanoalloy catalyst in the EG electrooxidation under alkaline conditions. The FeCoNi nanoalloy catalyst showed the highest selectivities toward the formation of C_2 products and to oxalic acid, i.e., 99 and 60%, respectively, at 0.4 V vs. the reversible hydrogen electrode (RHE), without CO_2 generation. We successfully generated power by a direct EG alkaline fuel cell employing the FeCoNi nanoalloy catalyst and a solid-oxide electrolyte with oxygen reduction ability, i.e., a completely precious-metal-free system.



Fig. 1.12. CO₂-free power generation by selective fuel oxidation with iron-group nanoalloy catalysts.

This work is related to the short-term milestone "Non-platinum catalysts: 50 mW·cm⁻¹" of Project 3 "development toward carbon-neutral power generation cycles" in the division's roadmap and it is the first report of completely precious-metal-free alkaline fuel cells.

Publication

T. Matsumoto, M. Sadakiyo, M. L. Ooi, S. Kitano, T. Yamamoto, S. Matsumura, K. Kato, T. Takeguchi, M. Yamauchi, CO₂-free power generation on an iron group nanoalloy catalyst via selective oxidation of ethylene glycol to oxalic acid in alkaline media, Scientific Reports, vol. 4, no. 5620, 2014.

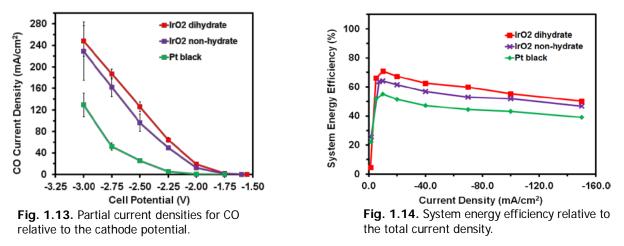
CO₂ Capture and Utilization (Lead Principal Investigator: Prof. Fujikawa)

The objective of this division is to develop: (1) highly efficient materials for CO_2 separation in power generation and industrial processes; and (2) electrochemical methods to convert CO₂ into value-added chemicals, such as a liquid fuels or their intermediates, in an energy-efficient and cost-effective way. In the area of CO_2 separation, the objective is to develop novel membrane technology to separate CO_2 in the process of pre-combustion for Integrated Coal Gasification Combined Cycle (IGCC), post-combustion at power plants and other industries, and for gas purification at natural gas wells. Membrane separation presents serious scientific challenges. Conventional membrane technologies are limited by low gas permeability, although their CO_2 selectivity is now reaching acceptable levels for application. The most promising approach to improve gas permeability is membrane thinning, because current membranes are still several microns thick. Thus, research in this division focuses on the design and development of materials for thinner membranes for selective gas separation. In the area of *electrochemical CO₂ conversion*, the objective is to develop better catalysts and electrodes. Most current catalysts require a high over-potential to drive electrochemical reduction of CO₂. Thus, the focus of the division is to develop catalysts that reduce this overpotential, thereby increasing the energetic efficiency of the process, while at the same time creating electrodes that eliminate mass-transport limitations in the electrolyzer cells. Selected representative results are:

Improving anode catalyst for the efficient electrochemical conversion of CO₂ to CO

In this project, we have achieved the highest current density for electroreduction of CO_2 to CO reported to date under ambient conditions through the optimization of anode catalysts. Recently, significant efforts have focused on the exploration of new cathode catalysts since the present high overpotential and low conversion rates on cathode catalysts prevent this process from being further developed for commercialization, however, considerably fewer efforts have studied how improvement the anode affects overall cell performance. Apart from our extensive research on the cathode catalyst, we believed that the optimization on the anode catalyst would improve the whole system performance In one of the projects we have accomplished this year, we showed that in combination significantly. with high performance Ag cathodes and 1 M KOH electrolyte, the use of IrO2 instead of Pt black (a widely used anode catalyst in CO₂ reduction applications) as the anode catalyst lowered ~0.2 V onset potential to 1.6 V, and achieved the highest partial current densities for CO (250 mA cm⁻², Fig. 1.13) reported to date under ambient conditions, compared to 130 mA cm⁻² when Pt black was used as the anode catalyst. Also, the use of IrO_2 anodes led to energy efficiencies as high as 70% (Fig. 1.14), which is about 40% improvement compared to the case using Pt as the anode catalyst. This work demonstrates that we have already reached the benchmark (Faradaic efficiency: 80~85%, energy efficiency: >70%, current density: 250 mA cm⁻²) in our Division's roadmap for CO production. Although highest energy efficiency and highest current density are not achieved at the same time, we believe that this finding, in combination with further development on the cathode catalyst, will finally help us produce high amount of CO at energy efficiency above 70%. This work is related to Project 2

"Electrochemical conversion" in the division's roadmap and addresses the closely related short-term milestones of "Catalysts for efficient CO_2 conversion" and "Optimize faradaic efficiency, current density, energetic efficiency". In fact this performance meets the division's CO production benchmark of "Faradaic Efficiency: 80~85%; Energy Efficiency: >70%; Current Density: 250 mA cm⁻²."



Publication

S. Ma, R. Luo, S. Moniri, Y. Lan, P.J.A. Kenis, Efficient Electrochemical Flow System with Improved Anode for the Conversion of CO_2 to CO, Journal of the Electrochemical Society, vol. 161, iss. 10, pp. F1124-F1131, 2014.

CO₂ Storage (Lead Principal Investigator: Prof. Tsuji)

The objective of this division is to: develop methods of reservoir characterization and modeling, and new effective monitoring of injected/leaked CO_2 to help ensure safe and permanent CO_2 sequestration in sub-seabed geologic formations; and propose and realize new carbon storage concepts suitable for geological formations and rock types typical of 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_2 injection in aquifer formations, and the requirement for long term monitoring of pressure variations near seismogenic faults. Selected representative results include:

Identify reservoir conditions for effective and safe CO_2 storage (pore-scale investigation)

To quantify capillary trapping mechanisms and access suitable reservoir conditions for efficient and safe CO_2 storage, we characterized CO_2 cluster within rock pore under different interfacial tension (IFT) conditions mainly using the lattice Boltzmann method (LBM) (see Fig. 1.14 (a)). Here we injected water into the CO_2 -saturated rock to evaluate capillary CO_2 trapping. A force balance factor N between capillary and viscous force is proposed to evaluate the instability of trapped CO_2 (Fig. 1.14 (b)). An increase of the instability factor N indicates that the capillary force becomes unable to balance the viscous pressure drop, and the shear force starts contributing to the face balance state. We found that the N increases with the size of CO_2 cluster, indicating larger CO_2 cluster is unstable and should be easier to remobilize (Fig. 1.14 (c)). We further demonstrated that N decreases at the condition of higher interfacial tension, Fig. 1.14 (c). Therefore, high interfacial tension conditions increase residual saturation (Fig. 1.14 (d)) and improve the both capacity and stability of residual trapping storage.

Complementary experiments porous micromodel experiments at reservoir conditions wherein water was displaced by liquid CO_2 revealed the dynamics of CO_2 fingering in porous media relevant to geologic CO_2 storage. In particular, finger penetration into the porous matrix was found to occur over very short, intermittent time scales at velocities orders larger than the injection velocity. Using the microscopic particle image velocimetry (micro-PIV) technique, these are the first measurements of this kind to quantify these flow dynamics and indicate that inertial forces may be an important aspect of the force balance at the pore scale, together with capillary and viscous forces (Fig. 1.15). By understanding the transient nature of CO_2 displacement of water, optimal conditions for effective and safe storage of CO_2 can be identified.

The accomplishment represents a transformation in our understanding of pore-scale flow processes, particularly those not captured in pore-scale models currently used in reservoir characterization, and contributes to the short-term milestone (Model injected CO_2 behavior (residual, solubility and mineral trapping) from laboratory expt. & simulation) of the Division's Project 1-1 (Pore-scale investigation of CO_2 fate).

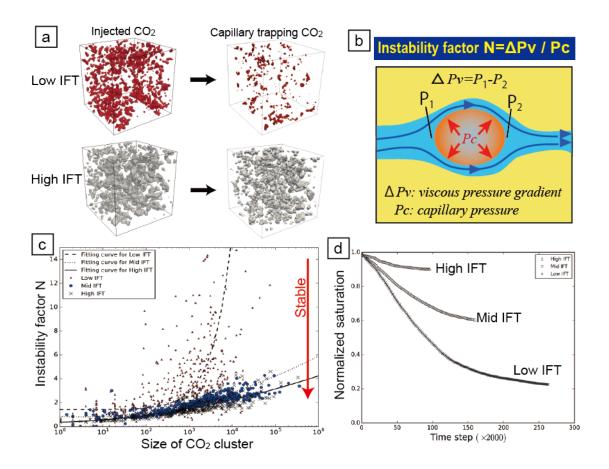


Fig. 1.14 (a) Injected CO_2 cluster (left) and capillary trapping CO_2 (right) simulated via LBM. (b) Schematic image of pore body and throat, and definition of instability factor. Blue region indicates pore space. (c) Instability factor N parameterized by size of CO_2 cluster and interfacial tension (IFT). (d) Normalized CO_2 saturation decreases due to water injection, but at the higher IFT conditions CO_2 is effectively trapped.

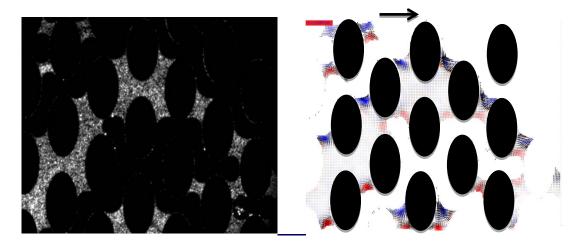


Fig. 1.15. (Left) Image showing liquid CO_2 infiltration (dark regions) from left to right at 80 bar into a water-saturated, periodic porous micromodel (porous pillars are dark ellipses). Water is seeded with fluorescent particles and this fluorescence is readily apparent above. (Right) Instantaneous velocity field in the water phase owing to liquid CO2 infiltration (white regions) from left to right at 80 bar into a water-saturated, periodic porous micromodel (porous pillars are dark ellipses). Vectors represent water velocity and contour represent vorticity (red: counter clockwise; blue: clockwise).

Publications

G. Blois, J.M. Barros, K.T. Christensen, A Microscopic Particle Image Velocimetry Method for Studying the Dynamics of Immiscible Liquid-Liquid Interactions in a Porous Micromodel, Microfluidics and Nanofluidics, vol. 18, pp. 1391-1406, 2015.

F. Jiang, T. Tsuji, Impact of interfacial tension on residual CO₂ clusters in porous sandstone, Water

Resources Research, vol. 51, iss. 3, pp. 1710-1722, 2015.

F. Kazemifar, G. Blois, D.C. Kyritsis, K.T. Christensen, A Methodology for Velocity Field Measurement in Multiphase High-Pressure Flow of CO₂ and Water in Micromodels, Water Resources Research, 2015, (DOI: 10.1002/2014WR016787)

F. Kazemifar, G. Blois, D.C. Kyritsis, K.T. Christensen, Quantifying the Flow Dynamics of Supercritical CO₂–Water Displacement in a 2D Porous Micro-Model using Fluorescent Microscopy and Microscopic PIV, Advances in Water Resources, 2015 (in revision).

Detection of localized heterogeneity in geological formation of the Tomakomai CO_2 capture and storage (CCS) site

We developed an advanced method using surface waves to estimate the 3D S-wave velocity (i.e. shear modulus) and the attenuation coefficient of geological formations. Using this method, we detected localized heterogeneity in the shallow geological formations in the Tomakomai CCS project site, which is the first large-scale CCS project in Japan. We successfully estimated a 3D S-wave velocity model (Fig. 1.16 (a)) whose resolution is ~10 times higher than that of conventional reflection profiles. Using information regarding amplitude decay of surface waves, we firstly estimated the 3D attenuation coefficient and detected localized heterogeneity in shallow geological formations (Figs. 1.16 (b) and (c)). Our study also showed that seismic attenuation is sensitive to the localized fracture (crack), compared to the S-wave velocity. This is the first result to identify the localized heterogeneity using surface waves in an actual CO_2 storage site. The estimated heterogeneous structure can provide vital information for CO_2 geological storage, including evaluation of CO_2 leakage paths, estimation of permeability heterogeneity for CO_2 modeling, and enhances estimations of lithology strength used to prevent CO_2 injection induced seismicity.

This accomplishment represents progress close to the realization of the short-term milestone on "Field-scale reservoir characterization in heterogeneous formation" in the division's roadmap for Project 2: Injected CO_2 monitoring and Field-scale investigation of CO_2 behavior.

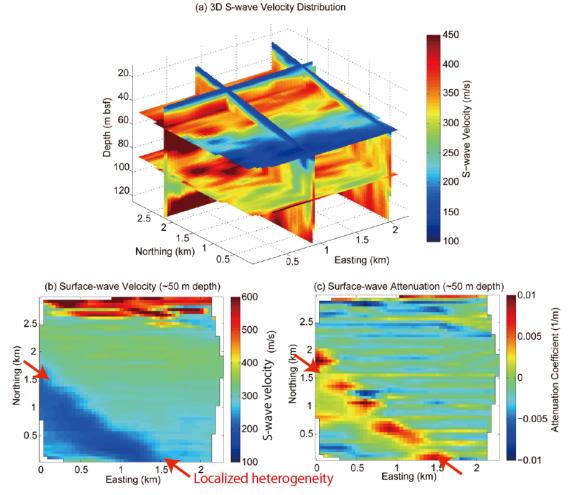


Fig. 1.16. (a) The estimated 3D S-wave velocity model in the Tomakomai CCS project site. Horizontal slices (map-views) of the (b) estimated surface-wave phase velocities and (c) attenuation coefficients at 2 Hz (~ 50 m depth from the seafloor). We firstly reveal NW-SE lithological boundary in this CCS site.

Publications

T. Ikeda, T. Tsuji, Advanced surface-wave analysis for 3D ocean bottom cable data to detect localized heterogeneity in shallow geological formation of a CO₂ storage site, International Journal of Greenhouse Gas Control, 2015 (DOI: 10.1016/j.ijggc.2015.04.020).

Energy Analysis (Acting Division Leader, Prof. Itaoka)

This division plays a critical role in I^2 CNER. It is responsible for providing carbon emission, energy efficiency, and cost analysis of current and emerging I^2 CNER and other energy processes, technology, and infrastructure. These analyses help ensure that I^2 CNER's and global energy related research are well targeted toward a carbon neutral society for Japan and the world as a whole. Also, in collaboration with the technical divisions, this division continuously reviews and revises the Institute's vision and roadmap toward a carbon-neutral society based on I^2 CNER and other energy system analyses.

Cost analysis of l^2 CNER's scenarios

To estimate the cost impact of implementing the I²CNER scenarios, the EAD developed a cost analysis module of electricity generation in Japan, adding to the energy model (technology bottom-up model) created in the previous year for the analysis of I²CNER's scenarios. The cost of a scenario is estimated as the difference between cost of energy supply, industrial activities, and transportation in a business as usual (BAU) scenario and those costs in each specific I²CNER scenario. The supply cost of energy includes the initial cost and operation cost, including fuel cost.

In the BAU scenario, we assumed that photovoltaics (PV) and wind power will increase following the historical trend; CCS will be deployed at a minimum level; and a fraction of existing nuclear plants will restart while no new plants beyond the plants under construction will be used. As we expected, we found the BAU scenario had the lowest cost. Among the other large emission reduction scenarios, excluding the "nuclear maintaining" scenario, which has yet great uncertainty regarding cost estimation on the back end, the "renewable scenario" is the least expensive in 2050 due to future cost reduction of PV. Meanwhile, the "renewable + battery" scenario, in which substantial battery power is required to mitigate the intermittency of PV and wind power is the most expensive in 2050 (Figure 1.17). This implies R&D should pursue not only cost reduction of renewables, but also technology to avoid negative impact on the quality of grid electricity due to the intermittency of PV and wind power, such as energy storage and dynamic demand response technology.

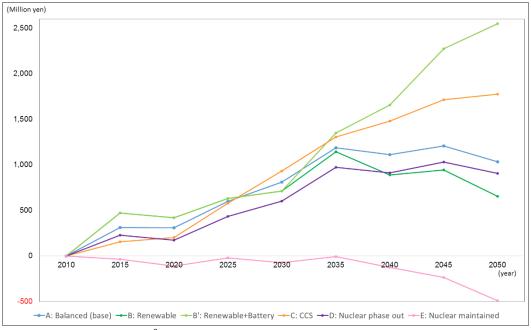


Fig. 1.17: Cost analysis of I²CNER's scenarios

Publication

K. Itaoka, S. Kimura, Energy technology analyses for deep GHG emission reduction by 2050 in Japan, Proceeding of Annual Conference 2014 of the Society for Environmental Economics and Policy Studies.

23

2. Advancing fusion of various research fields

I²CNER has undertaken multiple initiatives to advance fusion research, the primary one being the I²CNER Competitive Funding Program for young I²CNER researchers. The specific objective of the program is to foster interdisciplinary research and nurture young faculty and postdocs. The stringent criteria for the program include relevance to the I²CNER roadmap and a demonstrated potential for high-impact results. Participation in the program required proposal submission from young faculty and postdocs who have not collaborated with one another previously, and who have not had joint journal publications over the last two years. In FY 2014, the Director decided to require recipients of I²CNER Competitive Funds to give a progress report 3 times per year to keep the I²CNER Administration updated on the status of their interdisciplinary research projects. The success of the Competitive Funding Program will be assessed at the end of FY2015. Other efforts which encourage interdisciplinary research include the WPI Faculty Fellows Program (for full details, please see Section 3), the Institute Interest Seminar Series (for full details, please see Section 3), Collaborative Division Retreats (including more than 1 of I²CNER's divisions), and informal, young faculty-led seminars.

Our annual symposium this year focused on fuel generation and use. It was a symposium in which the leaders of the international scientific community came together and discussed interdisciplinary approaches to tackle key themes of I²CNER's roadmap: polarization in relation to the defect structure of the material components; the catalytic activity dependence on the surface structure and grain boundary species diffusion; dependence of the oxygen reduction reaction on proton transfer in non-precious catalysts; molecular design and dopant effects on stability for thermally activated delayed fluorescence; and the suggestion by Prof. Kunitake that we could consider amorphous membranes for fuel cells. Following this workshop, each of the I²CNER's research divisions ran similar workshops specifically focused on the interdisciplinary aspects of their research objectives. Indeed, it was a full week of interaction and debate over interdisciplinary research methodologies.

An outcome of the annual symposium and individual division workshops is that in FY 2015, I²CNER plans to host a workshop to explore cross-cutting themes for computational science, including catalysis, degradation, and select defect behaviors in order to discern what computational questions/problems I²CNER should address in the future. Possible deliverables for this workshop will include a "basic needs" report on I²CNER's computational science needs, which will serve as a prelusive roadmap for this effort; new interdisciplinary projects with computational elements; and improvements upon existing projects of the Institute through the addition of computational components (synergy). There are ongoing preliminary considerations for this workshop to be followed by one on "applied math for energy," which would follow a similar structure.

To further strengthen research collaboration between Kyushu and the Illinois Satellite, an interdisciplinary research grant was approved through the Competitive Funding program to foster the Sakai Group collaboration with Prof. Sharon Hammes-Schiffer, who is a world-renowned expert in the area of computational chemistry studies of molecular electrocatalysts for water oxidation and reduction. PI Sakai's group developed a new active water reduction catalyst, based on nickel dithiolate, and examined its electrochemical properties in order to understand the factors that lower the overpotential for water reduction, and ultimately fabricate a much more highly active catalyst for technology applications. The major part of the grant was used to introduce two sets of new 16-cored computational clusters (HPC-ProServer DPeT630/2667v3D128GRD21, CPU : E5-2667v3 (3.2GHz/16 Cores), Gaussian 09 pre-installed servers). The bridge for this collaboration is graduate student Keita Koshiba, who already visited Illinois with PI Sakai March 5-13, 2015, to get the collaboration started. Under the guidance of Prof. Hammes-Schiffer, the major reaction pathway leading to the observed electrocatalytic hydrogen generation from water with this molecular catalyst are being studied through density functional theory (DFT) calculations.

The Center's best interdisciplinary accomplishments by division are as follows:

i) <u>Hydrogen Production</u>: In collaboration with the Ishihara Group at Kyushu University, Prof. Xiuling Li has applied her remarkable MacEtch process for highly anisotropic wet etching of semiconductors to the fabrication of unique nanostructures that can potentially serve as outstanding material for photo electrochemical cells (*Solid State Physics, Materials Science, Analytical Chemistry and Surface Science*).
 ii) <u>Hydrogen Materials Compatibility</u>: A new fracture mechanics model for rolling contact fatigue

prediction was developed. This achievement impacts the reliable deployment of wind power generators by providing a state-of-the-art model for predicting the fatigue strength of bearings (*Metal fatigue, fracture mechanics, and tribology*)

iii) <u>Fuel Cells</u>: A well-defined system for electrochemical CO₂ reduction which utilizes Ag as the catalyst to reduce CO₂ to CO has been established by the CO₂ Capture and Utilization division. The Fuel Cell division developed a method to stabilize Pt-based electrocatalysts on carbon nanotube (CNT) for fuel cell applications. The observed onset potential for CO production was at a cell potential of -1.5 V comparable to the lowest found in the literature, and substantially better than that found using a Pt anode catalyst. The current density of 300 mA/cm² at -3.25 V cell potential is approaching that required for technology applications (*Cell technology and CNT-based novel Au electrocatalyst*)

iv) <u>Thermal Science and Engineering</u>: The reduction of lattice thermal conductivity is a critical goal of research on improving the thermal efficiency of thermoelectric materials for power generation from low grade heat sources. Silicon is earth abundant and the power factor of heavily doped Si is high, but the high lattice thermal conductivity prevents the use of silicon as a thermoelectric material. The lattice thermal conductivity of bulk crystalline silicon reduced by a factor of up to 20 when subjected to intense plastic strain under a pressure of 24 GPa using high-pressure torsion (HPT). (*Thermal science, material science, mechanical behavior*)

v) <u>Hydrogen Storage:</u> Carbon-based hydrogen storage materials is an entirely new class of potential candidates for on board hydrogen storage. PI Akiba and Prof. Hayashi of the Fuel Cells division have successfully designed the microstructure of such a carbon-based material with regard to the pore size, pore distribution and hydrophilicity/hydrophobicity. The technological impact of this new class of materials is that they operate below room temperature and do not need heat supply for the release of hydrogen (*Synthetic Chemistry, Surface Science, Materials science*).

vi) <u>Catalytic Materials Transformations</u>: Complementing their earlier work on the storage of hydrogen as formic acid, PI Ogo and his group have discovered a bio-inspired catalyst that converts formic acid into hydrogen; together, the processes define ways to store hydrogen as a liquid at room temperature and ambient pressure.

vii) <u>CO₂ Capture and Utilization</u>: We showed that high Faradaic efficiency (=selectivity) for CO and high utilization of CO₂ can be achieved with a dilute CO₂ feed, so flue gas from a power plant can be used directly as the feed for electroreduction of CO₂ to CO, thus eliminating the energy intensive process of CO₂ separation from flue gas (*Electrochemistry and Energy Saving System Process Optimization*).

viii) <u>CO₂ Storage</u>: Integrated experimental and numerical efforts identified key links between CO₂ migration in heterogeneous rock formations and elastic wave velocity measurements at the core scale that could potentially provide a new and robust method for monitoring CO₂ fate in actual reservoirs. Further, the numerical simulations confirmed that the small-scale heterogeneity characteristic of actual rock can actually provide an effective trap of CO₂ to increase the integrity of CO₂ storage (*fluid dynamics and geophysics, using both laboratory experiments and numerical simulations*).

