

World Premier International Research Center Initiative (WPI) FY2015 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 2016.

* 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)

Conducting research of the highest world level: Evidence of I²CNER's growing international stature and relevance can be seen in its 308 journal publications in FY2015, of which, 14 were published in journals with an impact factor greater than 10. On a related note, since its inception, 124 of the Institute's publications have been cited between 10 and 19 times, 50 have been cited 20-29 times, 15 have been cited 30-39 times, 13 have been cited 40-49 times, and 19 have been cited 50 or more times. In addition, in FY2015, I²CNER researchers received 37 national and international awards (including best poster presentations) from various societies and institutions, including Prof. T. Kunitake's 2015 Kyoto Prize in Advanced Technology for "Pioneering Contributions to Materials Science." As an Institute, in FY2015, we realized 5 of the short-term and 2 of the mid-term milestones in our division roadmaps, made significant progress toward 7 milestones in other projects, and realized a NEDO Target in the Hydrogen Storage division. In addition, our researchers have joint publications with researchers from 25 institutions around the world, and 52 internationally recognized researchers visited I²CNER for scientific interaction and exchange.

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 (57) of collaborative projects in which its researchers are involved with industry. A total of 22 projects resulted in technology transfer events. Moreover, 10 additional projects (5 in the CO₂ Capture and Utilization division, 1 in the Hydrogen Storage division, 1 in the Electrochemical Energy Conversion Division, and 3 in the Hydrogen Materials Compatibility Division) in collaboration with industry may result in technology transfer. In FY2015, I²CNER filed for 18 patents and was granted 20 patents (some of which were applied for in or before FY2014).

A selection of the Institute's breakthrough results in FY2015 are as follows: Coupling chemical synthesis, atomic resolution microscopy, and first-principles modeling, Illinois Professor Ertekin and PI Ishihara demonstrated for the first time that isolated dopant atoms embedded into titania can function as co-catalysts for the photocatalytic production of hydrogen gas at rates that can be as much as ten times as large as undoped systems. To our knowledge, this is the first direct comparison of measured activity across a spectrum of dopant species to computational predictions. PI Adachi was the first to identify that the increased number of hole traps lying above the valance band edge under solar illumination is the mechanism responsible for the degradation in a most exciting novel photovoltaic technology (hybrid perovskite devices). Moisture-induced degradation is the primary concern in moving this technology to manufacturing. The "polymer-wrapped carbon" approach of PI Nakashima to covering the carbon catalyst support in polymer electrolyte fuel cells and Li-O₂ batteries dramatically stabilizes and strengthens the function of the carbon surface. This discovery provides a radically new technique for the manufacturing of long lifetime electrodes with high performance. PI Takata developed a new platform for the design of novel mixed-wettability boiling surfaces for enhanced efficiency and reliability in energy and water applications by confirming that nanobubbles form preferentially on hydrophobic regions adjacent to hydrophobic domains. Using novel Raman spectroscopy methods, PI Zhang unlocked the fundamental physics governing charge and heat transport in suspended 2D nanomaterials. This increased fundamental understanding enables the easier integration of 2D materials in the semiconductor, electronics, battery energy, and composite materials industries. PI Akiba achieved hydrogen storage capacity of 9 wt% and on-set

temperature of 90°C through amide/hydride composites, which satisfies a NEDO target for on-board hydrogen storage applications. Continuing their work on biomimetic catalysis, the group of PI Ogo succeeded in developing a new synthetic [NiFe]-based catalyst for O₂ reduction via an O₂ adduct. This is the first example worldwide of a side-on iron (IV) peroxy complex of an O₂-tolerant hydrogenase mimic. Targeting the economic viability of the process that converts CO₂ from power plants to fuels and using optimized gas diffusion electrodes, Illinois Prof. Kenis achieved partial current densities for CO production at levels beyond the current benchmark. In an alternative collaborative approach, PI Yamauchi and Prof. Kenis utilized Cu catalysts with large surface roughness to achieve electroreduction of CO₂ to ethylene and ethanol at current densities 10 times larger than the levels reported prior to their work and at an overpotential that is the smallest reported in the literature. Using innovative numerical and experimental methodologies, PI Tsuji and PI Christensen demonstrated that inertial effects govern dynamic CO₂ migration and that CO₂ saturation is controlled by the flow capillary number and the viscosity ratio between CO₂ and water. These discoveries are transforming how we ascertain effective and safe CO₂ storage. In addition, PI Tsuji's new monitoring method (developed by fusing hydrology and geophysics) for the quantification of CO₂ saturation in reservoirs is currently deployed in an ongoing CO₂ sequestration project at a coal-fired power plant in Saskatchewan, Canada. PI Takaki attained a yield strength level of 600 MPa and acceptable hydrogen compatibility in the low-cost alloy Fe-16Cr-10Ni, which can be processed commercially. In addition, carrying out experiments with high strength martensitic stainless steel (JIS-SUS630), WPI researcher Dr. Yamabe demonstrated that barrier coatings may offer a viable pathway to deploying high-strength, low-cost steels for hydrogen service. Using geographic information system analysis, Prof. Itaoka of the Energy Analysis division and WPI Visiting Professor K. Hirose (Toyota Motor Corporation) identified prospective areas for hydrogen station locations for fuel cell vehicles and pointed to metropolitan areas which are not covered by the existing/planned stations.