In the following the Center's best interdisciplinary accomplishments are described in detail:

Hydrogen Production (Lead Principal Investigator: Prof. Ishihara)

Cd Doping of Cu Chalcopyrite Semiconductor Surfaces for Solar Cell Applications (Solid State Physics, Materials Science, Analytical Chemistry and Surface Science)

The nano-chemistry at the hetero-junction between CdS and Cu(In,Ga)Se₂ (CIGS), which determines the device performance, is the subject to considerable debate. This interdisciplinary research project seeks to clarify the composition of the interface by blending solid-state physics and thin film device fabrication (Prof. Rockett, UIUC) with expertise in surface analytical chemistry (Drs. Téllez and Druce, KU) and unique facilities at I²CNER (i.e. Low Energy Ion Scattering spectrometry). The interface chemistry is critical to controlling the electron concentration at the heterojunction of solar cells made from these materials and is necessary to achieving a high voltage output from the device. By examining the atomic-scale movement of atoms at the single-atomic-layer level we can show how this doping process occurs. To begin the analysis we have conducted a detailed study of methods to clean the sample and have shown that low-energy ion sputtering is the most effective method to remove any surface contamination prior to analysis of the sample surface. We have then performed a series of analyses on samples from which the CdS has been removed by chemical etching. This process typically yields a surface with residual Cd present. However, preliminary LEIS analysis did not find significant Cd doping of the heterojunction using conventional methods to prepare the materials. This shows that the Cd doping in the junction may be laterally non-uniform. Other studies by the Rockett

group have found that in some commercially-produced materials have significant Cd doping so relating the processing conditions to the level of doping is key to fabrication of efficient solar cells based on this material. The results of the study have been presented to the researchers at Solar Frontier, the world's leading manufacturer of CIGS solar cells, located in Tokyo to enhance their production process. The results also contribute to the short-term milestone of Hydrogen Production Division Project 1 (High Temperature Electrolysis) to increase the total H_2 formation efficiency of a photovoltaic powered electrolyser above 10 %.

Publication

H. Téllez, J. Druce, A. Hall, T. Ishihara, J. Kilner, A. Rockett, Low Energy Ion Scattering: Surface Preparation and Analysis of Cu(In,Ga)Se₂ for Photovoltaic Applications, Progress in Photovoltaics: Research and Applications, in press, (DOI: 10.1002/pip.2535).

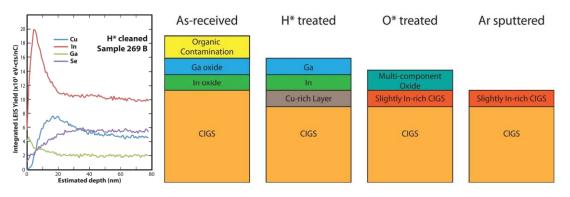


Fig.2.1. (Left) Depth profile for a hydrogen-cleaned CuInSe2 surface measured by low energy ion scattering (LEIS). The surface is highly enriched in In, underlying which is a Cu-rich region. (Right) A schematic illustration of the results of this study for methods of cleaning the sample surface and the anticipated compounds present in layers of the sample surface.

Fabrication of InP nanostructures using the MacEtch process (Solid State Physics, Materials Science, nano-machining and Surface Science)

Recently, an important Kyushu/Illinois collaboration was initiated in the hydrogen production division. This is the application of nanostructured semiconductors as photocatalysts. The work has been conducted as a collaboration between PI Ishihara and postdoc Guo at Kyushu University and Prof. Li at the University of Illinois. This collaboration has demonstrated the formation of highly anisotropic InP nanostructures with less than 20 nm feature sizes. The process is scalable to large areas and can be carried out at room temperature using the I-MacEtch method developed by Prof. Li. I-MacEtch is a unique and facile method to produce InP nanostructures, including linear, circular, and discrete features depending on the metal pattern, orientation, etchant composition, and etching time used. On the basis of extensive transmission electron microscopy and x-ray photoelectron spectroscopy characterization, Prof. Li's group has found that the inverse nature of the selective etching process is rooted in the formation of a thick oxide layer at the Au/InP interface that cannot be dissolved in the I-MacEtch solution. Remarkably, the sidewalls of the resultant nanostructures are not only nearly atomically smooth and free of porosity, but also are unaffected by the metal pattern edge roughness. I-MacEtch represents a highly economical and superior technique pertinent to the processing of various InP-based devices, including nanoscale field-effect transistors, solar cells, light emitters, and photocatalyst for modifying with organic dye. This interdisciplinary achievement represents progress toward the short-term milestone (Energy conversion efficiency >1%) of the division's Project 2: Photocatalytic water splitting through inorganic semiconductor for dye modified photocatalyst.

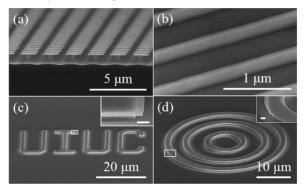


Fig. 2.2. InP nanostructures generated from I-MacEtch: (a) arrays of nanopillars generated from Pt square pads, (b) arrays of nanoscale fins from Au lines after Au removal, (c) the letters "UIUC" from Au pads with inset showing a high-magnification view of the outlined region (white box) corresponding to the letter "I", and (d) concentric InP microstructures generated from a set of Au rings, with inset showing the high-magnification view of the outlined region. The inset scale bars are 500 nm and metal catalyst layers were patterned by SL (a) and EBL (b–d).

Publication

S.H. Kim, P.K. Mohseni, J. Song, T. Ishihara, X. Li, Inverse Metal-Assisted Chemical Etching Produces Smooth High Aspect Ratio InP Nanostructures, Nanoletter, vol. 15, pp. 641-648, 2015.

Hydrogen Materials Compatibility (Lead Principal Investigator: Dr. Somerday)

A new fracture mechanics model for rolling contact fatigue (metal fatigue, fracture mechanics, and tribology)

The interdisciplinary achievement described below represents progress toward the milestone of developing models of mechanical and chemical processes relevant to tribo-failures and tribo-film formation. This short-term milestone is featured in Project 4: Environmental Effects on Friction and Tribological Failures.

In support of renewable energy development, a number of wind power generators have been constructed world-wide. Recently, the flaking fractures of large-scale bearings used in the generator, e.g., 0.4 m to 1 m outer diameter, have been frequently reported. The failure of bearings causes a significant economic loss since replacement of the large bearing mounted in the nacelle is costly. In such a situation, a novel strength-design method, which enables precise prediction of the fatigue strength, is required to enhance reliability.

In order to provide a solution, Prof. Matsunaga (WPI Professor) led an effort to establish a novel testing method to measure the threshold stress intensity factor ranges, ΔK_{IIth} and ΔK_{IIth} , for the shear-mode growth of small cracks. The results were embedded in a new fracture mechanics model suggested by collaborators with expertise in metal fatigue (Prof. Matsunaga, WPI Professor), tribology (Komata, NSK Ltd.), and fracture mechanics (Prof. Yamabe, WPI Associate Professor). This interdisciplinary collaboration incubated the novel method for evaluating the rolling contact fatigue strength of bearings with arbitrary shapes, dimensions, and material cleanliness, as shown in Fig. 2.3. In the past, such a fracture mechanics-based method has not successfully predicted the flaking failure of bearings, since it requires an interdisciplinary approach, i.e., measurement of growth-resistance of small shear-mode fatigue cracks as a function of crack size, establishment of rolling contact fatigue test methods using specimens with small defects having various sizes and depths, and the proper modeling of rolling contact fatigue phenomena based on fracture mechanics. As research products, three domestic patents were filed: one for a newly developed fatigue testing machine and the other two for the novel strength-design method. In the future, the design-method will be generalized for different hydrogen content in the material as well as different microstructures, e.g., bainitic structure.

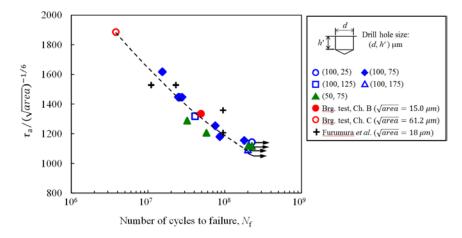


Fig. 2.3. Modified stress amplitude vs. cycles to failure diagram for rolling contact fatigue.

Publications

S. Okazaki, H. Matsunaga, T. Ueda, H. Komata, M. Endo, A practical expression for evaluating the small shear-mode fatigue crack threshold in bearing steel, Theoretical and Applied Fracture Mechanics, vol. 73, pp. 161-169, 2014.

H. Matsunaga, H. Komata, J. Yamabe, Y. Fukushima, S. Matsuoka, Effect of size and depth of small defect on the rolling contact fatigue strength of bearing steel JIS-SUJ2, Procedia Materials Science, vol. 3, pp. 1663-1668, 2014.

Prediction of subcritical crack propagation under sustained load (solid mechanics and mechanical metallurgy)

The interdisciplinary achievement described below represents progress toward the milestone of refining crack velocity vs. load models based on enhanced understanding of hydrogen-induced degradation in steels. This short-term milestone is featured in Project 3: Fracture and Fatigue Prognosis of Hydrogen Containment Systems.

Failure of hydrogen containment components is generally associated with subcritical cracking. Understanding subcritical crack growth behavior and its dependence on material and environmental variables can lead to more rigorous life-prediction models for structural components in hydrogen environments. In order to identify the issues underlying crack propagation and arrest, we developed a model for hydrogen induced stress-controlled crack propagation under sustained loading. The model was based on the assumptions that i) hydrogen reduces the material fracture strength and ii) crack propagation takes place when the opening stress over the characteristic distance ahead of a crack tip is greater than the local fracture strength. Formulating the modeling framework and its assumptions followed an interdisciplinary approach, in which the solid mechanics foundation is fully informed by mechanical metallurgy.

The model was used in a finite element simulation of crack propagation coupled with simultaneous hydrogen diffusion in a model material. The crack propagation model employed a nodal release technique in a simulated wedge opening load (WOL) specimen under constant displacement loading assuming plane strain conditions. The predicted crack velocity as a function of stress intensity factor (V-K curve) exhibited both stage I and II, which is characteristic of subcritical cracking (see Fig. 2.4). More importantly, both stage I and stage II of the V-K curve were captured through one mechanism of crack propagation, i.e. diffusion controlled crack propagation. This result suggests that it may not be necessary to treat stage I and II of the V-K curve differently in terms of mechanism-based modeling, which may allow advancements in models that are currently limited to stage II. Such advanced models are an essential component in state-of-the-art structural health monitoring systems applied to hydrogen containment components.

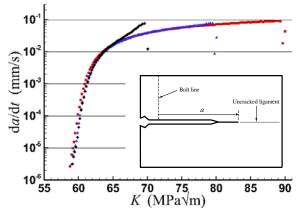


Fig. 2.4. Finite element simulation of crack velocity vs. stress intensity factor (V-K curve) for wedge opening load (WOL) specimens loaded to the initial stress intensity factors of 70, 80, and 90 MPa \sqrt{m} prior to hydrogen gas exposure. The inset shows a schematic of the simulated WOL specimen.

Publication

M. Dadfarnia, B.P. Somerday, P. Schembri, P. Sofronis, J.W. Foulk, III, K.A. Nibur, D.K. Balch, On modeling hydrogen induced crack propagation under sustained load, JOM, vol. 66, pp. 1390-1398, 2014.

Fuel Cells: (Lead Principal Investigator: Prof. Sasaki)

Electrochemical CO₂ reduction (Cell technology and CNT-based novel Au electrocatalyst)

The Paul Kenis group at the University of Illinois established a well-defined system for electrochemical CO_2 reduction, which utilizes Ag as the catalyst to reduce CO_2 to CO. The group of Prof. Nakashima in the Fuel Cell division developed a method to stabilize Pt-based electrocatalysts on carbon nanotube (CNT) for fuel cell applications. The metal nanoparticle stabilization methodology is generally applicable to a wide variety of nanoparticle materials, including those relevant to CO_2 reduction such as Ag and Au.

This research combines CNT-based supports with metal electrocatalysts for CO_2 reduction, and investigates the effect of the support on reactivity. We combined the best cathode (MWNT/PyPBI/Au; Fig. 2.5: left) with the best anode (IrO₂) to maximize the performance obtained for the electrochemical reduction of CO_2 to CO. The observed onset potential for CO production was at a cell potential of -1.5 V comparable to the lowest found in the literature (Fig. 2.5) and substantially better than that found using a Pt anode catalyst. The current density of 300 mA/cm² at -3.25 V cell potential is approaching that required for practical applications. This interdisciplinary achievement represents progress toward the short term milestone on durability and performance of electrocatalysts in Project 1 in the division roadmap.

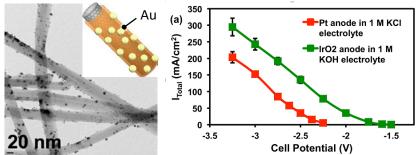


Fig. 2.5. (left) TEM image of MWNT/PyPBI/Au and (right) Total current density for CO when using different anode catalysts (cathode: 0.34 mg/cm² MWNT/PyPBI/Au catalyst painted on gas diffusion electrode).

Publication

H-R. Jhong, C.E. Tornow, C.R. Kim, J.L. Oberst, P.S. Anderson, A.A. Gewirth, T. Fujigaya, N. Nakashima, and P.J.A. Kenis, Gold Nanoparticles on Polymer-Wrapped Carbon Nanotubes: An Efficient and Selective Catalyst for CO₂ Reduction, (Submitted).

Thermal Science and Engineering (Lead Principal Investigator: Prof. Takata)

Thermal conductivity of suspended submicron graphene ribbons (thermal science and materials science) Thermophysical characterization of graphene is very important for both fundamental and technological research in relation to various energy devices. In particular thermal conductivity measurements of graphene ribbons are still very few. The temperature dependent thermal conductivity of a 169-nm wide and 846-nm long graphene ribbon has been investigated by the electrical self-heating method. The measured thermal conductivities range from (12.7 \pm 2.95) W/m/K at 80K to (932 \pm 333) W/m/K at 380 K, being (349 \pm 63) W/m/K at 300 K, following a ~T^{2.79} law for the full temperature range of 80K to 380K and a ~T^{1.23} law at low temperatures. The comparison of the measured thermal conductance with the ballistic transport limit indicates diffusive transport in this narrow and short ribbon due to phonon-edge as well as phonon-defect scattering. The data were also combined with an empirical model to predict possible width dependence of thermal conductivity for suspended graphene ribbons. These results help understand the 2D phonon transport in suspended submicron graphene ribbons and provide knowledge for controlling thermophysical properties of suspended graphene nanoribbons through size manipulation. This interdisciplinary achievement represents progress toward the short-term milestone of the development of measurement methods of physical properties of individual nanomaterials in the division's Thermophysical Properties Project 3 in the division roadmap.

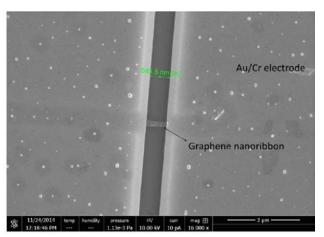


Fig. 2.6. SEM images of the suspended graphene ribbon (169×846 nm)

Publication

Q.-Y. Li, K. Takahashi, H. Ago, X. Zhang, T. Ikuta, T. Nishiyama, K. Kawahara, Temperature dependent thermal conductivity of a suspended submicron graphene ribbon, Journal of Applied Physics, vol. 117, No. 065102, 2015.

Reduction of thermal conductivity of crystalline silicon by high-pressure torsion (thermal science and materials science)

We report a dramatic and irreversible reduction in the lattice thermal conductivity of bulk crystalline silicon when subjected to intense plastic straining under pressure of 24 GPa by high-pressure torsion (HPT). Thermal conductivity of the HPT-processed samples were measured using picosecond time domain thermoreflectance. Thermal conductivity measurements show that the HPT-processed samples exhibit a lattice thermal conductivity reduction by a factor of approximately 20 (from intrinsic single crystalline value of 142 $Wm^{-1}K^{-1}$ to approximately 7.6 $Wm^{-1}K^{-1}$). Thermal conductivity reduction in HPT-processed silicon is attributed to the formation of nanograin boundaries and metastable Si-III/XII phases which act as phonon scattering sites, and the presence of a large density of lattice defects introduced by HPT processing. Annealing the samples at 873 K increases the thermal conductivity due to the reduction in the density of secondary phases and lattice defects. This interdisciplinary achievement represents progress toward the short-term milestone of the development of experimental techniques for interfacial thermal transport in the division's Thermophysical Properties Project 3 in the division roadmap.

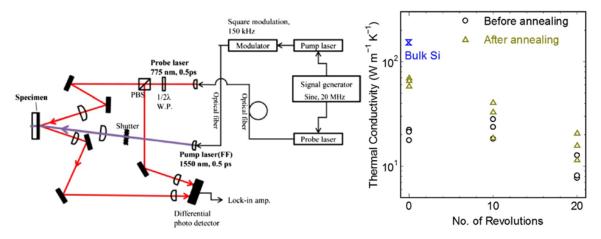


Fig. 2.7. (Left) Schematic of the picosecond time domain thermoreflectance setup. The violet and red lines show the optical transport path of the pump beam and probe beam. (Right) Thermal conductivities of the HPT-processed before and after annealing. An order of magnitude reduction in the thermal conductivity of Si upon HPT processing is observed. Annealing of the HPT samples show an increase in thermal conductivity due to the reverse transformation of metastable phases to Si-I cubic diamond phase.

Publication

S. Harish, M. Tabara, Y. Ikoma, Z. Horita, Y. Takata, D.G. Cahill, M. Kohno, Thermal conductivity reduction of crystalline silicon by high-pressure torsion, Nanoscale Research Letters, vol. 9, No. 326, 2014.

Hydrogen Storage (Lead Principal Investigator: Prof. Akiba)

Nanoporous materials as hydrogen storage media (Synthetic Chemistry, Surface Science, Materials science, and Hydrogen storage)

High surface area materials have attracted attention as potential hydrogen storage media because their storage capacity can reach more than several wt%. The US DOE envisions the high surface area materials as potential candidates for on board hydrogen storage. These materials operate below room temperature and do not need heat supply for the release of hydrogen. The design of the structure of high surface area is key to the development of hydrogen storage materials with enough capacity. The hydrogen storage division collaborates with Prof. Akari Hayashi of the Fuel cell division, an expert on carbon based materials, to create these new hydrogen absorbers. We have successfully designed the microstructure of a carbon-based material with regard to the pore size, pore distribution and hydrophilicity/hydrophobicity. We expect these materials to show favorable hydrogen absorbing properties and by tuning the microstructure we expect that we will achieve optimal hydrogen storage.

This interdisciplinary achievement represents progress toward the 5% wt short-term milestone of the division's Project 1: On board hydrogen storage.

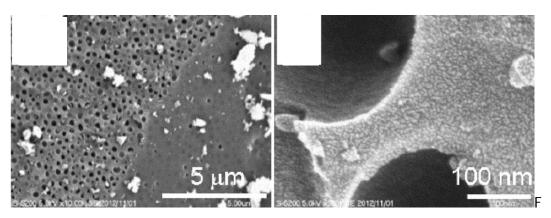


Fig. 2.8. SEM images of carbon materials synthesized by 50:50 mole ratios of resorcinol and 2,6-dihydropyridine hydrochloride.

Publication

Y. Sonoda, A. Hayashi, Y. Minamida, J. Matsuda, E. Akiba, Nanostructure Control of Porous Carbon Materials through Changing Acidity with a Soft-Template Method, Chemistry Letters, vol. 44, pp. 503-505, 2015.

Catalytic Materials Transformations (Lead Principal Investigator: Prof. Ogo)

A [NiFe]hydrogenase Model That Catalyses the Release of Hydrogen from Formic Acid (Bioinorganic Chemistry, Biochemistry, Coordination chemistry)

We report the decomposition of formic acid to hydrogen and carbon dioxide, catalysed by a NiRu complex originally developed as a [NiFe]hydrogenase model. This is the first example of H_2 evolution, catalysed by a [NiFe]hydrogenase model, which does not require additional energy. The catalyst plays the maximum value of turnover numbers (TONs, mol of H_2 evolved/mol of catalyst) of H_2 evolution is 857 for 1 h at 60°C at pH of 3.5. This is first [NiFe]hydrogenase model complex have been reported catalyzed for hydrogen production at ambient conditions, this model displays formate hydrogenlyase function without any need for additional energy input.

Building on previous biochemical studies published in 2014, we have achieved the short term milestone of isolating formate dehydrogenase and its model complex for CO_2 conversion. This achievement is part of the division's larger project on the development of novel biomimetic catalysts for H_2 , CO_2 , and H_2O activation based on naturally occurring enzymes (Project 1). This work is the benchmark in this area.

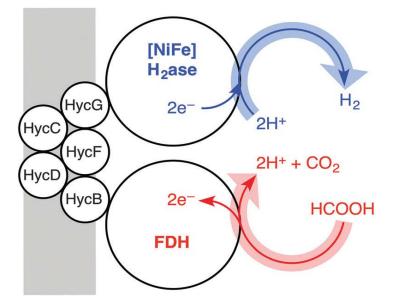


Fig. 2.9. A structure of formate hydrogen lyase (FHL) constructed from a [NiFe]hydrogenase ([NiFe]H2ase) and a formate dehydrogenase (FDH).

Publication

N.T. Nguyen, Y. Mori, T. Matsumoto, T. Yatabe, R. Kabe, H. Nakai, K.S. Yoon, S. Ogo, A [NiFe]hydrogenase model that catalyses the release of hydrogen from formic acid, Chem. Commun., vol. 50, pp. 13385–13387, 2014.

Ruthenium-Catalyzed Oxidative Kinetic Resolution of Unactivated and Activated Secondary Alcohols with Air as the Hydrogen Acceptor at Room Temperature. (Organic chemistry, Oxidation Chemistry, Asymmetric Catalytic Chemistry

Dioxygen (O_2) is a highly abundant, ubiquitous, and most efficient oxidant on the earth. However, the activation of O_2 required the addition of co-reductant, hearting, and pressurizing conditions in the chemical way. Recently, we found that ruthenium(aqua)-salen derivatives were efficient catalyst for the activation of O_2 under mild conditions. Herein, we could present that first example of aerobic oxidative kinetic resolution of unactivated secondary alcohols such as 2-ocatanol. The reaction carried out with good-to-high enantiomer differentiation using O_2 in air as a hydrogen acceptor.

Building on previous catalytic aerobic oxidation using iron or ruthenium complexes, we have achieved the short-term milestone of non-energy requiring aerobic oxidation. This achievement is part of the division's larger project on the energy conservation in material transformation (Project 2). This accomplishment is a monumental piece of work in the aerobic oxidative material transformation.

Publication

H. Mizoguchi, T. Uchida, T. Katsuki, Ruthenium-Catalyzed Oxidative Kinetic Resolution of Unactivated and Activated Secondary Alcohols with Air as the Hydrogen Acceptor at Room Temperature, Angew. Chem. Int. Ed. Vol. 53, pp. 3178-3182, 2014.

CO₂ Capture and Utilization (Lead Principal Investigator: Prof. Fujikawa)

Feasibility of using flue gas as a direct feed for efficient electroreduction of CO2 to CO (Electrochemistry and Energy Saving System Process Optimization)

We studied the effect of different CO₂ streams (e.g., the ~ 15% CO₂ in flue gas) on cathode performance in CO₂ reduction. Also, we examined and compared the effect of pH on performance with the effect variable CO₂ concentration. This study highlights that high Faradaic efficiency for CO and high utilization of CO₂ could be achieved at dilute CO₂ feed, which implies that the direct use of flue gas as a feed for electrochemical reduction to CO has promise.

One of the short term milestones of the division's Project 2 is to optimize important parameters in CO_2 reduction (e.g., Faradaic efficiency, current density and energetic efficiency). The use of flue gas directly as the feed for CO_2 reduction processes can possibly sidestep the energy intense of CO_2 capture and concentration so that we can increase overall energy efficiency of CO_2 reduction processes.

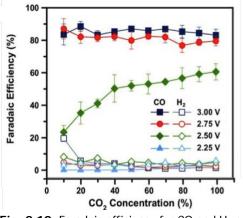


Fig. 2.10. Faradaic efficiency for CO and H_2 as a function of CO₂ concentration

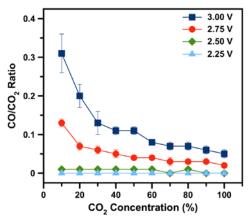


Fig. 2.11. Ratio of CO over CO_2 as a function of CO_2 concentration

Publication

B. Kim, S. Ma, H.R. Jhong, P.J.A. Kenis, Influence of dilute feed and pH on electrochemical reduction of CO₂ to CO, Electrochimica Acta, vol. 166, pp. 271-276, 2015.

CO₂ Storage (Lead Principal Investigator: Prof. Tsuji)

Two-phase flow within heterogeneous pore structure (fluid dynamics and geophysics, using both laboratory experiments and numerical simulations)

We revealed that two-phase fluid flow (CO₂ and water) is strongly controlled by small-scale heterogeneity in porous sandstone by (i) the measurement of elastic wave velocity at the sub-core scale (mm-cm; Fig. 2.13 (a)) and (ii) the two-phase fluid-flow simulation based on the Lattice-Boltzmann-Method at the pore-scale (nm-mm; Fig. 2.13 (b)). The lamina is a typical small-scale heterogeneity in the porous sandstone and has a smaller pore-size distribution than the surrounding porous zone. The geophysical observations indicate that CO₂ cannot pass through the lamina-rich zone in water-saturated porous sandstone. This restrictive CO₂ flow around the lamina-rich zone is caused by a gap in the pore pressure. These results highlight how it may be possible to accurately monitor the pore-scale CO₂ behavior external to the pore space using geophysical methods. This study also indicates that small-scale heterogeneity has a potential to be sub-sealed in the CO₂ reservoir and to increase the integrity of CO₂ storage. This work is related to Project (1) "Pore-scale investigation of CO₂ fate" of the CO₂ storage research division and addresses the short-term milestone "Model injected CO₂ behavior from laboratory experiment and simulation."

Benchmark: Current pore-scale models cannot capture dynamic nature of CO_2 migration nor do they embody the interconnected nature of the pore system and impact on CO_2 migration.

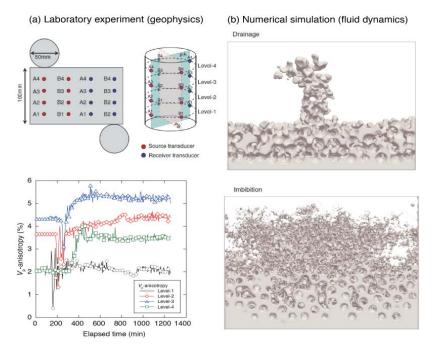


Fig. 2.12. (a) Geophysical observation to identify fluid flow along the lamina structure. (b) Flow paths of drainage and imbibition process.

Publication

K. Kitamura, F. Jiang, A.J. Valocchi, S. Chiyonobu, T. Tsuji, K.T. Christensen, The study of heterogeneous two-phase flow around small-scale heterogeneity in porous sandstone by measured elastic wave velocities and lattice Boltzmann method simulation, Journal of Geophysical Research (Solid Earth), vol. 119, pp. 7564-7577, 2014.

Energy Analysis (Acting Division Leader, Prof. Itaoka)

Decentralized carbon-free hydrogen production through natural gas steam reforming along with on-site CO_2 capture and storage (CCS). (chemical engineering, geological physics and economic analysis)

The production of carbon-free hydrogen is a key technology associated with the commercialization of the fuel cell vehicles. Currently, hydrogen is mainly produced by steam reforming of natural gas (NSR), a process which involves CO_2 emissions. In this study, we analyzed the potential and possible cost-advantage of producing carbon-free hydrogen by NSR along with on-site CCS (Fig. 2.13) against hydrogen production through water electrolysis (WER). In the comparison between the two approaches, we accounted for the storage potential and monitoring costs for the injected CO_2 . In particular, we analyzed CO_2 injection into shallow geological formations and prioritized the key methodologies for this CCS system. In addition, we accounted for the specific performance values of our developed separation membrane, such as gas flux, selectivity, cost of membrane, and usage period. Based on our system (Fig. 2.14) analysis, we concluded that NSR with a decentralized CCS system at the refueling stations has sufficient potential to produce reasonably priced

carbon-free hydrogen. We also demonstrated that such a hydrogen production system constitutes a bridge technology for the establishment of a carbon-free hydrogen supply system based on reusable energy sources. This work addresses the final objective of the CO_2 Storage division: "Propose and realize innovative CCS concepts suitable for geological formations typical of Japan (i.e. tectonically active area)." However, CO_2 onshore storage has the potential to cause concern on behalf of the public, as demonstrated in the Netherlands, so social science studies will be necessary to gauge public perception of this technology.

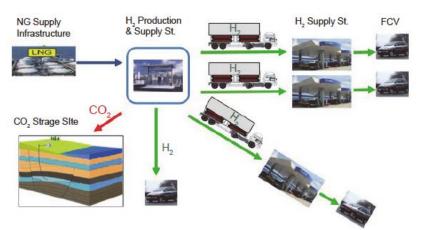


Fig. 2.13. Ideal carbon-free hydrogen supply system with decentralized natural gas reforming and on-site CCS.

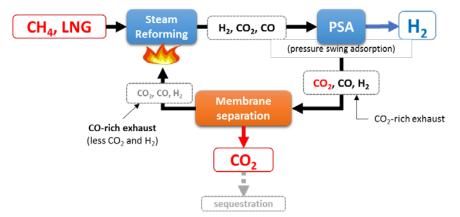


Fig. 2.14. Schematic diagram of CO_2 membrane capture and storage for H_2 from CH_4 or liquified natural gas (LNG): CH_4 or LNG is first converted to H_2 and CO_2 (and other gasses) by steam reforming. H_2 in this mixture gas is purified by PSA (pressure swing adsorption) which is the technology used to separate target gas species (H_2 , in this case) from a mixture of gases by using solid absorbent materials and controlling pressure. After the PSA process, CO_2 is separated by a membrane from the exhausted gas stream for CO_2 sequestration. The rest of the gasses comprising mainly of CO (and small amount of CO_2 and H_2) can be used as a fuel gas for steam reforming.

Publication

S. Kimura, K. Honda, K. Kitamura, I. Taniguchi, K. Shitashima, T. Tsuji, S. Fujikawa, Preliminary Feasibility Study for On-Site Hydrogen Station with Distributed CO₂ Capture and Storage System, Energy Procedia, vol. 63, pp. 4575-4584, 2014.

3. Globalization of the institution

* Describe what's been accomplished or recognized in the efforts to raise the center's international recognition as a genuine top world-level research institute, along with innovative efforts proactively being taken in accordance with the development stage of the center, including the following points, for example:

- Efforts being developed based on the analysis of number and state of world-leading, frontline researchers; number and state of visiting researchers; exchanges with overseas entities

- Proactive efforts to raise the level of the center's international recognition
- Efforts to make the center into one that attracts excellent young researchers from around the world (such as efforts fostering young researchers and contributing to advancing their career paths)

I²CNER added the Air Resources Board of the State of California (CARB) to its network of international collaborating institutions in FY 2014. Negotiations for a memorandum of understanding in the general field of hydrogen technology between I²CNER and the Helmholtz Zentrum Geesthacht (HZG) are underway. PI Akiba is already collaborating with researchers from HZG, e.g. from February-September 2015, HZG researchers will be working in Prof. Akiba's laboratory and a PhD student from HZG will visit I²CNER in August 2015. In addition, there has been communication between the Director of I²CNER, the Director of the Helmholtz Institute in Juelich, and PI Reiner Kirchheim to explore areas for possible collaboration between the two Institutes, in particular, in the areas of fuel cells, hydrogen production, storage, and delivery, and materials mechanical behavior. As of March 31, 2015, I²CNER has a total of 23 partner institutions in the US, Europe, and Asia, of which, I²CNER has agreements or MOUs with 4 (the University of Illinois, Norway SINTEF/NTNU, the Air Resources Board of the State of California (CARB), and the National Fuel Cell Research Center (NFCRC) at the University of California, Irvine). For the complete list of our international partner institutions, please see Appendix 3-1-2, "Satellites and partner institutions."

The researchers of the Institute have also had success at elevating the Institute's visibility on an individual level. By way of example, I²CNER researchers hosted a grand total of 42 distinguished visitors to Kyushu University from the United States, Canada, Europe, Korea, China, South Africa, Australia, France, Norway, Japan, and the United Kingdom. The Institute's researchers were responsible for organizing or co-organizing 8 international conferences, 6 international conference sessions, and 9 I²CNER international workshops. In addition, our researchers have joint publications with researchers from 26 institutions around the world.

Partnerships in International Research and Education (PIRE)

The I²CNER Director and Professors Elif Ertekin and Narayana Aluru from UIUC's Department of Mechanical Science and Engineering are working together with Kyushu University Profs. Tatsumi Ishihara, Hiroshige Matsumoto, and Nicola Perry to submit a joint "Partnerships for International Research and Education (PIRE)" Proposal focused on computation to NSF/JSPS. The project has already passed the pre-proposal stage and has been invited for a full proposal, which is due May 15, 2015. The decision to submit the pre-proposal was catalyzed by the fact that Kyushu and Illinois already have an ongoing relationship through the I²CNER project.

Air Resources Board of the State of California (CARB)

I²CNER initiated collaborations with the Air Resources Board of the State of California (CARB), which was formalized by a "Letter of Understanding," signed on May 19, 2014. Our first discussion was held via teleconference on December 1, 2014. Since the initial discussion, there have been several exchanges of information between CARB and I²CNER, including I²CNER's roadmaps and descriptions of each division, in order to familiarize CARB with the Institute and vice versa. Several mutual areas of interest have been identified, including a systems' approach to a sustainable society, SOFC/SOEC cathodes using proton conducting oxides, and challenges related to implementation of SOFCs operating in low and high pressure applications at both a systems and materials level. It is expected that this collaboration will continue to be strengthened in FY 2015 and beyond. The degree of mutual interests between I²CNER and CARB on renewable energy and the implementation thereof is demonstrated by the fact that CARB will hire one of the I²CNER Satellite postdoctoral researchers, Dr. Xuping Li, beginning in FY 2015.

Interactions with the US Department of Energy (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. A number of these projects which are focused on fundamental science are carried out at I²CNER. As a result of his recognized technical expertise and ability to productively manage projects, 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.

- Director Sofronis is in communication with the Fuel Cells Technology Office and exchanges information about mutual interests, which includes visits to Washington, D.C. and serving as a reviewer for the Department of Energy in the Annual Merit Review and Peer Evaluation Meetings.
- I²CNER was featured in a plenary lecture given by the Fuel Cell Technology Office at DOE's 2014 Annual Merit Review and Peer Evaluation Meeting on June 16, 2014.
- In FY 2014, former US DOE Energy Analyst Mark Paster was newly appointed as a member of the Institute's External Advisory Committee (EAC), after having played a vital role in the Energy Analysis Division (EAD).

National Fuel Cell Research Center (NFCRC)

In FY 2014, a delegation of I²CNER researchers visited NFCRC for the first time. In addition, the visit by the Associate Director of NFCRC, Prof. Jack Brouwer, to the 2015 I²CNER Annual Symposium set the stage for ongoing collaborations. NFCRC and I²CNER collaborate on challenges related to implementation of SOFCs operating in low and high pressure applications at both a systems and materials level. In particular, a research collaboration on cathode and SOFCs/SOECs using proton conducting oxides is under consideration.

ECOSTORE

I²CNER holds a four year consortium agreement with the ECOSTORE project, which is based in the European Union. 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. A 2-day ECOSTORE workshop was held at Kyushu University in March 2015.

University of Oxford

The Director serves on the Strategic Advisory Panel of the Hydrogen in Metals—From the Fundamentals to the Design of New Steels (HEmS) at the University of Oxford.

Influence on National and International Policy

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.

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.

Prof. Takeshi Tsuji is a member of the committee of the Japan CCS Corporation which will decide the next CO₂ storage site around the Japanese Islands.

Collaborative Foreign Exchange Program

I²CNER's "Collaborative Foreign Exchange Program" is in place 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. In FY 2014, 7 researchers (5 Japanese, 2 non-Japanese) had their proposals approved, 5 of which visited the Illinois Satellite. One of our female assistant professors visited Sandia National Laboratories for 6 months to collaborate with Dr. Somerday, the Lead PI of the Hydrogen Materials Compatibility Division.

WPI Faculty Fellows Program

In FY 2014, the Institute established a new 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/I²CNER for periods of three to six months. The program is intended to help recruit foreign researchers who may consider

accepting permanent positions at I²CNER. 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.

I²CNER Seminar Series

In FY 2014, I²CNER engaged key members of the international community from: academia, national laboratories, industry, and policy makers in government agencies. In FY 2014, the Institute hosted a total of 24 speakers (15 non-Japanese) in 22 I²CNER Seminars. The Director already gathered input from the young faculty on how to improve the climate, and the following measure is being implemented:

In order to make the visiting speakers more accessible to our young faculty, the Administration is
implementing a "sign-up sheet" system, where any I²CNER researcher can request a meeting with
visiting seminar speakers.

Institute Interest Seminar Series (IISS)

In order to advance interdisciplinary research amongst young researchers, the Institute regularly hosts the "Institute Interest Seminar Series (IISS)." A total of 24 speakers presented at 16 Institute Interest Seminars in FY 2014. The Director already gathered input from the young faculty on how to improve the climate, and the following measures are being implemented:

- The Administration plans to extend an open invitation to non-I²CNER young faculty within KU to participate in this seminar series in order to expand opportunities for collaboration for our young faculty.
- Question & Answer time will be extended to a half hour or more.
- More general research topics will be included, including social sciences or research ethics.
- Speakers will be encouraged to limit jargon and overly technical presentations in order to make the series marketable to an audience with a wide variety of scientific backgrounds.
- Some seminars in this series may be scheduled during lunch time to allow postdocs more time to participate in the discussion portion.

Role of the University of Illinois at Urbana-Champaign (UIUC) Satellite

From the very beginning, one of I²CNER's fundamental strategies for internationalization has been the Satellite Institute at the University of Illinois at Urbana-Champaign. The Illinois Satellite helps promote the Institute's overall international visibility through the participation of several world-leading researchers. In addition, the ongoing relationships between the faculty of Kyushu University and the University of Illinois at Urbana-Champaign are having a transformative impact upon I²CNER's overall research culture. Some of the efforts undertaken at the Satellite to promote the KU/UIUC relationship and the globalization of I²CNER are as follows:

Satellite Faculty Composition

The Illinois Satellite faculty members are all internationally recognized researchers in their respective areas of expertise. They were specifically invited to complement the I²CNER research activities at Kyushu, and they are continually re-assessed based upon their relevance to the overall I²CNER vision and roadmap. As of March 31, 2015, there are 8 Satellite Faculty and 1 WPI Principal Investigator participating at the Illinois Satellite. 1 member of I²CNER's External Advisory Committee (EAC), Dr. Robert Finley, is from the University of Illinois. In addition, there are several former Satellite Faculty members who are still working with I²CNER in some capacity: 1) Prof. Ian Robertson, Dean of the College of Engineering, University of Wisconsin-Madison, 2) Prof. Ken Christensen, University of Notre Dame, and 3) Prof. Lane Martin, University of California, Berkeley.

Chancellor Wise's Visit to Japan

In an effort to further strengthen the relationship between Kyushu University and the University of Illinois, the UIUC Chancellor, Phyllis Wise, visited Kyushu University in November 2014. During the Chancellor's visit, she had meetings with several important Kyushu University administrators, and she extended an open invitation to those administrators to travel to the Urbana-Champaign campus to further promote the ties between our universities. KU Executive Vice President in Charge of Research and Industrial Collaboration, Prof. Masato Wakayama, plans to visit UIUC May 21-22, 2015.

Revised Satellite Agreement

Upon I²CNER's renewal for a second term, Kyushu University administrators began working with

administrators at the University of Illinois at Urbana-Champaign to update the "Satellite Agreement," which will expire in November 2015. Though discussions and negotiations for the agreement are ongoing, some new details that will be addressed by the agreement include specific terms on Intellectual Property, provisions for the establishment of individual research agreements, etc. *Agreement on Academic Cooperation*

As part of the ongoing effort to promote mutual understanding and strengthen the relationship between Kyushu University and the University of Illinois at Urbana-Champaign, an "Agreement on Academic Cooperation" between the two universities was signed on May 26, 2014. The specific purpose of this agreement is to develop scientific, academic, and educational cooperation on the basis of equality and reciprocity.

Memorandum of Understanding on Intellectual Property

A "Memorandum of Understanding" between Kyushu University and the University of Illinois at Urbana-Champaign was negotiated cooperatively by KU's Industry-University-Government Collaboration Management Center (IMAQ) and UIUC's Office of Technology Management (OTM) to specify ownership and sharing of costs and revenue for the protection and commercialization of Intellectual Property created at the I²CNER Satellite. This MOU was signed on March 26, 2015. One of the stipulations of this MOU was that further clarification would be specified in the revised "Satellite Agreement," which will be signed in FY 2015. Please see above for more details.

Undergraduate Exchange Agreement

A "Student Exchange Program Agreement" between Kyushu University and the University of Illinois at Urbana-Champaign was signed on October 24, 2014. 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.

2nd Group of Undergraduate Exchange Students hosted at Illinois

From February 23-March 25, 2015, 6 Kyushu University undergraduate students from the Faculty of Engineering traveled to the University of Illinois at Urbana-Champaign as part of the I²CNER Undergraduate Exchange 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 of the Satellite, took tours of 2 local engineering companies, and interacted heavily with the Center for East Asian and Pacific Studies (CEAPS) to enhance their cultural experience of the university.

Faculty Promotion Process

I²CNER's promotion process is based upon the process used at Illinois, which maintains the high standards that are typical at top US universities. The process involves a confidential assessment by world-leading scientists from the international community in the candidate's area of expertise, and is carried out by a promotion committee involving senior faculty members from both KU and Illinois. Following this process, 2 of I²CNER's young researchers were promoted in FY 2014 (1 from Postdoctoral Researcher to Assistant Professor and 1 from Assistant Professor to Associate Professor). In addition, 2 more young researchers will be promoted as of April 1, 2015 (1 from Postdoctoral Researcher to Assistant Professor and 1 from Assistant Professor).

Satellite Advisory Committee

The I²CNER Satellite Advisory Committee has been in place since the inception of the Institute. With the transfer of the I²CNER Satellite Associate Director, Prof. Ken Christensen, to the University of Notre Dame, in FY 2014, the Satellite Advisory Committee has assumed a more prominent role. The committee members are Professors Ian Robertson, Andrew Gewirth, and Ken Christensen. This committee advises the Director on all science issues at the I²CNER Satellite, including, but not limited to proposal reviews, project reviews, and consultation on Satellite research directions and general research issues.

Fostering Young Researchers and Advancing their Career Paths

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.

Distribution of Funding to Young Faculty

Having an overall view of the progress and activities of the full time I²CNER faculty and researchers, the Director has at his disposal the "I²CNER Competitive Funding" and the "Director's Discretionary Funding," which are both intended to foster and advance interdisciplinary research. Competitive funding is allocated to those faculty members who are productive, and whose achievements (including papers, awards, winning external research funds, etc.) are relevant to I²CNER's fusion research. The productivity of those faculty who receive competitive funding is assessed each year, and the funding is reallocated based upon this assessment. In addition, we also allocate fundamental Start-up Research Funding to young faculty members in order to support their research programs, with specific instructions that the funds should be used to advance interdisciplinary research.

SRA Program

I²CNER's "Super Research Assistants (SRA)" Program is intended 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 I²CNER SRAs is demonstrated by the fact that our former SRAs have been hired as JSPS fellows (i.e. Research Fellowship for Young Scientists: doctoral course students). I²CNER employed a total of 8 SRAs 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. By way of example, the 3rd KAKENHI Seminar was held by Prof. Michihisa Koyama (Energy Analysis Division) and Prof. Shigenori Fujikawa (CO₂ Capture and Utilization Division) on September 8, 2014, and 23 of I²CNER's young researchers attended.

Post-1² CNER Appointments of Young Researchers

Throughout its first 5-year term, many of I²CNER's young researchers have leveraged their I²CNER appointments to advance their careers. Some examples are:

- Dr. Yuki Naganawa (Postdoctoral Researcher) accepted a position as an Assistant Professor at Nagoya University, Japan.
- Dr. Le Zhang (Postdoctoral Researcher) accepted a position as a Postdoctoral Researcher at Eindhoven University of Technology, Holland.
- Dr. Seiichiro Kimura (Postdoctoral Researcher) accepted a position as an Associate of the Matsushita Institute of Government and Management, Japan.
- Dr. Ryota Watanabe (Postdoctoral Researcher) accepted a position as a Researcher at the National Institute of Advanced Industrial Science and Technology (AIST), Japan.
- Dr. Shuai Wang (Postdoctoral Researcher) accepted a position as a Postdoctoral Researcher at the University of Wisconsin-Madison, USA.
- Dr. Xuping Li (Postdoctoral Researcher) accepted a position as an Air Resources Engineer at the State of California Air Resources Board (CARB), USA.
- Prof. Maki Matsuka (Assistant Professor) accepted a position as a Researcher at the National Institute of Advanced Industrial Science and Technology (AIST), Japan.
- Prof. Sean Bishop (Assistant Professor) accepted a position as a Research Associate at the Massachusetts Institute of Technology (MIT).
- Prof. Nobuo Nakada (Assistant Professor) accepted a position as an Associate Professor at the Tokyo Institute of Technology, Japan.

Visiting Students

In order to facilitate active exchange of students between Kyushu University and the University of Illinois (I²CNER Satellite Institute), and other collaborating institutions overseas, the Institute accepts short-term students from overseas as "Visiting Students" at Kyushu University. 2 visiting students from UIUC were hosted in FY 2014.

International Symposia

- On an annual basis, I²CNER holds a symposium addressing the current scientific state-of-the-art in its thematic research areas (divisions). The objective of this series of international symposia is to identify what I²CNER researchers see as the major roadblocks, challenges, and opportunities in those fields, to demonstrate how the Institute's efforts are addressing these, and to show where the Institute's research activities lie in terms of excellence, successful fusion, and interdisciplinary impact relative to the spectrum of research being carried out today in the global scientific community. Each year, the symposium is followed by more specific workshops organized by each division. These workshops are brainstorming for awhich provide opportunities to identify strengths and weaknesses in our research portfolio, and explore how we might best accomplish critical growth in scientific breadth of the thematic research areas. In FY 2014, the "I²CNER Annual Symposium 2015: Fuel Generation and Use for the 21st Century" was held on February 2, 2015 and was attended by 141 scientists. Holding with the I²CNER tradition, follow-up workshops were hosted by each division as part of the "I²CNER International Workshop" on February 4 and 5, 2015. The topics of these 9 workshops included the hydrogen economy, hydrogen production by photocatalytic water splitting, sustainable material conversion systems, innovative CO₂ capture, CO₂ geological storage, hydrogen materials interactions (fatigue and fracture, and tribology), and thermal issues for hydrogen and related energy systems.
- The hosting of the Tokyo Symposium, which is sponsored by the U.S. Embassy in order to bring I²CNER research activities to the attention of the energy stakeholders in the capital of Japan and the international community, is another growing I²CNER tradition. So far, two symposia were hosted in 2012 and 2014, both with the presence of the US Ambassador to Japan and high-ranking government officials from MEXT, DOE, and the White House. The stated objective of the 2014 symposium was to show how merging Japan and the US academic and research cultures is impacting and transforming multidisciplinary international research and academic infrastructures, and explore what can be done to improve, enhance, and accelerate the transition of our research to impactful energy solutions.
- 4 WPI institutes (AIMR, iCeMS, MANA and I²CNER) organized a workshop at the E-MRS (European Materials Research Society) Spring Meeting in Lille, France in May 2014. Director Sofronis and Professors Sakai and Adachi gave presentations at the workshop.

4. Implementing organizational reforms

* If innovated system reforms generated by the center have had a ripple effect on other departments of the host institutions or on other research institutions, clearly describe in what ways.

O *I²CNER's Merit-based Salary System/ KU's New Merit-based Annual Salary System* Compensation considerations are based upon a special agreement between I²CNER 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, I²CNER follows a special merit-based salary system which deviates from the established salary ranges. Upon KU's review of the effectiveness of this system in I²CNER, it was determined that the university should adopt this system across all units in order to make KU an attractive place for young scientists to initiate their career, and for senior scientists to expand their research programs. Kyushu University's new merit-based annual salary system for faculty members is intended to promote revitalization by securing diverse, international, and competent personnel. As of April 1, 2015, 6 Kyushu University faculty will be paid within this system. Kyushu University's long-term goal is to pay approximately 20% of its faculty within this system.

O Cross-Appointment Employment System

In view of the successful model of Director Sofronis' cross-appointment case, which was the first ever at Kyushu University, KU institutionalized a cross-appointment employment system in March 2015. Though there are no cross appointments through the system yet since it is brand new, the Kyushu University Administration is working to promote/encourage new appointments through this system, which may include researchers from the private sector (industry) within and outside Japan, and other universities and institutes, both foreign and domestic. The KU Administration views this

system as an excellent way to identify and leverage resources for hiring elite young faculty at Kyushu University. By way of example, a possible cross appointment case is being explored between the Institute of Mathematics for Industry (IMI) and an Australian institution. In addition, the Kyushu University Administration plans to utilize this system in the hiring of new faculty for its new undergraduate school, which will fall within the framework of the Super Global University (Top Global University) initiative.

O Intra-University Faculty Transfer System

Kyushu University's "Intra-University Faculty Transfer System" was designed to enable flexibility in allocating faculty within the University for the purpose of improving the standards of education and research conducted at KU. Utilizing this personnel-system reform, 9 senior-level Kyushu faculty have been transferred to I²CNER and serve as the core Kyushu-based PIs of I²CNER. These tenured faculty can return to their original departments after they have spent a reasonable amount of time in I²CNER. After having utilized this system for the past 2 years, the current Kyushu University Administration is working together with I²CNER to assess the effectiveness of the system and to explore ways in which the system could be improved. By way of example, discussions have been initiated between the KU Administration, I²CNER, and other academic units of KU to consider whether or not the transfers may better serve Kyushu University and the WPI vision if they are made permanent.

O Travel Expenses for Inviting Researchers from Overseas

Under authorization of the Kyushu University Administration, when inviting renowned researchers from overseas, I²CNER implemented a unique practice of paying increased per diem rates to offset higher travel expenses for more prestigious/internationally visible researchers (i.e. in special circumstances) in order to ensure that travel costs did not become a barrier to their visiting Kyushu University. The idea behind this practice is to increase the overall international visibility of I²CNER/Kyushu University by attracting the world's best researchers to visit to give seminar presentations, interact with our researchers, etc. Due to the success of this practice in I²CNER, the Kyushu University Administration has authorized this practice in other units of KU, as well. By way of example, the Ultramicroscopy Research Center, the Graduate School of Integrated Sciences for Global Society, and the Faculty of Information Science and Electrical Engineering have all issued increased per diem payments to world-renowned visiting researchers.

\circ *I*²*CNER Faculty Involvement with Teaching*

I²CNER faculty are involved with teaching. Three (3) new "Education and Research Fields," which Kyushu University has established in the School and Graduate School of Engineering, and the Department of Automotive Science of the Graduate School of Integrated Frontier Sciences, are all engaged in research areas which overlap with those of I²CNER. The university has already ensured that the Institute's full-time faculty members can remain involved with both the teaching and supervision of students within the university in these schools. In fact, KU values this involvement and views it as essential to the revitalization of its programs because it brings into the classroom faculty with international experiences with cutting-edge research. The load will be flexible in order to help maintain the highest possible standards of performance, both for their research and teaching obligations. I²CNER's young faculty have already begun teaching joint courses on energy. These courses are part of the globalization program of KU, such as the former GLOBAL 30 and the recent Top Global University (TGU) Program of MEXT. As such, the average teaching load for I²CNER's young faculty is low (co-teaching of a single course per academic term). In addition, KU is planning to establish an International Liberal Arts and Sciences College (this is a tentative name and it is a new undergraduate school) within the coming 4 years in the framework of the TGU This college will encompass both physical and social sciences. We envision that program. I²CNER's young faculty will help the educational mission of the new college by offering science and technology courses in their relevant fields, again, in a way that balances research and teaching obligations. Since, according to President Kubo's vision, 10-15 of I²CNER's PIs will come from other units of KU or industry, either through the Intra-University Transfer System or cross-appointments, it is our vision that these tenured PIs in I²CNER will supervise the graduate students they bring with them from their home departments jointly with other I²CNER faculty. For the faculty of Kyushu University contributing to the project through the transfer system or cross appointments, the university will work with the home departments to provide the support needed for the employment of substitutes for their educational mission. The I²CNER faculty's involvement in teaching will be used as a model for other, similar units of Kyushu University.

O *l²CNER's Role in Kyushu University's Internationalization Initiative*

Kyushu University is implementing a project for internationalization of research and education throughout the University. As a part of this plan, efforts have been made in collaboration with the International Affairs Division of Kyushu University to introduce undergraduate and postgraduate degree programs in English; to increase the number of international students and excellent lecturers; to prepare internal documents and the university webpage in English; to assist students and staff members to improve their English language skills; and to establish international student and researcher support centers at every campus in order to further accelerate the establishment of international education and research environments. In this regard, I²CNER provides an unparalleled opportunity for many permanent Kyushu University employees, especially those who serve in the Institute's Administrative Office, to strengthen their English language skills, which can then be used in subsequent posts at KU. By way of example, a former I²CNER Associate Administrative Director was promoted to the Head of the International Student Exchange Division of the International Affairs Department as of September 1, 2014.

O *Revision of KU Systems*

In addition, Kyushu University works in cooperation with I²CNER for flexible implementation, adjustment, and modification of the university's internal systems, upon the requests from the Institute Director, in order to ensure smooth management of the Institute. For example, the Executive Vice President in charge of Research is currently working with the I²CNER Director and other academic units of Kyushu to explore cross appointments, improvement of the intra-university faculty transfer system, and identify ways for I²CNER to leverage the existing Kyushu University Joint Research Department System.

5. Efforts to secure the center's future development over the mid- to long term

* Please address the following items, which are essential to mid- to long-term center development:
 - Future Prospects with regard to the research plan, research organization and PI composition; prospects for the fostering and securing of next-generation researchers

- Prospects for securing resources such as permanent positions and revenues; plan and/or implementation for defining the center's role and/or positioning the center within the host institution's institutional structure - Measures to sustain the center as a world premier international research center after program funding ends (including measures of support by the host institution)

O President Kubo's Vision

I²CNER embarks upon its second term as a permanent unit of KU. According to President Kubo's vision, there are going to be (10) tenured PIs organically in I²CNER. The rest of the 10-15 PI positions in I²CNER (out of the 20-25) will come from either: a) other units of KU through the Intra-University Transfer System (this means that those tenured faculty can return to their original departments after they have spent a reasonable amount of time in I²CNER), b) through cross-appointments between I²CNER and other units of KU, e.g. economics, sciences, mathematics, life sciences, etc., or c) through cross-appointments between I²CNER and its international partner institutes and industry. In addition, the vision is that 3 to 4 PIs amongst the 10 tenured faculty will be non-Japanese. In order to support the recruitment of such distinguished researchers as tenured I²CNER PIs from abroad, Kyushu University has recently introduced in its Education and Research Council the new Merit-based Annual Salary System, which allows for these foreign faculty to be compensated with a competitive salary, according to international standards. Lastly, apart from the PI categories (a), (b), and (c) above, following the Institute's policy on Faculty Fellows, I²CNER will host Faculty Fellows at the PI level.

O University Reform Revitalization Program

Kyushu University implements the "University Reform Revitalization (URR) Program" in order to encourage individual units of the University to actively review their structure and promote reform in order to revitalize the University. In line with this policy and the President's Vision for tenured PIs in I²CNER as described above, I²CNER competes for tenured positions through this program by annual proposal submissions, and will make continued efforts to secure additional tenured positions. As of April 1, 2015, I²CNER has a total of 2 tenured full-professor and 7 tenured associate professor

positions, of which, 2 positions will be used to hire foreign PIs, as required by the KU Administration. International recruitment efforts are ongoing.

O Kyushu University Administration Support of the Diversification of I²CNER Faculty Kyushu University will help the Director to diversify the population of I²CNER PIs and expertise in areas such as mathematics, economics, social and life sciences, and computational science. Faculty appointments in I²CNER from other KU units will be viewed as prestigious positions in Kyushu University.

O Computational Sciences and Mathematics within \hat{I}^2 CNER Already, efforts have been initiated to expand I^2 CNER's current research plans to include computational sciences and mathematics. This is to be accomplished through exploratory workshops.

O *P*²CNER Synergy with Kyushu University

Under the advisement of the KU President, meetings are underway with other Kyushu University units and Executive Vice Presidents to discuss the expansion of I²CNER's engagement with Kyushu University. The idea is to expand the research platform of I²CNER to leverage Kyushu University's resources beyond those of the Faculty of Engineering. By way of example, I²CNER is in discussions with the Executive Vice President for International Programs about leading Kyushu University's participation in the RENKEI program. The KU President personally facilitates and oversees the discussions between I²CNER and other KU units about the personnel structure and personnel allocation framework within I²CNER, in consideration of the Director's policy and expectations. At the request of the President, the Executive Vice President in charge of Research will make necessary arrangements within the university/nurture I²CNER's relationships with other KU units. Specifically, by encouraging permanent faculty transfers and cross-appointments, the President has provided a framework in which I²CNER can develop a synergistic relationship with other Kyushu units. All of this is done in support of the Director's efforts to execute the WPI vision for the university.

O Leveraging l^2 CNER infrastructure to compete for research funding

With regard to securing revenue, I²CNER researchers leverage the established infrastructure and research culture of the Institute to aggressively pursue funding. By way of example, efforts are currently underway through the Core-to-Core international program of JSPS and the PIRE program of NSF. In addition, I²CNER PIs are pursuing large funding for their research efforts in the form of research centers. By way of example, Prof. Ogo directs the Center for Small Molecule Energy (CSME) and Prof. Horita has proposed the "International Research Center of Giant Straining for Advanced Materials (IRC-GSAM). As an Institute, I²CNER will leverage the initiatives of the government of Japan for globalization of the national universities. Due to its linkage with the University of Illinois, I²CNER, along with KU, is in a unique position to compete for resources in these government initiatives. Additional resources are expected to come from technology transfer or patent sales and corporation-supported non-tenured faculty members whose research is impactful to the corporation's operations (e.g. Air Liquide's support of Prof. Alex Staykov).

O Kyushu University's Mid-term Plan

I²CNER is at the center of Kyushu University's (KU) mid-term plan, which specifies that KU will "promote leading-edge research related to the carbon-neutral energy research domain in collaboration with the University of Illinois, which is conducted at the International Institute for Carbon-Neutral Energy Research (I²CNER). I²CNER is one of the research centers funded by the "World Premier International Research Center Initiative (WPI)" of MEXT and possesses the strength and unique characteristics of Kyushu University." Also, in its third-period mid-term goal and plans, KU is considering developing an energy-related plan centered on I²CNER.

\circ *l²CNER Research Hub*

In order to continue developing a research environment befitting a top world-level research institute, and to promote collaboration and fusion research, I²CNER Building 2 was completed at the end of February 2015, following the completion of I²CNER Building 1 in FY 2012. Both buildings are designed to promote interdisciplinary research in an "under one roof" spirit, and are home to several common laboratories which are available for use by any I²CNER researcher. The I²CNER Buildings are located at the heart of the Center Zone on the Ito Campus of Kyushu University, which is being developed rapidly into the 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 the

I²CNER Buildings. KU's Center of Innovation (COI) project, the Center for Co-Evolutional Social Systems (CESS), is also in the same vicinity.

O *l²CNER's Permanent Position within Kyushu University*

Effective April 1, 2013, with the revision of the Regulations of Kyushu University, which are the most significant among its rules and regulations, I²CNER's position is clearly defined as a permanent Research Institute of Kyushu University without regard to the length of the WPI Program. In addition, the revised General Regulations of Faculty Councils and the Regulations of I²CNER enable the Institute to have a Faculty Council within the institution in light of the Director's top-down decision making system, which is the intent of the WPI Program. These revisions make I²CNER's Faculty Council substantially different from conventional Faculty Councils. This unconventional approach not only serves as a catalyst for improving the members' mindset, but also as a challenge to impact the very concept of the faculty council system in Japan.

O Options for long-term funding of $l^2 CNER$

With regard to additional funding sources for the operation of I²CNER, the following financial measures are under consideration:

- In addition to the KU management expense grants, which are spent for the operation of I²CNER, external funding acquired by the core researchers will be allotted to management, personnel, research, and any other expenditures of their own research activities.
- 2. Hiring of 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 (IMAQ) is expected to play an active role in this development.
- 4. Foundations associated with KU could contribute to I²CNER's sustainability. Example cases within KU are the Inamori Frontier Research Center, which is supported by Kyocera, and the research support provided by the Gas Association of Japan to the Faculty of Engineering.
- Leverage the initiatives of the Government of Japan for globalization of the National Universities. Thanks to its linkage with the University of Illinois, I²CNER, along with KU, is in a unique position to utilize these government initiatives for resources and future expansion.
- 6. I²CNER will promote/advance the "open innovation process," and aggressively pursue relationships with industry and government programs to identify mission-oriented basic science that will support technology implementation in industry.

O Maintaining the International Culture of P²CNER

To attract leading researchers from overseas universities and research institutes to I²CNER, new initiatives, such as I²CNER's Faculty Fellows Program, and KU's "Cross-Appoint System" (established in March 2015) will be utilized. More active engagement and interactions between KU and Illinois researchers will be promoted through mutual PI sabbaticals, etc. based on the Agreement on Academic Cooperation between the two universities (signed in FY2014). The Agreement on Student Exchange, which was also signed in FY2014, will help further promote student exchange between Kyushu and Illinois, and may lead to the development of a "Joint-Degree Program," etc.

O *l²CNER-Industry Collaboration*

Kyushu University plans to further promote I²CNER's collaboration with industry through its unique "Joint Research Department System," which has been implemented successfully in other KU units, such as the Faculty of Engineering, the Faculty of Information Science and Engineering, the Center for Advanced Medical Innovation, the Faculty of Agriculture, the Institute of Mathematics for Industry, etc. The Kyushu University Administration is working with the I²CNER Director to establish such a Joint Research Department within I²CNER in the near future. In addition, strong cooperation between the Industry-University- Government Collaboration Management Center of Kyushu University (IMAQ) and the Office of Technology Management (OTM) of the University of Illinois has already started. IMAQ and OTM signed an agreement on IP Management on March 26, 2015. Visits amongst the two offices are planned for discussions on both national and international technology transfer.

O Support from KU's Office for Strategic Research Planning

The Office for Strategic Research Planning and other related offices of Kyushu University will continue to proactively support researchers in their efforts to secure large competitive research grants. Such assistance involves information gathering and thorough advice on grant applications. By way of example, Prof. Horita has applied for the "International Research Center of Giant Straining for Advanced Materials (IRC-GSAM). In addition, the Office will assist I²CNER in its efforts to compete for research funds from the local government and industries in related areas.

O I²CNER Director's Authority and Access to the KU President

Regular meetings will be held between the Director and the Executive Vice President in charge of Research and Industry Collaboration. Advice and counsel from the President will be given as needed. With regard to matters relating to the promotion of university-industry collaboration, the Executive Vice President in charge of Research and Industry Collaboration will provide the Director with necessary support and advice. I²CNER is in line with the mid-term goal and plans of Kyushu University, and organized directly under the President of Kyushu University. The Institute Director, Prof. Sofronis, has direct access to the Office of the President and the Office of the Executive Vice President in charge of Research and Industry Collaboration. Support to the Institute Director from the University President, and from all individual departments of Kyushu University, will continue to be guaranteed. In addition, the Executive Vice President in Charge of Research and Industry Collaboration is working to further strengthen awareness and support of I²CNER amongst the other Vice Presidents. The decision-making system of the Institute has been set so that the Director is solely responsible for making decisions regarding the planning and conduct of the research activities, the formation and composition of the research program areas or divisions, potential division reorganization and redirection of research efforts in response to the feedback from the annual site visit reviews of the Institute, the recruitment of postdocs and faculty, the establishment of international collaborations and interactions with top research Institutions, the administration of the peer evaluation process of the Institute's research output, and budget implementation, the idea being that the Director's authority will affect future organizational reforms, developments, etc.

Kyushu University Administration Support of I²CNER Administrative Office As part of the university's continued efforts to strengthen the administrative support for I²CNER, a Head of Administration, which is a management-level position, was assigned to the Administrative Office in FY2014. I²CNER is the only permanent research institute at Kyushu University that has its own support office, making this the first such assignment ever made at the university.

O I² CNER as a Model for Kyushu University Internationalization

Kyushu University promotes the concept of this Institute as the model project for internationalization of research and education in the University, and applies the concept to the entire University body, with the aim of transforming Kyushu University's academic culture so that it exemplifies the WPI vision for international reputation, training of young scientists in an international environment, advancing knowledge through an open research platform, and attracting scientists and students from around the globe.

6. Others

* In addition to the above 1-5 evaluation items, only if there is anything else that deserves mention regarding the center project's progress, please note it.

Internal Programs Review Committee (IPRC)

The Internal Programs Review Committee (IPRC) is an important standing committee of the Institute which is called by the Director whenever necessary to review individual programs within the Institute. The members of the IPRC and the Chair of the Committee are appointed by the Director. Once the review(s) are complete, the IPRC provides the Director with a written advisory report. The final decision about what action to take regarding any individual research program is the responsibility of the Director. In FY 2015, the composition of our Internal Programs Review Committee (IPRC) will be revisited in order to make it more efficient (meetings involving discussion and debate), so as to enable it to reach more concrete and evaluative conclusions (e.g. more critical assessments of underperforming research efforts).

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, a member of the IPRC, and a member of the Satellite Advisory Committee, but also as the Chief Science Advisor to the Director in order to further strengthen the management of the Institute in relation to its research activities.

FY 2014 Recruitment Campaigns

In FY 2014, the Institute ran 1 open recruitment campaign for foreign PIs from which we received 12 applications and made 0 hires. Similarly, the Institute ran 1 open recruitment campaign for faculty positions from which we received 3 applications and made 0 hires. In the area of postdoc recruitment, we ran 2 open recruitment campaigns resulting in a total of 29 applications and hired 1 foreign researcher. In addition, we ran 2 recruitment campaigns specifically for researchers for the Energy Analysis Division which resulted in 3 applications for faculty positions and 10 applications for postdoc positions, but 0 hires were made.

7. Center's response to interim evaluation

Transcribe each item from the "7. Actions required and recommendations" section and note how the center has responded to them. However, if you have already provided this information, please indicate where in the report.

1) The current composition of researchers is limited to a few areas of engineering, lacking theorists, mathematicians, environmental specialists and social scientists. Diversification of PIs and their expertise is indispensable if I²CNER wants to challenge mid- to long-term disruptive technology targets.

I²CNER's status in KU President Kubo's vision, specifically, his plan for I²CNER's interaction with other units of Kyushu, will help transition I²CNER into a center that involves additional key components, such as technology forecasting, social return on investment, science communication with the public, mathematics, and computational science. The Director has regular meetings with the Executive Vice Presidents for Research and International Programs, and discusses precisely strategies through which the university can help I²CNER diversify its core of PIs.

Meetings with Prof. Sharon Hammes-Schiffer of the University of Illinois (UIUC) on computational science capabilities have already occurred. In fact, Prof. Hammes-Schiffer, a world authority on computational sciences, already began working with I²CNER. A workshop which focuses on and explores computational sciences in carbon neutral energy, and which will involve a few relevant, well-regarded academic and industrial research partners, is planned for FY 2015. This summer, I²CNER PIs Christensen and Tsuji will participate and give a presentation in the meeting of the Mathematics for Industry Study Group, which will be held from July 29 to August 4 at Kyushu University and the University of Tokyo. The idea is to work in collaboration with the Executive Vice President for Research of KU to explore interactions with the mathematics community which hopefully will result in a workshop on applied math for energy. Another area under consideration is related to modeling of the network. Prof. Fujii from the University of Tokyo has been appointed as a WPI Visiting Professor to help with exploratory discussions on subject.

Regarding the recommendation on social science, the EAD is aggressively searching for new members, (postdocs and faculty) through continuous recruitment calls, and is also looking for an expert in social science who will assess the economic and social aspects of technology deployment. This person's objective will be to understand the deployment barriers to energy technologies as they depend upon risk and communication.

2) Serious effort should always be made to identify next research focus and research topics with the help of EAD. Make much better use of roadmaps and concretely integrate them in the decision making vis. future research priorities.

The EAD has already engaged with each of the technical divisions to revisit and revise their respective roadmaps, including reconsideration, consolidation, and elimination of select projects. The roadmaps

have been revised from the versions that were presented in the Interim evaluation, and whenever possible, projects' milestones were placed within a time period of 15-20 yrs. from now so that projects could finish by 2030 or 2035, rather than 2050. Lastly, benchmarks for the targets of each I²CNER research project have been identified, and some of these benchmarks reflect our accomplishments (e.g. hydrogen activation catalysts, materials for on board hydrogen storage). All research presented in Sections 1 & 2 of this report reflects the revised/updated roadmaps as of March 31, 2015. In addition, the composition of our Internal Programs Review Committee (IPRC) will be revisited in order to make it more efficient (meetings involving discussion and debate), so as to enable it to reach more concrete and evaluative conclusions (e.g. more critical assessments of underperforming research efforts). The advice of I²CNER's External Advisory Committee (EAC) will be taken into consideration, as well. As described above, plans are being finalized for a workshop on computation which will take place in FY 2015. The EAD is planning to investigate the feasibility of importing renewables, such as biofuels, to Japan from sources outside Japan, and the related technologies, such as integration of renewable energy to the grid. Depending on the conclusions of these efforts, I²CNER will consider investing in the fundamental science related with these technologies.

3) The research on CO_2 and CCS at I^2 CNER is needed to redesign and enhance to reach a world top level institution.

CO₂ Storage: Following reorganization of its personnel and research focus areas in 2012, including replacing the Division Lead PI with a younger researcher of I²CNER, and the addition of a preeminent expert in pore scale simulations at Illinois, the CO₂ storage division has focused its efforts on becoming an international leader in the area of pore-scale flow processes central to CO₂ migration within water-saturated heterogeneous rock formations typical of Japan and many other countries considering geologic sequestration of CO₂. Evidence of this international achievement includes the development and implementation of transformational simulation and experimental techniques that have revealed new and critical physics central to CO_2 fate in rock. For example, I^2CNER is a world leader in the use of the Lattice Boltzmann Method (LBM) for simulating the flow of CO₂ and brine in digital rock models (i.e., porous simulation domains generated from scans of actual rock samples) that have now clarified, for the first time, optimal injection conditions for maximizing CO₂ capacity in the reservoir while minimizing CO_2 mobility for long-term and safe storage. Now, I²CNER is also a world leader in laboratory experimental studies of such flow processes at reservoir conditions (i.e., very high pressures) wherein the flow physics is directly quantified. The tools that I²CNER has developed have transformed our understanding of how CO₂ migrates through the pore space, particularly the transient nature of this migration, and highlight significant deficiencies in present modeling strategies that are often used to predict CO_2 fate in actual reservoirs. Finally, I²CNER is making transformational advances in linking pore-scale flow physics with geological monitoring methodologies to provide a step-change in our ability to remotely monitor CO₂ once it has been injected into geologic reservoirs. By linking laboratory experiments on actual rock core with the LBM simulations mentioned above, I²CNER has advanced the world's understanding of how rock heterogeneity can actually improve the trapping of CO₂ for safe and efficient geologic CO₂ storage while also providing a clear link between elastic wave velocities often monitored in the field with trapped CO_2 in the pore structure. Thus, post-reorganization and realignment, I²CNER's CO₂ Storage Division has rapidly ascended to become an international authority on pore-scale flow processes central to geologic CO₂ storage, and we expect our impact and visibility to continue its rapid rise in this regard. Lastly, the CO₂ storage division researchers are deeply involved in many international collaborations on geologic CCS, including 1) a new US Department of Energy (DOE) Energy Frontiers Research Center based at the University of Illinois focused on understanding pore-scale flow processes relevant to geologic CO₂ storage in the United States, 2) the Tomakomai CCS projects in Japan, and 3) the Spitsbergen CCS effort in Norway. The involvement of I²CNER researchers in such international collaborations further validates the international leadership of I²CNER's CO₂ storage division, particularly noting that this division, in its current structure and associated research portfolio, is only 2+ years old.

 CO_2 Capture and Utilization: The original focus of the division was to use an electrochemical method for CO_2 separation. These efforts were not very successful. In 2012, Kenis from Illinois was asked to join I²CNER with a program focusing on conversion of CO_2 to value-added products. In the spring of 2013, the original research roadmap of the division was revised to focus on (1) CO_2 Capture, specifically separation of CO_2 using membrane-based approaches (Fujikawa, Taniguchi); and (2) CO_2

Utilization, specifically via electroreduction (Kenis in collaboration with members of the fuel cell division). The division was renamed the CO_2 Capture and Utilization Division. Dr. Fujikawa, an expert in membrane technology, became the new Lead PI of the division. Associate Professor Ikuo Taniguchi, an expert in materials synthesis, was hired to further strengthen the separation effort. In summary, the CO_2 Capture and Utilization Division started its research from scratch in January 2013—there were only 18 months between start of the new work and the Interim Evaluation Review of l^2CNER in June 2014. In FY 2014, Dr. Benny Freeman (University of Texas at Austin), world leader on separation processes, was added as an additional member of the division to strengthen the membrane separation efforts.

The reorganization of the division has had a positive outcome. In only 1.5 years, significant and impactful results have been obtained in both the capture and the utilization efforts. For example, a key breakthrough in developing ultrathin membranes with promising permeance and selectivity for CO_2 has been achieved. These are the world's thinnest (<30 nm), leak-free membranes that can be handled and transferred without a support material. These membranes represent a new class of materials for gas separations, but also open up new interdisciplinary research on ultrathin gas diffusion electrodes, ion conductive membranes, developments that have been rapidly emerging after the restructuring of the division. In addition, the work on the electroreduction of CO_2 is has already reached at the level of world class: the work at I²CNER has resulted in the very best catalysts and the best gas diffusion electrodes for production of desired products such as CO, ethylene, and ethanol, with the Faradaic efficiencies (=product selectivity), current densities (rate of production), and overall energetic efficiencies obtained exceeding (at times by a factor of 10) those obtained by others in this active research field, and these world record performance levels have almost met the first benchmarks of the division's roadmap. Also note that in close collaboration with the Energy Analysis Division, members of this division have completed a techno-economic feasibility study of the membrane-based capture and the electrochemical conversion processes being pursued, with the outcome that both approaches hold promise compared to current practice and compared to alternative approaches being studied.

In summary, the requested redesign of the research efforts of the CO_2 Capture and Utilization Division took place 1.5 years ago, and has successfully created a path towards world class research, a promise which is already being fulfilled, in part.

4) *Nuclear energy should be reconsidered and preferably removed from the portfolio of future research themes.*

The EAD will continue to update I²CNER's vision scenarios for carbon neutral energy in Japan. In these scenarios, we will recognize the possibilities for contributions from nuclear energy at various levels, including future technology developments; however, I²CNER will not create any research efforts associated with nuclear energy.

5) A particular effort should be made to invite world-leading top scientists who can join as foreign PIs residing at l^2 CNER.

In accord with President Kubo's vision, the long-term goal of I²CNER is to have 3 to 4 PIs among the 10 total tenured PIs in I²CNER be non-Japanese. Of the 3 positions which were won in the University Reform Revitalization Program in FY 2014, 2 of them will be used to hire foreign PIs, <u>as required by the KU Administration</u>. For the full details of I²CNER's tenured positions, please see *President Kubo's Vision* in Section 5 above. The new Annual Salary Scheme of KU to support recruitment of distinguished foreign researchers is helpful in this recruitment effort. I²CNER's Faculty Fellows Program will also be used to identify and help transition such foreign hires from their home institutions to KU. In February 2015, the Institute's reinvigorated recruiting campaign to hire permanent-staying foreign principal investigators began, including advertising in journals of related-societies, such as the Japan Research Career Information Network (JREC-IN) by the Japan Society of Mechanical Engineers, and the Chemical Society of Japan. This ongoing recruiting effort for foreign PIs will close on May 29, 2015. An additional campaign for postdoctoral researchers in the Energy Analysis Division and tenured faculty members at all ranks is also underway and closes on June 30, 2015. It should be noted that in our pursuit of foreign PIs, we shall never compromise our standards for I²CNER's established research culture.

6) A technology transfer system should be developed following many successful models internationally that can serve as examples (MIT, Stanford, ETH etc.).

It is the vision of President Kubo that technology transfer will be carried out through the concerted efforts of IMAQ of Kyushu University and OTM of the University of Illinois. A Memorandum of Understanding between Kyushu University and the University of Illinois at Urbana-Champaign on Intellectual Property created by these two offices has been signed. For full details on the memorandum, please see Section 3 above. IMAQ held an orientation seminar for all I²CNER researchers on September 30, 2014. A similar meeting was held by OTM at the Illinois Satellite on February 26, 2015. Leveraging the existing resources both at Illinois and Kyushu University, IMAQ and OTM will continue to work collaboratively to create a technology transfer system for I²CNER which may involve outreach to industry in Japan and the US. In addition, relationships between I²CNER and industry will be fostered using KU's "Joint Research Department System." For full details, please see Section 5 above.

7) The external advisory committee membership can be expanded in its number, expertise and nationality to seek advice for long-term strategy of l^2 CNER.

The membership of I²CNER's External Advisory Committee was expanded and diversified in FY 2014. In October 2014, Prof. Fraser Armstrong, University of Oxford, UK, an expert on catalysis and Fellow of the Royal Society, officially accepted our invitation to serve on the EAC. In November 2014, Mr. Mark Paster, Retired Analyst from the Energy Efficiency & Renewable Energy (EERE) Office, U.S. Department of Energy (DOE), officially transitioned into an EAC member role from his former position in I²CNER's Energy Analysis Division. Finally, Prof. Michael Celia, Princeton University, expert on CO₂ storage, specifically on pore scale behavior and upscaling to reservoir behavior, has officially accepted our invitation to join the EAC in FY 2015, effective April 12, 2015. The list of full members is as follows:

- Prof. Ronald J. Adrian (Chair), Arizona State University, USA, *National Academy of Engineering (NAE)*
- o Dr. Deborah Myers (Co-Chair), Argonne National Laboratory, USA
- o Dr. Robert J. Finley, Illinois State Geological Survey, USA
- Prof. Reiner Kirchheim, University of GÖttingen, Germany
- o Prof. Robert McMeeking, University of California, USA, National Academy of Engineering (NAE)
- o Dr. Kevin Ott, Retired, Los Alamos National Laboratory, USA
- Prof. Tetsuo Shoji, Tohoku University, Japan
- Prof. Fraser Armstrong, University of Oxford, UK, Fellow of the Royal Society (FRS)
- Mr. Mark Paster, Retired Analyst from the Energy Efficiency & Renewable Energy (EERE) Office, U.S. Department of Energy (DOE)
- o Prof. Michael Celia, Princeton University, USA (as of April 12, 2015)
- 8) For the sustainability of I²CNER after ten years, efforts should be started to design the finance and seek stable funding resources.

I²CNER's permanent position within Kyushu University has been ensured by the KU Administration, as is reflected in President Kubo's vision (please see Section 5 for full details). According the President's vision, I²CNER will have a core of 25 PIs, including 10 tenured PIs, with the remaining 10-15 PI positions coming from other departments of KU or from industry through various channels that the university currently has in place (e.g. cross-appointment system, etc.). Aside from the longevity which is guaranteed by the tenured positions, I²CNER's vital role in KU will be further enhanced by the involvement of these personnel from other units of Kyushu, including the planned International Liberal Arts and Sciences College, which will naturally allow these I²CNER PIs to step into roles (e.g. teaching) within those units that will extend beyond the I²CNER funding period.

With regard to additional funding sources for the operation of I²CNER, the following financial measures are under consideration:

 In addition to the KU management expense grants, which are spent for the operation of I²CNER, external funding acquired by the above-mentioned 25 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).
- Resources from technology transfer or patent sales. Kyushu University plans to further promote collaboration with industry through its unique "Joint Research Department System." Strengthening cooperation between the Industry-University- Government Collaboration Management Center of Kyushu University (IMAQ) and the Office of Technology Management (OTM) of the University of Illinois will help advance IP management and technology transfer, both nationally and internationally.
- 4. Foundations associated with KU could contribute to I²CNER'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.
- Leverage the initiatives of the Government of Japan for globalization of the National Universities. Thanks to its linkage with the University of Illinois, I²CNER, along with KU, is in a unique position to utilize these government initiatives for resources and future expansion.
- 8. Center's response to the site-visit report

Transcribe each item from the "7. Actions required and recommendations" section and note how the center has responded to them. However, if you have already provided this information, please indicate where in the report.

1) The mindset of the PIs, all other participants and the host institutions has been much improved, but they still have to strive for excellence, prestige and status by keep a strong sense of responsibility that they are developing and running a truly international, world top-level research center to meet the expectations of the general public.

As mentioned previously, President Kubo has formulated a specific vision for I^2CNER 's position and future within Kyushu University, and he intends to implement that vision along with Executive Vice President Wakayama, both through policy and progressive change of I^2CNER 's standing within Kyushu University. For complete details regarding the KU Administration's efforts in this regard, please see Sections 4 & 5 above. As mentioned in Section 3, UIUC Chancellor Phyllis Wise visited Kyushu University in FY 2014 and issued an open invitation to KU Administrators to visit the UIUC campus. For more details regarding the Illinois Satellite efforts to develop a truly international research center, please see Section 3. At the Institute level, the I^2CNER Administration is making every effort to reinforce an I^2CNER -centric mindset in all of its researchers.

<u>Efforts are underway to recast the framework in which our research divisions operate in consideration</u> <u>of I²CNER's roadmap for a carbon-neutral energy Japan</u>. By way of example, a reconfiguration of the hydrogen production and fuel cells divisions is almost complete. This includes a change of the Lead Principal Investigator in one of the divisions.

2) The current composition of researchers is limited to a few areas of engineering, lacking theorists, mathematicians, environmental specialists and social scientists. Diversification of PIs and their expertise is indispensable. More collaboration with basic science is needed by inviting PIs first from a closest school, the Faculty of Science of KU. Physical, material, life and computational sciences are highly recommended. This is necessary if P²CNER wants to challenge mid- to long-term disruptive technology targets.

Please see response under Section 7-1) above.

3) Serious effort should always be made to identify next research focus and research topics with the help of EAD. Make better much use of roadmaps and concretely integrate them in the decision making vis. future research priorities.

4) For I²CNER's scenarios, it seems appropriate to include renewable energy sources imported from outside Japan. The renewable energy could be much cheaper being produced in more suitable places in the world.

Transport of low carbon fuel from sources outside Japan, including hydrogen based on renewable energy such as wind, solar, and hydro, as well as brown coal reforming with CCS, will be carefully analyzed by the I²CNER EAD, including an examination of the viability of the process. In addition, I²CNER will explore required basic science breakthroughs for the development of technologies that utilize abundant renewable energy outside Japan, especially technologies that efficiently convert strong direct solar radiation in sun belts into hydrogen, including not only PV and CSP (Concentrating Solar Power) with electrolysis, but also technologies of thermal–chemical conversion and bio-chemical conversion.

In particular, biofuels are among the imported renewable energy sources from outside Japan that the EAD will analyze. For example, it is possible to gasify biomass and turn it into diesels or gasoline fuels. Biofuels could be used directly in standard or hybrid vehicles. Biofuels could be used with SOFCs to generate electricity or a combination of electricity and heat. They could be used with conventional combustion for heating homes and buildings, or to generate electricity. An important question is to identify which countries have "excess" biomass, or enough potential to produce it without compromising food production, and to determine whether those countries could export large quantities of biomass, and at what cost.

An additional project will involve the detailed analysis of the electricity grid relative to the use of new technologies and energy storage requirements. It is an uncontested realization that the future of most renewable energy solutions relies on their smooth integration into the electric grid.

5) The research activity related to CO_2 and CCS at I^2CNER is not at a world top-level and should be redesigned and enhanced if it is continued.

Please see response under Section 7-3) above.

6) Nuclear energy should be reconsidered and preferably removed from the portfolio of future research themes.

Please see response under Section 7-4) above.

7) Refocus, reduce, and/or eliminate few areas that are below par and are unlikely to become internationally competitive. Replace them with high-risk, high return original projects.

Efforts are underway to reformulate the framework under which our research on hydrogen production and fuel cells is being carried out. This includes divisional reconfigurations and Lead Principal Investigator changes.

The effort of identifying projects which are underperforming and which do not hold promise for international recognition has already started at the young researcher/faculty level. In fact, one postdoctoral researcher was terminated as of March 31, 2015. In addition, the appointments of an additional 2 assistant professors, 1 associate professor, and 1 postdoctoral researcher will be terminated as of March 31, 2016.

The Energy Analysis Division has revisited and updated the roadmaps, and any effort that does not hold promise for producing tangible results against the milestones or targets of the Division's roadmap will be reassessed. Plans will be underway pending the involvement of the IPRC.

8) A particular effort should be made to invite world-leading top scientists who can join as foreign PIs residing at I^2 CNER.

Please see response under Section 7-5) above.

9) *I²CNER* is recommended to develop more intimate and long-term connections or collaborations with researchers outside *I²CNER* to be a leader in this field. Working with leading groups in Japan in respective fields and collaboration outside US should be intensified.

I²CNER added the Air Resources Board of the State of California (CARB) to its network of international collaborating institutions in FY 2014. Negotiations for a <u>memorandum of understanding in the general</u> field of hydrogen technology between I²CNER and the Helmholtz Zentrum Geesthacht (HZG) are underway. In addition, there has been communication between the Director of I²CNER, the Director of the Helmholtz Institute in Juelich, and PI Reiner Kirchheim to explore areas for possible collaboration between the two Institutes, in particular, the areas of fuel cells, hydrogen production, storage, and delivery, and materials mechanical behavior.

Very recently, in FY 2014, Professor Khellil Sefiane, Head of the Institute for Materials and Processes, University of Edinburgh, Scotland, UK, became heavily engaged with I²CNER, spending about 3 months at I²CNER. He was appointed as a WPI Professor. In FY 2015, Prof. Sefiane plans to spend four months in residence at Kyushu through a cross appointment in the "Progress 100" Program. The possibility of a future/continuing cross-appointment for Prof. Sefiane will be explored in FY 2015.

We appointed Dr. Kurosawa from the Institute of Applied Energy as a WPI Visiting Professor to work with the EAD on the MARKAL-TIMES energy model developed by the International Energy Agency to analyze feasibility and impact of energy scenarios. We also appointed Prof. Fujii from the University of Tokyo as a WPI Visiting Professor to help the EAD with the analysis of the integration of renewables with the grid. In FY 2015, Dr. K. Hirose from TOYOTA Motor Corporation will be appointed as a WPI Visiting Professor to help the EAD with assessing and analyzing hurdles or opportunities to achieve a carbon-neutral energy society in Japan with regard to the needs and deployment of a hydrogen infrastructure for the production and delivery of hydrogen for fuel cell vehicles and other potential hydrogen applications.

The I²CNER Director serves on the Strategic Advisory Panel of HEmS, a research center at Oxford University whose goal is to study hydrogen in metals—from fundamentals to the design of new steels. Collaborations with other centers outside the US are in place with the Norwegian University of Science and Technology (NTNU) and SINTEF. The relevant MoU was signed on March 17, 2014.

10) Developing a technology transfer system should be focused on in the second WPI phase. There are many successful models internationally that can serve as examples (MIT, Stanford, ETH etc.).

Please see response under Section 7-6) above.

11) The external advisory committee membership can be expanded in its number, expertise and nationality to seek advice for long-term strategy of *l*²CNER.

Please see response under Section 7-7) above.

12) For the sustainability of I²CNER after ten years, efforts should be started to design the finance and seek stable funding resources.

Please see response under Section 7-8) above.

List of Center's Research Results and Main Awards

A. Refereed Papers

List only the Center's papers published in 2014. (Note: The list should be for the calendar year, not the fiscal year.)

- (1) Divide the papers into two categories, A and B.
 - A. WPI papers

List papers whose author(s) can be identified as affiliated with the WPI program (e.g., that state the name of his/her WPI center). (Not including papers whose acknowledgements contain the names of persons affiliated with the WPI program.)

B. WPI-related papers

Among papers published in 2014, list those related to the WPI program but whose authors are not noted in the institutional affiliations as WPI affiliated. (Including papers whose acknowledgements contain the names of researchers affiliated with the WPI program.)

Note: On 14 December 2011, the Basic Research Promotion Division in MEXT's Research Promotion Bureau circulated an instruction requiring paper authors to include the name or abbreviation of their WPI center among their institutional affiliations. As some WPI-affiliated authors of papers published up to 2011 may not be aware of this requirement, their papers are treated as "WPI-related papers." From 2012, however, the authors' affiliations must be clearly noted and only category A papers will be listed.

Newly selected centers are to list papers under category C below (in addition to categories A and B above).

(2) Method of listing paper

- List only referred papers. Divide them into categories (e.g., original articles, reviews, proceedings).

- 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 (say, more than 20), all of their names do not need to be listed.

- If the papers are written in languages other than English, divide them into language categories when listing them.

- Assign a serial number to each paper to be used to identify it throughout the system.

(3) Submission of electronic data

- In addition to the above, for each paper provide a .cvs file output from the Web of Science (e.g.) or other database giving the paper's raw data including Document ID. (Note: the Document ID is assigned by paper database.)

- These files do not need to be divided into paper categories.
- (4) Use in assessments
 - The lists of papers will be used in assessing the state of WPI project's progress in FY 2014.
 - They will be used as reference in analyzing the trends and states of research in all the WPI centers, not to evaluate individual researcher performance.
 - The special characteristics of each research domain will be considered when conducting assessments.
- (5) Additional documents

After all documents, including these paper listings, showing the state of research progress have been submitted, additional documents may be requested.

Order of Listing

- A. WPI papers
 - 1. Original articles
 - 2. Review articles
 - 3. Proceedings
 - 4. Other English articles
 - 5. Articles written in other than English

B. WPI-related papers

1. Original articles

- 2. Review articles
- 3. Proceedings
- 4. Other English articles5. Articles written in other than English

Note: The list includes the refereed papers published in the calendar year

2014 either online or in print whichever comes first.

No.	Description
	A. WPI papers
	A.1. Original articles
1	Ju, YW., Hyodo, J., Inoishi, A., Ida, S., and Ishihara, T. (2015), A dense La(Sr)Fe(Mn)O _{3-δ} nano-film anode for intermediate-temperature solid oxide fuel cells, Journal of Materials Chemistry A, 3 (7), 3586-3593
2	Noguchi, Y., Kim, HJ., Ishino, R., Goushi, K., Adachi, C., Nakayama, Y. and Ishii, H. (2015), Charge carrier dynamics and degradation phenomena in organic light-emitting diodes doped by a thermally activated delayed fluorescence emitter, Organic Electronics: physics, materials, applications, 17, 184-191
3	Li, M., Zhang, H., Cook, S.N., Li, L., Kilner, J.A., Reaney, I.M. and Sinclair, D.C. (2015), Dramatic influence of A-site nonstoichiometry on the electrical conductivity and conduction mechanisms in the perovskite oxide Na _{0.5} Bi _{0.5} TiO ₃ , Chemistry of Materials, 27 (2), 629-634
4	Hyodo, J., Tominaga, K., Hong, JE., Ida, S. and Ishihara, T. (2015), Effects of three-dimensional strain on electric conductivity in au-dispersed Pr _{1.90} Ni _{0.71} Cu _{0.24} Ga _{0.05} O _{4+δ} , Journal of Physical Chemistry C, 119 (1), 5-13
5	Fukuhara, L., Kosugi, K., Yamamoto, Y., Jinnai, H., Nishioka, H., Ishii, H. and Kawahara, S. (2015), FIB processing for natural rubber with nanomatrix structure, Polymer (United Kingdom), 57, 143- 149
6	Li, P., He, X., Huang, T.C., White, K.L., Zhang, X., Liang, H., Nishimura, R. and Sue, HJ. (2015), Highly effective anti-corrosion epoxy spray coatings containing self-assembled clay in smectic order, Journal of Materials Chemistry A, 3 (6), 2669-2679
7	Hirata, S., Sakai, Y., Masui, K., Tanaka, H., Lee, S.Y., Nomura, H., Nakamura, N., Yasumatsu, M., Nakanotani, H., Zhang, Q., Shizu, K., Miyazaki, H. and Adachi, C. (2015), Highly efficient blue electroluminescence based on thermally activated delayed fluorescence, Nature Materials, 14 (3), 330-336
8	Sagara, Y., Shizu, K., Tanaka, H., Miyazaki, H., Goushi, K., Kaji, H. and Adachi, C. (2015), Highly efficient thermally activated delayed fluorescence emitters with a small singlet-triplet energy gap and large oscillator strength, Chemistry Letters, 44 (3), 360-362
9	Zheng, YQ., Potscavage, W.J., Zhang, JH., Wei, B. and Huang, RJ. (2015), Hole transporting material 5, 10, 15-tribenzyl-5H-diindolo[3, 2-a:3', 2'-c]-carbazole for efficient optoelectronic applications as an active layer, Chinese Physics B, 24 (2), 027801
10	Inoishi, A., Matsuka, M., Sakai, T., Ju, YW., Ida, S. and Ishihara, T. (2015), Lithium–Air Oxygen Shuttle Battery with a ZrO ₂ -Based Ion-Conducting Oxide Electrolyte, ChemPlusChem, 80 (2), 359- 362
11	Takenaka, S., Mikami, D., Tanabe, E., Matsune, H. and Kishida, M. (2015), Modification of carbon nanotube surfaces with precious metal and transition metal oxide nanoparticles using thin silica layers, Applied Catalysis A: General, 492, 60-67
12	Harada, K., Oishi, T., Hamamoto, S., Kawasaki, T. and Ishihara, T. (2015), Oxygen desorption properties of Pr ₆ O ₁₁ doped with Bi and Ce for low temperature particulate matter oxidation, Applied Catalysis A: General, 492, 223-230
13	Ida, S., Kim, N., Ertekin, E., Takenaka, S. and Ishihara, T. (2015), Photocatalytic Reaction Centers in Two-Dimensional Titanium Oxide Crystals, Journal of the American Chemical Society, 137 (1), 239-244
14	Matsuno, H., Ohta, T., Shundo, A., Fukunaga, Y. and Tanaka, K. (2014), Simple surface treatment of cell-culture scaffolds with ultrafine bubble water, Langmuir, 30 (50), 15238-15243
15	Shizu, K., Tanaka, H., Uejima, M., Sato, T., Tanaka, K., Kaji, H. and Adachi, C. (2015), Strategy for designing electron donors for thermally activated delayed fluorescence emitters, Journal of Physical Chemistry C, 119 (3), 1291-1297
16	Higaki, Y., Hatae, K., Ishikawa, T., Takanohashi, T., Hayashi, J. and Takahara, A. (2014), Adsorption and desorption behavior of asphaltene on polymer-brush-immobilized surfaces, ACS Applied Materials & Interfaces, 6 (22), 20385-20389

	Appendix 1
17	Baba, T., Takizawa, T., Harada, K., Yamada, H., Ishihara, T. and Takami, A. (2015), Effect of Pr doping on catalytic properties of oxide ion conductor, Zr–Nd–O, for soot oxidation, Catalysis Today, 251, 2-6
18	White, K.L., Wong, M., Li, P., Miyamoto, M., Higaki, Y., Takahara, A. and Sue, HJ. (2015), Interlayer structure and self-healing in suspensions of brush-stabilized nanoplatelets with smectic order, Soft Matter, 11 (5), 954-971
19	Matsumoto, K., Shundo, A., Ohno, M., Fujita, S., Saruhashi, K., Miyachi, N., Miyaji, K. and Tanaka, K. (2015), Modulation of physical properties of supramolecular hydrogels based on a hydrophobic core, Physical Chemistry Chemical Physics, 17 (3), 2192-2198
20	Shibahara, M., Watanabe, M., Goto, K., Miyazaki, T., Zhang, H., Nakayama, Y. and Shinmyozu, T. (2014), Structural properties of five- and six-layered [3.3]metacyclophanes, Tetrahedron Letters, 55 (51), 7089-7093
21	Ishihara, T., Xie, J., Shin, T.H., Ju, YW., Ida, S. and Kilner, J.A. (2015), Bi doped Pr ₆ O ₁₁ as fluorite oxide cathode for all-fluorite solid oxide fuel cells, Journal of Power Sources, 275, 167-174
22	Higaki, Y., Okazaki, R., Ishikawa, T., Kikuchi, M., Ohta, N. and Takahara, A. (2014), Chain stiffness and chain conformation of poly(α-methylene-γ-butyrolactone) in dilute solutions, Polymer (United Kingdom), 55 (25), 6539-6545
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797	Chair, J.M., Yamaguchi, S., Eguchi, K., Ishihara, T. and Tatsumisago, M. (2014), The 19th International Conference on Solid State Ionics (SSI-19) Preface, Solid State Ionics, 262, 1-1
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804	Hirai, T., Kido, M., Shinohara, T., Nojima, S., Kim, J., Ota, N., Ishige, R., White, K., Higaki, Y. and Takahara, A. (2014), Synthesis of polymer with perylene diimide pendant side chains and characterization of its higher order structure, Abstracts of Papers of the American Chemical Society, 248, 405-POLY
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821	Funahashi, M., Yasuda, T. and Kato, T. (2014), Liquid Crystal Semiconductors: Oligothiophene and Related Materials, Handbook of Liquid Crystals, 2nd edition, Chap. 21, 8, 675-708
822	Isoda, K., Yasuda, T., Funahashi, T. and Kato, T. (2014), Redox-Active (Electrochromic) Liquid Crystals, Handbook of Liquid Crystals, 2nd edition, Chap. 22, 8, 709-725
823	Rupp, J.L.M. (2014), Solid Oxide Fuel Cells: Introduction, Encyclopedia of Applied Electrochemistry, 2018-2023
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824	Kirchheim, R. and Pundt, A. (2014), Hydrogen in Metals, Physical Metallurgy, 3, 2597-2705
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825	Gogotsi, Y., McCreery, R., Lyth, S.M., et al. (2014), Carbon electrode interfaces for synthesis, sensing and electrocatalysis: General discussion, Faraday Discussions, 172, 497-520
	B.5. Articles written in other than English (Original articles in Japanese)
826	Yoshinaga, K., Yonezawa, A., Motokucho, S. and Kojio, K (2014), Synthesis of ZnO Nanoparticles Using Reverse Micelles of Block Copolymer Hybridized with ZnO/PMMA, Kobunshi Ronbunshu, 71 (12), 644-650
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836	health risk management for middle-stream industrial processes in the supply chain, Kagaku
000	Kogaku Ronbunshu, 40 (3), 174-186
	B.5. Articles written in other than English (Original articles in Chinese)
	Liu, JH., Wang, HD., Hu, YD., Ma, WG., Zhang, X. (2014), Experimental study of
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838	and convective heat transfer coefficient of individual carbon fiber using Raman spectroscopy,
000	Huagong Xuebao/CIESC Journal, 65, SUPPL. 1, 251-257
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	B.5. Articles written in other than English (Review article in Japanese)
0.41	Matsuno, H. and Tanaka, K. (2014), An Effect of Mechanical Properties of Polymer Surface on
841	Fibroblast Adhesion, Nippon Gomu Gyokaishi (Journal of the Society of Rubber Science and Technology), 87 (10), 434-439
	B.5. Articles written in other than English (Editorial material in Japanese)
	Tsuchiyama, T. (2014), Preface to the 100th volume memorial special issue on physical metallurgy
842	1-microstructure control and material properties, Tetsu-To-Hagane/Journal of the Iron and Steel
	Institute of Japan, 100 (9), 1049
	B.5. Articles written in other than English (Book chapter in Japanese)
843	Nishihara, M., et al. Energy conversion technologies, Kagaku-binran (Handbook of Chemistry),
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0.1.1	B.5. Articles written in other than English (Note in Japanese)
844	Takahara, A. (2014), Fundamental science of polymer thin films, Kobunshi, 63 (2), 95
	B.5. Articles written in other than English (Magazine article in Japanese)
015	Yamabe, J., Matsunaga, H., Hamada, S. and Matsuoka, S. (2014), Proposal of Design Method for
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B. Invited Lectures, Plenary Addresses (etc.) at International Conferences and International Research Meetings

- List up to 10 main presentations during FY2014 in order from most recent.
- For each, write the lecturer/presenter's name, presentation title, conference name and date(s)

No.	Lecturer/presenter names and details
1	Ishihara, T., New Technology for Carbon Neutral Energy, 8th International Conference on Materials Science and Technology MSAT-8, Bangkok, Thailand, Dec. 15, 2014 (Plenary)
2	Matsunaga, H., Dominant Factors for Very High Cycle Fatigue of High Strength Steels, The Sixth International Conference on Very High Cycle Fatigue (VHCF-6), Chengdu, China, Oct. 17, 2014 (Keynote)
3	Nakashima, N., Design and Creation of Advanced Nanomaterials Based on Soluble Carbon Nanotubes, 2014 MRS Spring Meeting & Exhibit, San Francisco, CA, USA, Apr. 23, 2014 (Invited)
4	Takata, Y., Effect of Dissolved Air and Subcooling on Bubble Nucleation from a Hydrophobic Spot, Gordon Research Conference "Micro & Nanoscale Phase Change Heat Transfer", Galveston, TX, USA, Jan. 12, 2015 (Invited)
5	Akiba, E., Hydrogen Storage in Japan -Recent Progress and Future prospect-, Hy-SEA 2014 Hydrogen Storage - Embrittlement – Applications, Rio de Janeiro, Brazil, Oct. 26-30, 2014 (Plenary)
6	Yamauchi, M., Fe-Group Nanoalloy Catalysts : Toward Realization of a Sustainable Society, 97th Canadian Chemistry Conference and Exhibition, Vancouver, Vancouver, Canada, Jun. 5, 2014 (Invited)
7	Fujikawa, S., Fabrication and application of nanometer-thick membrane, Special symposium on the celebration for the Order of Culture of Prof. Toyoki Kunitake, Tokyo, Japan, Nov. 21, 2014 (Invited)
8	Tsuji, T., Digital rock physics: Insight into fluid flow and elastic deformation of porous media, GeoMod2014, Potsdam, Germany, Sep. 3, 2014 (Keynote)
9	Itaoka, K., Public understanding on CCS in Japan, International CCS Symposium for Low- Carbon Society, Tokyo, Japan, Feb. 12, 2015 (Invited)
10	Christensen, K.T., Quantitative Studies of Environmental Flows at the Micro- and Macro-Scales, 16 th International Symposium on Flow Visualization, Okinawa, Japan, June 27, 2014 (Keynote)

C. Major Awards

List up to 10 main awards received during FY2014 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.

No.	Recipient names and details
1	Ian Robertson 2014 Edward DeMille Campbell Memorial Lecture ASM International, 2015
2	Takeshi Tsuji Young Researcher Award, The Seismological Society of Japan, 2015
3	Toyoki Kunitake Order of Culture 2014, Government of Japan, 2014
4	Akihide Nagao Invention and Innovation Award 2014-Encouragement Prize, Japan Institute of Invention and Innovation, 2014
5	Atsushi Takahara Outstanding Contribution and Innovation in Fluoropolymer Science at FLUOROPOLYMER 2014, French Fluorine Network
6	Hellena Téllez-Lozano Best Scientific Contribution Award for Decrease of the electrochemically active surface in mixed ionic-electronic conductors (MIECs) by impurity segregation, 11th European SOFC&COE FORUM 2014
7	Hellena Téllez-Lozano, John Druce, Ju, YW., Tatsumi Ishihara, and John Kilner Christian Friedrich Schonbein Contribution to Science Medal, European Fuel Cell Forum 2014 (EFCF 2014)
8	Brian Somerday DOE Hydrogen and Fuel Cells Program Achievement Award for Hydrogen Delivery and Safety, Codes and Standards, 2014
9	Harry Tuller Fellow, Electrochemical Society, 2014

FY 2014 List of Principal Investigators

NOTE:
Underline names of principal investigators who belong to an overseas research institution.
In case of researchers not listed in the latest report, attach "Biographical Sketch of a New Principal Investigator".

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	Principal Investigators To	otal:24							
	Affiliation	Academic degree,	(To Work or	tal working	ng hours g hours: 100)%)	Starting date	Status of project participation	Contributions by PIs
Name (Age)	(Position title, department, organization)	specialty	Research activities	ect Other	Research	other activities	of project participation	(Describe in concrete terms)	from overseas research institutions
Center director <u>Petros Sofronis</u> (57)	Prof., International Institute for Carbon-Neutral Energy Research, Kyushu University	Ph.D., Micromechanics of materials, Environmental degradation of materials	15%	75%	5%	5%	2010, Dec.1 st	 Manages the Institute from Illinois Satellite Travels to the Institute to participate in events and exchange with researchers (48% time) Promotes I²CNER's interests to various research institutions and industries on a daily basis Daily exchange of e-mails Participates in meetings/events via videoconference system 	directs I ² CNER's operations
Tatsumi Ishihara (53)	Prof., International Institute for Carbon-Neutral Energy Research, Kyushu University	Dr. of Eng., Catalyst and solid state electrochemistry	90%	10%	0%	0%	2010, Dec.1 st	 Located at I²CNER Participates in research/events as Associate Director, Head of Hydrogen Production Division 	
Chihaya Adachi (51)	Prof., Department of Applied Chemistry, Kyushu University	Dr. of Eng., Materials science and device physics	60%	20%	10%	10%	2010, Dec.1 st	 Located at I²CNER Participates in research/events 	

Appendix 2 Dr. of Eng., Prof. Atsushi Takahara Institute for Materials Surface and Located at I²CNER 2010, • (59) 60% 20% 10% 10% Chemistry and Engineering Dec.1st Participates in research/events Interface Kyushu University Characterization Prof., Located at I²CNER • Seiji Ogo International Institute for Participates in research/events as Dr. of Science. 2010, • (51) Carbon-Neutral Energy 90% 10% 0% 0% Dec.1st Green Chemistry Head of Catalytic Materials Research, **Transformations Division** Kyushu University Prof., Zenji Horita International Institute for Ph.D., Dr. of Located at I²CNER 2010, (61) Carbon-Neutral Energy Eng., Materials 10% 0% 90% 0% Dec.1st · Participates in research/event Research, Science Kyushu University Prof., Ph. D., International Institute for Nanocarbon I ocated at I²CNFR Naotoshi Nakashima 2010, Carbon-Neutral Energy science, 85% 15% 0% 0% Dec.1st (63) • Participates in research/events Research, Supramolecular Kyushu University science Dr. of Science Prof., and technology, Located at I²CNER Kazunari Sasaki International Institute for Fuel cell 2010, (50) Carbon-Neutral Energy 90% 10% 0% 0% · Participates in research/events as materials, Dec.1st Head of Fuel Cell Division Research, Inorganic Kyushu University materials Prof., International Institute for Located at I²CNER Etsuo Akiba Dr. of Science, 2010, • Participates in research/events as (63) Carbon-Neutral Energy 70% 30% 0% 0% Dec.1st Materials science Head of Hydrogen Storage Division Research, Kyushu University · Primarily located at partner institution Prof. Eng. Sc. D., Participates in research Harry L. Tuller Department of Materials Functional • Visited I²CNER for four weeks to 2010, 15% (69) Science and Engineering, 35% 5% 45% electroceramic Dec.1st participate in events and exchange Massachusetts Institute of materials opinions for collaborative research Technology projects Discussion via Internet

									Appendix 2
<u>John A Kilner</u> (68)	Prof., Department of Materials, Imperial College, London	PhD., Materials for solid oxide fuel cells and electrolysers	35%	5%	45%	15%	2010, Dec.1 st	 Primarily located at partner institution Participates in research Visited I²CNER for six weeks for research to participate in events and exchange opinions for collaboration Regular discussion via Internet 	
Joichi Sugimura (57)	Prof., International Institute for Carbon-Neutral Energy Research, Kyushu University	Dr. of Eng., Tribology and Machine Design	70%	30%	0%	0%	2010, Dec.1 st	 Located at I²CNER Participates in research/events 	
Yasuyuki Takata (58)	Prof., International Institute for Carbon-Neutral Energy Research, Kyushu University	Dr. of Eng., Thermal Engineering	70%	30%	0%	0%	2010, Dec.1 st	 Located at I²CNER Participates in research/events as Associate Director, Head of Thermal Sciences and Engineering Division 	
<u>Xing Zhang</u> (53)	Prof., Department of Engineering Mechanics, Tsinghua University	Ph.D., Thermal Science	10%	10%	45%	35%	2010, Dec.1 st	 Primarily located at partner institution Participates in research/events Visited I²CNER for seven weeks to conduct research, participate in events, and exchange opinions for collaboration Discussion via Internet 	
<u>Brian P. Somerday</u> (46)	Dr., Sandia National Laboratories	Ph.D., Materials Science and Engineering	20%	15%	35%	30%	2010, Dec.1 st	 Primarily located at partner institution Participates in research as Head of Hydrogen Materials Compatibility Division Stayed at I²CNER for two weeks to participate in events and exchange opinions for collaboration Participates in meetings/events via videoconference system 	 Accepting researchers from I²CNER

Prof., International Institute for 2011, • Located at I²CNFR Setsuo Takaki Dr. of Carbon-Neutral Energy 90% 10% 0% 0% April.1st (62) Engineering Participates in research/events Research, Kyushu University Ph.D., Primarily located at partner Hydrogen in Metals, institution Prof., Thermodynamics • Participates in research Reiner Kirchheim The Institut für 2011, • Stayed at I²CNER for one week to (71) of alloys, 20% 20% 40% 20% April.1st Metallphysik, participate in events and exchange Interstitial University of Göttingen opinions for collaboration solution and Discussion via Internet diffusion in glasses Associate Prof., Located at I²CNER Miho Yamauchi International Institute for Dr. of Science, 2012, Participates in research/events (41) Carbon-Neutral Energy 100% 0% 0% 0% Jan. 1st Chemistry Hosted a student from UIUC Research, Kyushu University Prof., Ph.D., Ken Sakai Department of Chemistry • Located at I²CNER 2012, Inorganic 80% 10% 0% 10% Jan.16th (53) Faculty of Sciences, Kyushu • Participates in research/events Chemistry University Primarily located at partner institution Participates in research/events as Prof., Chief Science Advisor to the Dean of Engineering, • Sent Director University of Ian Robertson Ph.D., 2012, graduate 5% 20% 25% 50% • Serves as a member of the Illinois April.1st (57) Wisconsin-Madison, Metallurgy students to Satellite Advisory Committee Chief Science Advisor to the Institute • Visited I²CNER for one week to Director participate in events and exchange opinions for collaboration **Discussion via Internet**

Appendix 2

	-			:	:		1	Appendix 2
<u>Andrew A. Gewirth</u> (55)	Prof., Chemistry, University of Illinois	Ph.D., Chemistry	20%	5%	60%	15%	2012, April.1 st	 Primarily located at partner institution Participates in research Serves as a member of the Illinois Satellite Advisory Committee Visited I²CNER for one week to participate in events and exchange opinions for collaboration Discussion via Internet
<u>Kenneth T.</u> <u>Christensen</u> (41)	Prof. , College of Engineering, University of Notre Dame	Ph.D., Theoretical and Applied Mechanics specializing in experimental fluid mechanics	20%	5%	60%	15%	2012, April.1 st	 Primarily located at partner institution Participated in research/events as Associate Director of the Illinois Satellite (until August 2014) Serves as a member of the Illinois Satellite Advisory Committee Visited I²CNER for three weeks to participate in events and exchange opinions for collaboration Discussion via Internet
Shigenori Fujikawa (44)	Associate Prof., International Institute for Carbon-Neutral Energy Research, Kyushu University	Dr. of Eng., Nanoscience and engineering	100%	0%	0%	0%	2013, June.1 st	 Located at I²CNER Participates in research/events as Head of CO₂ Capture and Utilization Division
Takeshi Tsuji (35)	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 st	 Located at I²CNER Participates in research/events as Head of CO₂ Storage Division

Researchers unable to participate in project in FY 2014

Name	Affiliation (Position title, department, organization)	Starting date of project participation	Reasons	Measures taken
Tsutomu Katsuki	Prof., International Institute for Carbon-Neutral Energy Research, Kyushu University	2010, Dec.1	Deceased	
Katsuki Kusakabe	Prof., Department of Nanoscience, Sojo University	2010, Dec.1	Appointment changed to WPI Visiting Professor	

Records of FY2014 Center Activities

- 1. Researchers and center staffs, satellites, partner institutions
- 1-1. Number of researchers in the "core" established within the host institution
- Enter the total number of people in the columns below. In the "Researchers" column, put the number and percentage of overseas researchers in the < > brackets and the number and percentage of female researchers in the [] brackets.
- In the "Administrative staffs" column, put the number and percentage of bilingual staffs in the () brackets.
- In the "Final Goal" column, enter the currently projected goal and the estimated date for achieving it [OO month, OO year].

	Goal set in the "Post-interim evaluation revised center project"	Results at end of FY 2014	Final goal (Date: March 2020)
Researchers	172	166	177
	<78, 45%> [29, 17%]	<75, 45%> [18, 11%]	<81, 46%> [33, 19%]
Principal	25	24	25
investigators	<9, 36%> [1, 4%]	<9, 38%> [1, 4%]	<9, 36%> [3, 12%]
Other	147	142	152
researchers	<69, 47%> [28, 19%]	<66, 46%> [17, 12%]	<72, 47%> [31, 20%]
Research support staffs	70	56	70
Administrative	21	22	21
staffs	(17, 81%)	(18, 82%)	(17, 81%)
Total	263	244	268

Other matters of special mention

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

As described in Section 5 of the Report, President Kubo envisions that there will to be (10) tenured PIs organically in I²CNER. The rest of the 10-15 PI positions in I²CNER (out of the 20-25) will come from either: a) other units of KU through the Intra-University Transfer System (this means that those tenured faculty can return to their original departments after they have spent a reasonable amount of time in I²CNER), b) through cross-appointments between I²CNER and other units of KU, e.g. economics, sciences, mathematics, life sciences, etc., or c) through cross-appointments between I²CNER and its international partner institutes and industry. In addition, the vision is that 3 to 4 PIs amongst the 10 tenured faculty will be non-Japanese. In order to support the recruitment of such distinguished researchers as tenured I²CNER PIs from abroad, Kyushu University has recently introduced in its Education and Research Council the new Merit-based Annual Salary System, which allows for these foreign faculty to be compensated with a competitive salary, according to international standards. Lastly, apart from the PI categories (a), (b), and (c) above, following the Institute's policy on Faculty Fellows, I²CNER will host Faculty Fellows at the PI level.

As of March 31, 2015, we are conducting open recruitment campaigns to hire 2 foreign tenured PIs (our goal is for one of the positions to be filled by a female, if possible), and several tenured faculty members (Japanese or non-Japanese, either full professor or associate professor). These campaigns will close on May 29, 2015 and June 30, 2015, respectively.

- As background to how the Center is working to mobilize/circulate the world's best brains, give good examples, if any, of how career paths are being established for the Center's researchers; that is, from which top-world research institutions do researchers come to the Center and to which research institutions do the Center's researchers go, and how long are their stays at those institutions.

Researcher	Position at I ² CNER	Affiliated with I ² CNER for:	Former Affiliation	Affiliation after I ² CNER
Keigo Kitamura	Assistant Professor	4 years and 3 months	Research Institute of Innovative Technology for the Earth, Japan	(Currently at I ² CNER)
Aleksandar Staykov	Assistant Professor (1), Associate Professor (2)	3 years and 7 months (1), 5 months (2)	Kyushu University, Japan	(Currently at I ² CNER)
Junko Matsuda	Assistant Professor	4 years	National Institute of Advanced Industrial Science and Technology, Japan	(Currently at I ² CNER)
Shao Huaiyu	Assistant Professor	3 years and 11 months	Max-Planck, Germany	(Currently at I ² CNER)
Stephen Lyth	Assistant Professor	3 years and 10 months	Tokyo Institute of Technology, Japan	(Currently at I ² CNER)
Kiminori Shitashima	Associate Professor	3 years and 10 months	Central Research Institute of Electric Power Industry, Japan	(Currently at I ² CNER)
Shigenori Fujikawa	Associate Professor	3 years and 5 months	Institute of Chemical and Physical Research, Japan	(Currently at I ² CNER)
Miho Yamauchi	Principal Investigator, Associate Professor	3 years and 3 months	Hokkaido University, Japan	(Currently at I ² CNER)
John Druce	Postdoctoral Researcher	3 years and 3 months	Imperial Collage of London, UK	(Currently at I ² CNER)
Takeshi Tsuji	Associate Professor	3 years	Kyoto University, Japan	(Currently at I ² CNER)
Masaaki Sadakiyo	Assistant Professor	3 years	Kyoto University, Japan	(Currently at I ² CNER)
Arnaud Macadre	Postdoctoral Researcher	3 years	Kyushu University, Japan	(Currently at I ² CNER)
Nicola Perry	Postdoctoral Researcher(1), Assistant Professor (2)	2 years (1), 7 months (2)	Northwestern University, USA	(Currently at I ² CNER)
Chungsik Kim	Postdoctoral Researcher	2 years and 6 months	Kyushu University, Japan	(Currently at I ² CNER)
Ikuo Taniguchi	Associate Professor	2 years and 4 months	Research Institute of Innovate Technology for the Earth, Japan	(Currently at I ² CNER)
Limin Guo	Postdoctoral Researcher	2 years and 4 months	Tohoku University, Japan	(Currently at I ² CNER)
Wei Ma	Postdoctoral Researcher	2 years and 4 months	Kyushu University, Japan	(Currently at I ² CNER)
Motonori Watanabe	Assistant Professor	2 years and 3 months	Institute of Chemistry, Academic Sinica, Taiwan	(Currently at I ² CNER)
Ki-Seok Yoon	Associate Professor	2 years and 2 months	Kyushu University, Japan	Currently at I ² CNER)
Kenshi Itaoka	Professor	2 years and	Mizuho Information &	(Currently at I ² CNER)

(Listed chronologically, as of March 31, 2015)

		1 month	Research Institute. Inc., Japan	
Hoda Sadat Emami Meibody	Postdoctoral Researcher	2 years	CNRS, France	(Currently at I ² CNER)
Alexander Rene Parent	Postdoctoral Researcher	2 years	Yale University, USA	(Currently at I ² CNER)
Kaveh Edalati	Postdoctoral Researcher	2 years	Kyushu University, Japan	(Currently at I ² CNER)
Fei Jiang	Postdoctoral Researcher	2 years	Kyushu University, Japan	(Currently at I ² CNER)
Mohamed Reda Berber	Postdoctoral Researcher	2 years	Kyushu University, Japan	(Currently at I ² CNER)
Kwati Leonard	Postdoctoral Researcher	1 year and 6 months	Kyushu University, Japan	(Currently at I ² CNER)
Daniel Orejon	Postdoctoral Researcher	1 year and 6 months	University of Edinburgh, UK	(Currently at I ² CNER)
Roman Selyachyn	Postdoctoral Researcher	1 year and 3 months	University of Kitakyushu, Japan	(Currently at I ² CNER)
Biao Shen	Postdoctoral Researcher	1 year and 2 months	Kyushu University, Japan	(Currently at I ² CNER)
Sho Kitano	Postdoctoral Researcher	1 year	Kinki University, Japan	(Currently at I ² CNER)
Tatsunori Ikeda	Postdoctoral Researcher	1 year	Kyoto University, Japan	(Currently at I ² CNER)
Kevin White	Postdoctoral Researcher	1 year	Kyushu University, Japan	(Currently at I ² CNER)
Hideaki Komiyama	Postdoctoral Researcher	1 month	Tokyo Institute of Technology, Japan	(Currently at I ² CNER)
Pravakaran Saravanan	Postdoctoral Researcher	1 months	National University of Singapore, Singapore	(Currently at I ² CNER)
Nobuo Nakada	Assistant Professor	4 years	Kyushu University, Japan	Associate Professor, Tokyo Institute of Technology, Japan
Sean Bishop	Assistant Professor	3 years and 3 months	Massachusetts Institute of Technology (MIT), USA	Research Associate, Massachusetts Institute of Technology (MIT), USA
Xuping Li	Satellite Postdoctoral Researcher	2 years and 3 months	University of California, Davis, USA	Air Resources Engineer, Air Resources Board of the State of California (CARB), USA
Masaru Konno	Postdoctoral Researcher	2 years	Kyushu University, Japan	Researcher, Iwate University, Japan
May Martin	Graduate Research Assistant	2 years	University of Illinois at Urbana-Champaign	Humboldt Fellow, University of Göttingen, Germany
Maki Matsuka	Lecturer (1), Associate Professor (2)	4 months (1), 1 year (2)	Kyushu University, Japan	Researcher, National Institute of Advanced Industrial Science and Technology, Japan
Yuki Naganawa	Postdoctoral Researcher	1 year and 2 months	Kyoto University, Japan	Assistant Professor, Nagoya University, Japan
Shuai Wang	Postdoctoral Researcher	1 year and 2 months	Hokkaido University, Japan	Postdoctoral Researcher, University of Wisconsin-Madison, USA
Seiichiro Kimura	Postdoctoral Researcher	1 year	Kyushu University, Japan	Associate, Matsushita Institute of Government and Management, Japan
Takeshi Matsumoto	Postdoctoral Researcher	1 year	Hokkaido University, Japan	Assistant Professor, Chuo University, Japan
Ryota Watanabe	Postdoctoral Researcher	11 months	Toyota Central R&D Labs., Inc., Japan	Researcher, National Institute of Advanced Industrial Science and Technology, Japan

Le Zhang	Postdoctoral Researcher	10 months	Tokyo Institute of Technology, Japan	Postdoctoral Researcher, Eindhoven University of Technology, Holland
Ju-Hyung kim	Postdoctoral Researcher	10 months	Kyushu University, Japan	Assistant Professor, Pukyung National University, Korea
Myo Minn	Postdoctoral Researcher	8 months	Kyushu University, Japan	Postdoctoral Researcher, Singapore University of Technology and Design, Singapore

1-2. Satellites and partner institutions

- List the satellite and partner institutions in the table below.
- Indicate newly added and deleted institutions in the "Notes" column.
- If satellite institutions have been established, describe by satellite the Center's achievements in coauthored papers and researcher exchanges in Appendix 4.

<Satellite institutions>

Institution name	Principal Investigator(s), if any	Notes
University of Illinois	Andrew Gewirth	
at Urbana-Champaign (UIUC)		

< Partner institutions>

< Partner Institutions>		
Institution name	Principal Investigator(s), if any	Notes
Air Resources Board of the State		Newly added
of California (CARB)		(Letter of Understanding, signed)
Bandung Institute of Technology		
Dalian Institute of Chemical		
Physics		
Department of Energy, Energy		
Efficiency and Renewable Energy		
Helmholtz Zentrum Geesthacht		Newly added
(HZG)		(Agreement underway)
Imperial College London	John Kilner	
Massachusetts Institute of	Harry Tuller	
Technology		
Max-Planck Institute		
Mohawk Innovative Technology		
Norwegian University of Science		
and Technology (NTNU)/SINTEF		
Sandia National Laboratories	Brian Somerday	
Swiss Federal Institute of		
Technology Zurich (ETH)		
Tsinghua University	Xing Zhang	
Universiti Teknologi Malaysia		
University of Bergen		
University of California at Berkeley		
University of California at		
		4

Irvine/NFCRC		
University of Göttingen	Reiner Kirchheim	
University of Norte Dame	Kenneth Christensen	Newly added
University of Oxford		
University of Texas at Austin		
University of Thessaly		
University of Wisconsin-Madison	Ian Robertson	

2. Securing competitive research funding

- Competitive and other research funding secured in FY2014:

Total: 2,883,991,176 yen

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

COMPETITIVE FUND			
RECIPIENT	NAME OF GRANT	FUNDED BY:	TOTAL (Yen)
Joichi Sugimura	R&D Project (Useful Technology of Hydrogen)	NEDO	828,346,000
Chihaya Adachi	Exploratory Research for Advanced Technology (ERATO)	JST	253,800,000
Seiji Ogo	KAKENHI (Specially Promoted Research)	JSPS	174,800,000
Kazunari Sasaki	The Center of Innovation (COI) Program	MEXT	126,960,000

COMPETITIVE FUND				
RECIPIENT	NAME OF GRANT	FUNDED BY:	PERIOD	TOTAL (Yen)
Nicola Perry	KAKENHI (Young Researcher B)	JSPS	FY 2013-14	2,470,000
	Enhancement of fuel cell electrode kinetics by control of Fermi level			
Miho Yamauchi	KAKENHI (Scientific Research B)	JSPS	FY 2013-15	18,590,000
	Development of highly active iron-group catalysts by precise alloy-structure control			
Xing Zhang	KAKENHI (Scientific Research B)	JSPS	FY 2013-15	18,720,000
	Experimental study on ballistic thermal characteristics of an individual SWCNT and its application in nanofluids			
Shigenori Fujikawa	KAKENHI (Scientific Research B)	JSPS	FY 2014-16	16,250,000
	Large scale fabrication of Au nanofin array for efficient trapping near-infrared light			
Masamichi Nishihara	KAKENHI (Scientific Research C)	JSPS	FY 2014-16	4,940,000
	Development and structural and functional evaluation of charge-transfer complex hybrid films with various electron-donating molecules			
Hiroshige Matsumoto	KAKENHI (Challenging Exploratory Research)	JSPS	FY 2014-15	3,900,000
	Water electrolysis using water-absorbing porous electrolyte cell for oxygen production under micro gravity			
Masaaki Sadakiyo	KAKENHI (Young Researcher B)	JSPS	FY 2014-16	3,510,000
	Development of ionic conductivity of hydroxide ion-including metal-organic frameworks prepared by salt inclusion			
Motonori Watanabe	KAKENHI (Young Researcher B)	JSPS	FY 2014-15	4,030,000
	Synthesis of alcohol soluble indigo and O2 sensor application			
Guo Limin	KAKENHI (Young Researcher B)	JSPS	FY 2014-15	4,030,000
	Dye-sensitized mesoporous Ta3N5 photocatalysts for water splitting under visible light with longer wavelengths up to ~600 nm			
Sean Bishop	KAKENHI (Young Researcher B)	JSPS	FY 2014-15	3,900,000

	Development of Si impurity tolerant SOFC electrodes using reactive additives				
Mohamed Reda Berber	KAKENHI (Young Rese	archer B)	JSPS	FY 2014-15	4,030,000
	A step towards the real world application of polymer electroly of durability		olyte fuel cells:	improvement	
Yuki Honda	KAKENHI (Young Rese	archer B)	JSPS	FY 2014-15	3,900,000
	Mechanism Analysis Fluorescent Protein-ba			ce Changes of	f the Green
Miho Yamauchi	CREST		JST	FY 2012-15	31,206,500 (FY2014)
	Development of highly selective nanoalloy catalysts for the realization of carbon-neutral energy cycles				arbon-neutral
Tsutomu Katsuki (Tatsuya Uchida)	ACT-C	JST		FY 2012-15	14,300,000 (FY2014)
	Development of efficient methods for asymmetric carbon-carbon bond formation				
Hiroshige Matsumoto	ALCA	JST		FY 2013-19	72,213,000
	Novel steam electrolys	is			
Hiroshige Matsumoto	SIP	JST		FY 2014-18	48,750,500
	Novel steam electrolysis				
Ikuo Taniguchi	ALCA	JST		FY 2014-15	4,550,500
	Advanced Low Carbon Technology Research and Development Program, Preparation of nanogel immobilized membranes and the CO2 separation properties				

COMMISIONED RESEA	ARCH					
RECIPIENT	FUNDED BY:	PERIOD	TOTAL (Yen)			
Ikuo Taniguchi	RITE	FY 2014	3,024,000			
	Development of novel catalysts assisting bicarbonate format	Development of novel catalysts assisting bicarbonate formation reaction				
Masanobu Kubota	Air Liquid Laboratories	FY 2014-15	7,509,000			
	Research and Development on Welded Joints of a High-Nitrogen and High-Strength Stainless Steel Tube for High-Pressure Hydrogen Gas					
Kenshi Itaoka	Quintessa (note: research consulting firm in Yokohama)	FY 2014-15	7,509,000			
	Research on public understanding of CCS					
Kenshi Itaoka	TOYOTA FY 2014 3,486,587					
	Research for domestic hydrogen station deployment model					
Kiminori Shitashima	University of Tokyo FY 2014 16,173,710					
	Ocean resource use promotion technical development program, Development of large-area survey system for discovery for ocean mineral resources					

JOINT RESEARCH					
RECIPIENT	FUNDED BY:	PERIOD	TOTAL (Yen)		
Hiroshige Matsumoto	MITSUI KINZOKU (MINING & SMELTING)	FY 2013-14	679,740		
	Development of high-ion-conducting solid electrolyte operating at low temperature				
Hiroshige Matsumoto	ΤΟΥΟΤΑ	FY 2013-14	5,405,600		
	Joint research on the development of high performance electrodes for SOFC				
Petros Sofronis	JFE Steel	FY 2014-15	2,040,000		
	Effect of Hydrogen on Fatigue S-N Curves (Co-researcher: Masanobu Kubota)				
Hiroshige Matsumoto	Panasonic	FY 2014	2,000,000		
	Joint research on the development of high proton conducting metal oxides				
Masanobu Kubota	Nippon Steel & Sumitomo Metal Corporation	FY 2014-15	1,944,000		
	Fundamental Studies on Fretting Fatigue and Crack Growth Behavior of Small Crack				

Appendix 3

Hiroshige Matsumoto	Panasonic	FY 2014	2,160,000		
<u> </u>	Joint research on epitaxially-prepared high-proton-conduct	ing thin film me	etal oxides		
Takeshi Tsuji	Shikoku Research Institute	bikoku Research InstituteFY 2014600			
	Q-value estimation around the fault using P-S logging data				
Tsutomu Katsuki (Tatsuya Uchida)	Nissan Chemical Industries	FY 2014	7,000,000		
	construction of new strategy for environmentally friendly catalytic organic ransformation				
Hiroshige Matsumoto	KYOCERA FY 2014-15				
	Research on low-temperature sintering of ceramic materia	s			
Miho Yamauchi	Toyota Central R&D Labs	FY 2014	1,000,000		
	Synthesis of homogeneous solid-solution Fe-Ni nanoalloys	for sensor appli	cations		
Hiroshige Matsumoto	atsumoto Honda FY 2014-15 1,000,0				
	Development of novel hydrogen production method				
Masanobu Kubota	Air Liquid Laboratories FY 2014-15 20,400,00				
	Effect of Impurities Contained in Hydrogen Gas on Inhibition of Hydrogen Embrittlemen in Steels (Co-researcher: Alex Staykov)				
Ikuo Taniguchi Tokyo Boeki Mechanics FY 2014					
	Development of novel CO2 separation membranes with properties	progressive CC	02 separation		

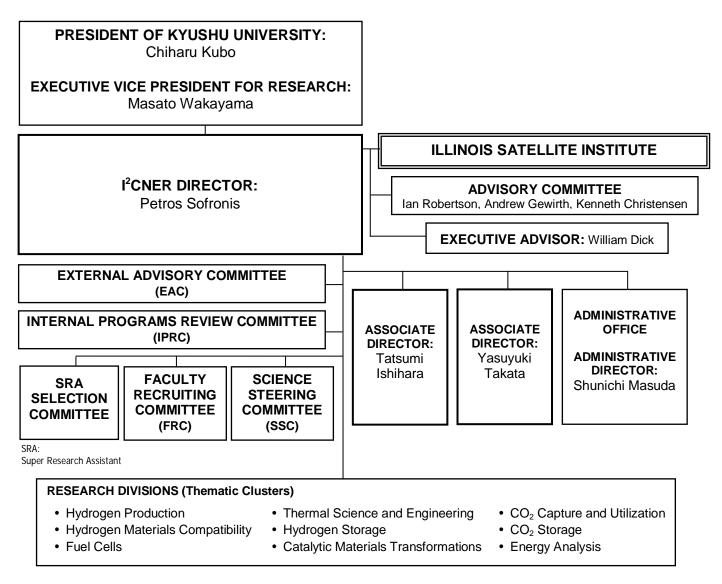
- 3. International research conferences or symposiums held to bring world's leading researchers together
- Indicate the number of international research conferences or symposiums held in FY2014 and give up to three examples of the most representative ones using the table below.

FY 2014: 6 meetings	
Major examples (meeting title and place held)	Number of participants
I ² CNER Tokyo Symposium TKP Garden City Shinagawa, Tokyo	From domestic institutions: 98 From overseas institutions: 27
I ² CNER Annual Symposium 2015 I ² CNER Hall, Ito Campus, Kyushu University	From domestic institutions: 79 From overseas institutions: 62
I ² CNER International Workshop 2015 Ito Campus, Kyushu University	From domestic institutions: 321 From overseas institutions: 83

- 4. Center's management system
- Please diagram management system in an easily understood manner.

I²CNER ORGANIZATIONAL STRUCTURE

(As of April 1, 2015)



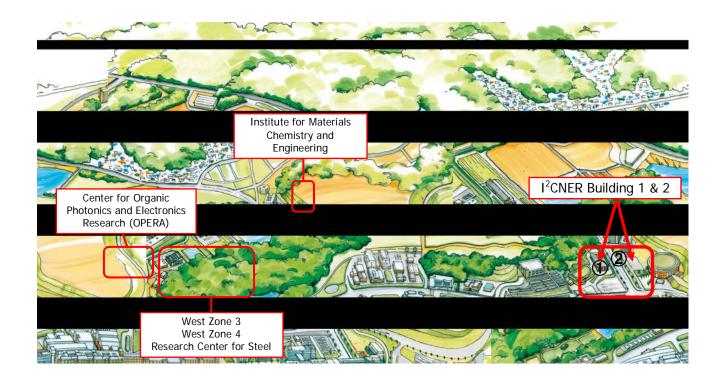
- If any changes have been made in the management system from that in the "Post-interim evaluation revised center project," please describe them. Please describe any changes made in the administrative director, head of host institution, and officer(s) in charge at the host institution (e.g., executive vice president for research)

As of October 1, 2014, Professor Chiharu Kubo replaced Professor Setsuo Arikawa as President of Kyushu University. The new Executive Vice President for Research and Industrial Collaboration, Professor Masato Wakayama oversees I²CNER's interactions with all of Kyushu University. Executive Vice President Reiko Aoki interacts with I²CNER on international collaborations and visibility of both I²CNER and Kyushu University.

Beginning April 1, 2015, Shunichi Masuda joined I²CNER as the new Administrative Director, replacing Yukio Fujiki, who resigned from the position as of March 31, 2015. Mr. Masuda's main function is to administer the affairs of the office to facilitate the operations of the Institute, and provide administrative support to the research personnel.

5. Campus Map

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



i) Overall project funding

Cost Items	Details	Costs (10,000 dollars)
	Center director and Administrative director	22
	Principal investigators (no. of persons):16	217
Personnel	Other researchers (no. of persons):79	394
	Research support staffs (no. of persons):29	60
	Administrative staffs (no. of persons):25	100
	Total	793
	Gratuities and honoraria paid to invited principal investigators (no. of persons):60	8
	Cost of dispatching scientists (no. of persons):0	0
	Research startup cost (no. of persons):30	43
Project activities	Cost of satellite organizations (no. of satellite organizations):1	214
	Cost of international symposiums (no. of symposiums):3	10
	Rental fees for facilities	264
	Cost of consumables	24
	Cost of utilities	24
	Other costs	173
	Total	759
	Domestic travel costs	18
	Overseas travel costs	52
Travel	Travel and accommodations cost for invited scientists (no. of domestic scientists):33 (no. of overseas scientists):31	24
	Travel cost for scientists on secondment (no. of domestic scientists):3 (no. of overseas scientists):1	1
	Total	95
	Depreciation of buildings	10
Equipment	Depreciation of equipment	1,160
	Total	1,170
	Projects supported by other government subsidies, etc.	145
Other research	Commissioned research projects, etc.	1,304
projects	Grants-in-Aid for Scientific Research, etc.	181
	Total	1,630
	Total	4,447

	Ten thousand	d dollars
WPI grant		1,310
Costs of establishing and maintaining fac	cilities	1,766
Establishing new facilities (Building 2) (Number of facilities:5,000m ²)	Costs paid:	1,765
Repairing facilities (Number of facilities:0m ²)	Costs paid:	0
Others		1
Cost of againment produced		1 240
Cost of equipment procured		1,248
Name of equipment: Ventilation Device	e for Draft	
Chamber		13
Number of units:1 Name of equipment:Simultaneous ICP	Costs paid: Atomic Emission	9

Costs paid:

Number of units:1

Spectrometer

Others

ii) Costs of Satellites and Partner institutions

Cost Items	Details	Costs (10,000 dollars)
	Principal investigators (no. of persons):3	
	Other researchers (no. of persons):6	
Personnel	Research support staffs (no. of persons):21	
	Administrative staffs	
	Total	147
Project activities		52
Travel		15
Equipment		0
Other research		0
projects		0

9

1,226

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Status of Collaboration with Overseas Satellites

1. Coauthored Papers

- List the refereed papers published in FY2014 that were coauthored between the center's researcher(s) in domestic institution(s) and overseas satellite institution(s). List them by overseas satellite institution in the below blocks.
- Transcribe data in same format as in Appendix 1. Italicize the names of authors affiliated with overseas satellite institutions.
- For reference write the Appendix 1 item number in parentheses after the item number in the blocks below. Let it free, if the paper is published in between Jan.-Mar. 2015 and not described in Appendix 1.

Overseas Satellite: University of Illinois, Urbana-Champaign (Total: 9 papers)

No.	Author names and details
1- (-)	Robertson, I.M., Sofronis, P., Nagao, A., <i>Martin, M.L.</i> , Wang, S., Gross, D.W. and Nygren, K.E. (2015), Hydrogen embrittlement understood, Metallurgical and Materials Transactions B, 46 (3), 1085-1103
2- (-)	<i>Dadfarnia, M., Martin, M.L.</i> , Nagao, A., Sofronis, P. and Robertson, I.M. (2015), Modeling hydrogen transport by dislocations, Journal of the Mechanics and Physics of Solids, 78, 511-525)
3- (13)	Ida, S., Kim, N., <i>Ertekin, E.</i> , Takenaka, S. and Ishihara, T. (2014), Photocatalytic Reaction Centers in Two-Dimensional Titanium Oxide Crystals, Journal of the American Chemical Society, 137 (1), 239-244
4- (47)	Téllez, H., Druce, J., Hall, A., Ishihara, T., Kilner, J. and <i>Rockett, A.</i> (2015), Low energy ion scattering: Surface preparation and analysis of Cu(In,Ga)Se ₂ for photovoltaic applications, Progress in Photovoltaics: Research and Applications, 23 (10), 1219-1227
5- (137)	<i>Dadfarnia, M.</i> , Somerday, B. P., Schembri, P.E., Sofronis, P., Foulk III, J.W., Nibur, K.A. and Balch, D.K. (2014), On Modeling Hydrogen-Induced Crack Propagation Under Sustained Load, JOM, 66 (8), 1390-1398
6- (139)	Nagao, A., <i>Martin, M.L.</i> , <i>Dadfarnia, M.</i> , Sofronis, P. and <i>Robertson, I.M.</i> (2014), The effect of nanosized (Ti,Mo)C precipitates on hydrogen embrittlement of tempered lath martensitic steel, Acta Materialia, 74, 244-254
7- (144)	Wang, S., <i>Martin, M.L.</i> , Sofronis, P., Ohnuki, S., Hashimoto, N., <i>Robertson, I.M.</i> (2014), Hydrogen-induced intergranular failure of iron, Acta Materialia, 69, 275-282
8- (221)	Harish, S., Tabara, M., Ikoma, Y., Horita, Z., Takata, Y., <i>Cahill, D.G.</i> , Kohno, M. (2014), Thermal conductivity reduction of crystalline silicon by high-pressure torsion, Nanoscale Research Letters, 9, 326
9- (291)	Kitamura, K., Jiang, F., <i>Valocchi, A.J.</i> , Chiyonobu, S., Tsuji, T. and <i>Christensen, K. T.</i> (2014), The study of heterogeneous two-phase flow around small-scale heterogeneity in porous sandstone by measured elastic wave velocities and lattice Boltzmann method simulation, Journal of Geophysical Research: Solid Earth, 119 (10), 7564-7577

2. Status of Researcher Exchanges

- Using the below tables, indicate the number and length of researcher exchanges in FY2014. Enter by institution 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.

Overseas Satellite: University of Illinois at Urbana-Champaign, USA

<To satellite>

1							
		Under 1 week	From 1 week to 1 month	From 1 month to 3 months	3 months or longer	Total	
	FY2014	4 6	0 0	0 0	0 0	4 6	

<From satellite>

	Under 1 week	From 1 week to 1 month	From 1 month to 3 months	3 months or longer	Total
FY2014	5	0	0	0	5
	9	4	0	0	13

FY 2014 Visit Records of World Top-caliber Researchers from Abroad

Researchers	Total: 34	1	ſ	1	
Name (Age)	Affiliation (Position title, department, organization)	Academic degree, specialty	Record of research activities (Awards record, etc.)	Time, duration	Summary of activities during stay at center (e.g., participation as principal investigator; short-term stay for joint research; participation in symposium)
Taeghwan Hyeon	Professor, School of Chemical and Biological Engineering, Seoul National University, Korea	Ph. D., Nanostructured Catalytic and Magnetic Materials, Sonochemical Synthesis and Characterization	 Top 100 Chemists of the decade (2000-2010) by UNESCO & IUPAC (ranked at 37th in chemistry area; 19th in Materials Science, 2011) 	2014/4/4	I ² CNER Seminar Series Presentation
Harry Tuller	Prof. Department of Materials Science and Engineering, Massachusetts Institute of Technology, USA	Eng. Sc. D., Functional Electroceramic Materials	 Helmholtz International Fellow Award (2012) Somiya Award of the International Union of Materials Research Society (2012) Outstanding Achievement Award, High Temperature Division, Electrochemical Society (2010) Docteur Honoris Causa, University of Oulu, Finland (2009) McMahon Award, Alfred University, NY (2009) Orton Award, American Ceramic Society (2008) FH Norton Award, American Ceramic Society (2007) Docteur Honoris Causa, University of Provence, Marseille, France (2004) Von Humboldt Award (1997-2002) Fulbright Award (1989-1990) 	2014/5/31- 2014/6/7 2015/1/24- 2015/2/12	Joint Research, Participation in Site Visit as Principal Investigator, Division Meetings Joint Research, Participation in I ² CNER Annual Symposium, Hydrogen Forum and International Workshop as Principal Investigator

Appendix 5

John Kilner	Prof.,	PhD., Materials	•	Platinum Medal,	2014/5/31-	Participation in Site Visit,
	Department of Materials,	for Solid Oxide Fuel Cells and		Institute of Materials Minerals	2014/6/14	Division Retreat, and Joint Research as Principal
	Imperial	Electrolysers		and Mining (2012)		Investigator
	College, London, UK		•	Somiya Award, International	2014/11/7-	Joint Research
	London, or			Union of Materials	2014/11/22	
				Research Societies		Douticination in 120NED
			•	(2012) Royal Society Armourers and Braziers Award, Royal Society (2005) Schoenbein Medal, European Solid Oxide Forum (2004) Verulam Medal, Institute Of Materials, Minerals and Mining (2005) Fellow, City and Guilds Institute of London (2007) Excellence in Teaching, Imperial College (1997)	2015/1/24- 2015/2/12	Participation in I ² CNER Annual Symposium, Hydrogen Forum and International Workshop, and Joint Research as Principal Investigator
Brian Somerday	Dr., Sandia National Laboratories,	Ph.D., Materials Science and Engineering	•	DOE Hydrogen and Fuel Cell Program	2014/6/1- 2014/6/9	Participation in Site Visit, and Division Retreat as Principal Investigator
	USA		•	Achievement Award (2014) Best Poster Award, ASME 12 th Fuel Cell Science, Engineering, and Technology Conference (2014)	2015/1/31- 2015/2/7	Participation in I ² CNER Annual Symposium, Hydrogen Forum, International Workshop, and Joint Research as Principal Investigator
Kenneth Christensen	Prof., College of Engineering, University of Notre Dame,	Ph.D., Theoretical and Applied Mechanics specializing in	•	Dean's Award for Excellence in Research from the College of Engineering, UIUC	2014/6/2- 2014/6/6	Participation in Site Visit, and Division Meetings as Principal Investigator
	USA	experimental		(2012)	2014/6/2-	Participation in I ² CNER
		fluid mechanics	•	Francois Frenkiel Award for Fluid	2014/6/6	Tokyo Symposium
				Mechanics from	2015/2/1-	Participation in I ² CNER
			•	APS-DFD (2011) NSF CAREER	2015/2/5	Annual Symposium, Hydrogen Forum and
				Award (2007)		International Workshop
				AFOSR Young		as Principal Investigator

Elif Ertekin	Assistant Prof., Department of Mechanical Science & Engineering, University of Illinois	Ph.D., Materials Science & Engineering	•	Materials Research Society Best Poster Award (2005 and 2012) Intel Corporation Graduate Fellowship (2004-2005) National Science Foundation Graduate Fellowship (1999-2002) Xerox Undergraduate Research Award, Penn State University (2000) Frank Fenlon Undergraduate Thesis Presentation Award, Penn State	2014/6/2- 2014/6/9	Participation in Site Visit, and Division Retreat as Satellite Faculty Member
Xing Zhang	Prof., Department of Engineering Mechanics, Tsinghua University	Ph.D., Thermal Science	•	University (1999) Significant Contribution Awards from the 10 th Asian Thermophysical Properties Conference (2013) National Nature Science Award (Second Class) from the State Council of the People's Republic of China (2011) Best Paper Award from the Heat Transfer Society of Japan (2008)	2014/6/3- 2014/6/12 2014/7/21- 2014/8/16 2015/1/29- 2015/2/14	Participation in Site Visit, and Division Meetings as Principal Investigator Joint Research Participation in I ² CNER Annual Symposium, International Workshop, and Joint Research as Principal Investigator
Josua Meyer	Professor, University of Pretoria, South Africa	PhD., Mechanical Engineering	•	Thomas Price Award (1988)	2014/8/8	I ² CNER Seminar Series Presentation
C.N.R. RAO	National Research Professor, Linus Pauling Research Professor, Honorary President, Jawaharlal Nehru Centre for Advanced Scientific Research, India	D.Sc., Ph.D., Solid State and Materials Chemistry, Structural Chemistry	•	International Award (Gold Medal) of the Chinese Academy of Sciences (2012) The Royal Medal (Queen's Medal), by the Royal Society, London, U.K (2009) Chemical Pioneer, American Institute of Chemists (2005)	2014/8/25	I ² CNER Seminar Series Presentation

			•	Somiya Award of the International Union of Materials Research Society (IUMRS) (2004)		
Shahrum Abdullah	Professor, Universiti Kebangsaan Malaysia, Malaysia	Ph.D., Mechanical Engineering, Fatigue Life Assessment	•	Bronze Medal in the World Design Exhibition (2007) Second Best Paper Award, National Conference on Design and Concurrent Engineering (2006) Gold Medal in the Design Competition, 17th ITEX (2006) Best Paper Award for the 12th International Conference in Experimental Mechanics (ICEM12) (2004)	2014/9/5	I ² CNER Seminar Series Presentation
Xavier Sauvage	Research Scientist, CNRS (National Center for Scientific Research), France	Ph.D., Material Science	•	FEMS Young Lecturer Award, Federation of European Materials Societies (2010)	2014/9/12	I ² CNER Seminar Series Presentation
Ruzhu Wang	Professor, Shanghai Jiao Tong University, China	Ph.D., Refrigeration and Cryogenics	•	Second National Award of Invention for the Advancement of Science and Technology (2010)	2014/9/12	I ² CNER Seminar Series Presentation
Satish Kandlikar	Gleason Professor of Mechanical Engineering, Rochester Institute of Technology, USA	Ph.D., Electronics Cooling	•	2012 Heat Transfer Memorial Award, Heat Transfer Division, ASME	2014/10/24	I ² CNER Seminar Series Presentation
Sylviane Sabo-Etienne	CNRS Research Director, Universite de Toulouse, France	Ph.D., Organometallic Chemistry, Catalysis, Coordination Chemistry	•	RSC Frankland Award (2010) Glenn T. Seaborg Memorial Lecturer, the University of California, Berkeley (2010)	2014/10/31	I ² CNER Seminar Series Presentation

Thomas McCarthy	Professor, Department of Polymer Science and Engineering, University of Massachusetts, USA	Ph.D., Organic Chemistry	•	Univ of Mass "Milestone Award" (2006) Univ of Mass "Centennial Award - Outstanding Faculty Member" (2008)	2014/11/7	I ² CNER Seminar Series Presentation
			•	Univ of Mass "Outstanding Accomplishments in Research and Creative Activity" (2008)		
Curtis Berlinguette	Professor, University of British Columbia, Canada	Ph.D., Solar Cells, Solar Fuels, Energy Storage, Catalysis	•	Alfred P. Sloan Research Fellow (2011)	2014/11/21	I ² CNER Seminar Series Presentation
Thomas Meyer	Arey Distinguished Professor of Chemistry, University of North Carolina at Chapel Hill, USA	Ph.D., Solar Energy Conversion, Artificial Photosynthesis	•	Samson Prime Minister's Prize for Innovation in Alternative Fuels for Transportation (2014) Honda-Fujishima Lectureship Award (2013)	2014/12/1	I ² CNER Seminar Series Presentation
Cyrus Wadia	Assistant Director, Clean Energy & Materials R&D, White House Office of Science and Technology Policy, USA	Ph.D. Energy and Resources	•	World Top Young Innovator Award (MIT Technology Review TR35), (2009) DOE Entrepreneur In Residence Grant (2009) 1st Place Research Competition, B.E.R.C Symposium (2008)		Participation in I ² CNER Tokyo Symposium
Peng Zhang	Professor, Shanghai Jiao Tong University, China	Ph. D., Thermal Energy Storage, Heat Transfer and Fluid Flow, CO ₂ Capture and Storage	•	Young Investigator Award, Chinese Society of Engineering Thermophysics (2012) Young Scientist Award, Chinese Association of Refrigeration (2007)	2015/1/23	I ² CNER Seminar Series Presentation
Scott Barnett	Prof., Northwestern University, USA	Ph.D. Metallurgy	•	Fellow, American Vacuum Society (1998) Department Teacher of the Year (1993)	2015/2/1- 2015/2/3	Participation in I ² CNER Annual Symposium

Kevin Nibur	Principal, Hy-Performance Materials Testing, LLC., USA	Engineer		Owner of Hy-Performance Materials Testing, LLC.	2015/2/1- 2015/2/5	Participation in I ² CNER Annual Symposium, Hydrogen Forum and International Workshop
Minghui Yang	Prof., Dalian Institute of Chemical Physics, Chinese Academy of Science, China	Ph.D. Materials Chemistry	•	China National "Thousand Youth Talents" Award for Distinguished Professorship (2013)	2015/2/1- 2015/2/5	Participation in I ² CNER Annual Symposium, Hydrogen Forum and International Workshop
Ian Robertson	Prof., Dean of Engineering, University of Wisconsin-Madi son, Chief Science Advisor to the Director	Ph.D., Metallurgy	•	ASM Edward DeMille Campbell Memorial Lecturer (2014) Donald Burnett Teacher of the Year Award (1992) DOE Award (with H. K. Birnbaum) for Outstanding Scientific Accomplishment (1984)	2015/2/1- 2015/2/5	Participation in I ² CNER Annual Symposium, Hydrogen Forum and International Workshop as Principal Investigator
Andrew Gewirth	Prof., Chemistry, University of Illinois	Ph.D., Chemistry	•	University of Illinois Scholar (1995) Alfred P. Sloan Fellowship (1993) DOE Outstanding Accomplishment in Materials Science (1993) Fellow, UIUC Center for Advanced Study (1991) Presidential Young Investigator Award (1990)	2015/2/1- 2015/2/6	Participation in I ² CNER Annual Symposium, Forum and International Workshop as Principal Investigator
Jack Brouwer	Assoc. Prof., National Fuel Cell Research Center, University of California, Irvine, USA	Ph.D. Mechanical Engineering	•	Honored Member, International Who's Who of Professionals (2006)	2015/2/1- 2015/2/6	Participation in I ² CNER Annual Symposium, Division Retreat and Division Symposium
Joan Ogden	Prof., University of California, Davis, USA	Ph.D. Theoretical Plasma Physics	•	R&D Excellence Awards, DOE (2005-2006)	2015/2/1- 2015/2/6	Participation in I ² CNER Annual Symposium, Hydrogen Forum, International Workshop and Research Discussion
Yuying Yan	Prof., University of Nottingham, UK	Ph.D. Mechanical Engineering		Reported by Royal Society's Excellence Supported by the UK EPSRC, Royal Society, Royal Academy of	2015/2/1- 2015/2/6	Participation in I ² CNER Annual Symposium, Hydrogen Forum, International Workshop, and Division Symposium

				Engineering, European FP7 and industries		
Reiner Kirchheim	Prof., The Institut für Metallphysik, University of Göttingen, Germany	Ph.D., Hydrogen in Metals, Thermodynamics of Alloys, Interstital Solution and Diffusion in Glasses	•	industries Leibniz-Medaille of the IFW Dresden (2013) Hydrogen & Energy Award, H&E-Symposium (2010) Lee Hsun Lecture Award, IMR Shenyang, Chinese Academy of Sciences (2007) International Award of Materials Engineering for Recourses, Akita, Japan (2005) Heyn-Denkmünze (highest award of the German Materials Society, DGM) (2004) Honda Memorial Award, Tohoku University (2003) Highly Cited Author in Materials Science (1980-2000) Carl Wagner Prize (1990) Scripta Metallurgica Outstanding Paper Award (1987)	2015/2/1- 2015/2/7	Participation in I ² CNER Annual Symposium, Hydrogen Forum and International Workshop as Principal Investigator
Jürgen Fleig	Prof., Vienna University of Technology, Austria	Ph.D. Chemistry	•	Edward C. Henry Award, American Ceramic Society (2005) Tajima-Prize, International Society of Electrochemistry (2004)	2015/2/2, 2/5	Participation in I ² CNER Annual Symposium and Division Symposium
Christopher Pickett	Prof., University of East Anglia, England	Ph.D. Chemistry	•	RSC Ludwig Mond Award (2009)	2015/2/2- 2015/2/7	Participation in I ² CNER International Workshop , Hydrogen Forum and Research Discussion
May-Britt Hägg	Prof., Norwegian University of Science and Technology, Norway	Ph.D. Chemical Engineering	•	Participation in 8 EU-projects since mid 1990 Heading several national projects with grants from Norwegian Research Council	2015/2/3- 2015/2/5	Participation in I ² CNER International Workshop

Appendix 5

Michael Felderhoff	Max-Planck Institute for Kohlenforschung, Germany	Ph.D., Chemistry	•	Expert of the International Energy Agency (IEA) Task 32 "Hydrogen-based energy storage" of the Hydrogen Implementation Agreement since 2013	2015/2/3- 2015/2/6	Participation in I ² CNER International Workshop and Research Discussion
Rodney Ruoff	Professor, Ulsan National Institute of Science and Technology, Korea	Ph.D., Global environment and energy	•	Lee Hsun Lecture Award, Institute of Metal Research, Chinese Academy of Sciences (2009) 16th most cited materials scientist of top 100 most cited	2015/2/13	I ² CNER Seminar Series Presentation
David Smith	Regents' Professor, Department of Physics, Arizona State University, USA	D.Sc., Ph.D., Electron Microscopy and Materials Physics	•	Helmholtz International Fellow Award (2014) Distinguished Physical Scientist Award, Microscopy Society of America (2014)	2015/3/6	I ² CNER Seminar Series Presentation

State of Outreach Activities

- Using the table below, show the achievements of the Center's outreach activities in FY2014(number of activities, times held).

- Describe those activities that have yielded novel results or that warrant special mention in the "Special Achievements" space below.

- In appendix 7, list and describe media coverage (e.g., articles published, programs aired) in FY2014 resulting from press releases and reporting.

Activities	FY2014 (number of activities, times held)
PR brochure, pamphlet	5
Lectures, seminars for general public	14
Teaching, experiments, training for elementary and secondary school students	16
Science café	1
Open houses	1
Participating in, exhibiting at events	5
Press releases	14

Special Achievements

Super Science High Schools (SSH) Student Workshop

• Prof. Takeshi Tsuji gave a lecture for students. (August 7, 2014)

European Materials Research Society (E-MRS) 2014 Spring Meeting

 Director Sofronis, Prof. Ken Sakai and Prof. Adachi gave lectures at the workshop, jointly organized by 4 WPI institutes (AIMR, iCeMS, MANA, and I²CNER). (May 28, 2014)

Kyushu University Homecoming Day

• I²CNER hosted over 60 Kyushu University alumni for a facility tour. (October 18, 2014)

4th WPI Joint Symposium

• Prof. Aleksandar Staykov gave a lecture. (December 13, 2014)

Books for general readers

• Prof. Seiji Ogo published "The Story of Hydrogen Energy." (December 2014)

Kyushu University Soft Engineering Open Lecture 2015

• Prof. Yamauchi and Prof. Taniguchi gave lectures for general public. (January 24, 2015)

FY 2014 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	2014/9/6 2014/9/8	Nikkei Shimbun Nishinippon Shimbun Nikkan Kogyo Shimbun Nikkei Sangyo Shimbun	Development of a future-generation of PEFCs using a minimal amount of Pt (Naotoshi Nakashima, Fuel Cells Division)
2	2014/5/5	Nishinippon Shimbun Zaikei Shimbun Yomiuri Shimbun	Pore pressure distribution around the seismogenic fault (Takeshi Tsuji, CO ₂ Storage Division)
3	2014/5/31	Nikkei Technology Online Nishinippon Shimbun Nikkan Kogyo Shimbun	Development of EL devices with 100% of luminous efficiency (Chihaya Adachi, Hydrogen Production Division)
4	2014/6/4 2014/6/5		[NiFe]Hydrogenase from Citrobacter sp. S–77 Surpasses Platinum as an Electrode for H ₂ Oxidation Reaction (Seiji Ogo, Catalytic Materials Transformations Division)
5	2014/6/5	Nikkei Shimbun	Raising the level of industrial might (Director Sofronis, Hydrogen Materials Compatibility Division)
6	2014/6/27	Kagaku Shimbun	Development of facile strain analysis of largely bending films (Shigenori Fujikawa, CO ₂ Capture and Utilization Division)
7	2014/7/3	Mynavi News (Web) Zaikei Shimbun	Vacuum generation by hydrogen permeation to atmosphere (Yasuyuki Takata, Thermal Science and Engineering Division)
8	2014/9/29	Denki Shimbun Nikkan Kogyo Shimbun Nikkei Shimbun	World-first experiment on a controlled sub-seabed CO ₂ leak demonstrates minimal environmental impact and rapid recovery (Kiminori Shitashima, CO ₂ Storage Division)

	2014/10/6	Zaikei Shimbun	
9		Nikkei Sangyo Shimbun Nikkan Kogyo Shimbun Kagaku Shimbun	Semiconducting carbon nanotube sorting (Naotoshi Nakashima, Fuel Cells Division)
10	2014/10/24	National Institute for Environmental Studies (Web)	Surface termination and subsurface restructuring of perovskite-based solid oxide electrode materials (Tatsumi Ishihara, John Kilner, John Druce and
	2014/10/26	Zaikei Shimbun	Hellena Téllez, Hydrogen Production Division)
11	2014/10	Nikkan Tekko Shimbun	Challenge of new automotive materials development (Setsuo Takaki, Hydrogen Materials Compatibility Division)
12	2014/11/10	Japan Times	Time for underground CO_2 storage is now (Ziqiu Xue, CO_2 Storage Division)
13	2014/12/15	Television Nishinippon Corporation (TNC)	Short interview: (Stephen Lyth, Fuel Cells Division)
14	2015/1	NHK Fukuoka	Short interview about her research, I ² CNER, and what it's like to be an international researcher at KU (Nicola Perry, Fuel Cells Division)
15	2015/2/14	Mainichi Shimbun	Effect of molecular motion on carrier formation in a poly (3-hexylthiophene) film (Keiji Tanaka, Hydrogen Production Division)
16	2015/2/20	NHK Fukuoka	Development of long lifetermoelectric conversion sheet (Tsuyohiko Fujigaya, Fuel Cells Division)
17	2015/2	Economist Seattle Times Washington Times	Wendy Schmidt Ocean Health XPRIZE: selected as Team SINDEN Japan Team Leader (Kiminori Shitashima, CO ₂ Storage Division)