Advancing fusion: In response to the recommendation by JSPS that I²CNER expand beyond engineering into different academic fields, such as mathematics or social sciences, in FY2015, in consultation with the KU Executive Vice President in Charge of Research and Industrial Collaboration, Prof. Masato Wakayama, the I²CNER Director decided to utilize the competitive fund to support the Institute's new initiative on Applied Math for Energy. After rigorous screening by the IPRC, 5 applications from throughout Kyushu University have been selected as "seed projects" the idea being to foster close, ongoing collaboration between I²CNER and other KU units, in particular, the Institute of Mathematics for Industry (IMI). Further, EVP Wakayama and the I²CNER Director are working on establishing a joint math institute between IMI at KU and the Math Department at UIUC, called the "US-Japan Institute for Applied Math for Energy" (IAME). A joint I²CNER-AIMR workshop was organized by Prof. A. Staykov at I²CNER on Sept. 2, 2015 in order to bring together young researchers who are involved in top-level interdisciplinary research on carbon materials and nanographenes so that they could exchange information and experiences, and explore possible collaborations. The workshop led to a successful KAKENHI grant application by Dr. Han (AIMR) and Dr. Watanabe (I²CNER).

The 2016 I²CNER Annual Symposium, "Computational Solutions to Fundamental Problems in Carbon-Neutral Energy Research," was held in order to i) bring together experts from the computational and experimental community, and ii) discuss and converge upon the most critical needed advances in computation relevant to the mission of I²CNER, with the overarching goal being to accelerate the transition from basic science to orders of magnitude improvements in performance through coupling of computational modeling and key experiments (fusion). The workshop focused on 5 subthemes, and the deliverable of the symposium was a "Basic Needs" report on computation in I²CNER, which will be used to guide future initiatives/investments related with computation and how it can inform I²CNER's existing research themes.

Globalization of the Institute: I²CNER is currently considering initiating interactions in an official capacity with the Helmholtz Institute Forschungszentrum Juelich, Germany. As of March 31, 2016, I²CNER has a total of 26 partner institutions in the US, Europe, and Asia. Specific highlights of our globalization efforts in FY2015 include visits by 2 KU Executive Vice Presidents to the UIUC Satellite; visits by the 2 upper level UIUC Administrators to KU; the exchange visit of 1 student from the KU School of Letters to UIUC for 3.5 months under the KU-UIUC exchange program; the exchange visit of 6 KU undergraduates, including 2 female students, to UIUC for about 1 month; and the visits of 3 KU researchers to the UIUC Satellite under the I²CNER Collaborative Foreign Exchange Program.

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 52 distinguished visitors to Kyushu University from the United States, Canada, Korea, China, Indonesia, Australia, Finland, Scotland, Germany, France, Italy, Denmark, Japan, and England and others. The Institute's researchers were responsible for organizing, co-organizing, or serving on the scientific committee for 13 international conferences, 23 international conference sessions/symposia or workshops, and 9 I²CNER international workshops. In addition, our researchers have joint publications with researchers from 25 institutions around the world. In FY2015, I²CNER placed 7 of our researchers at different international institutions.

I²CNER's permanent position within Kyushu University: In support of the vision of Prof. Chiharu Kubo, KU's President, in FY2015, the Institute filled 2 tenured foreign faculty positions, including 1 foreign principal investigator position. In this same spirit, the KU Administration awarded I²CNER 2 tenured positions (1 associate professor and 1 professor) through the University Reform Revitalization Program, and 1 joint assistant professor position with the Institute of Mathematics for Industry (IMI), bringing the total of tenured faculty in the Institute to 6, with 4.66 points (about 6 positions) left to fill in FY2016. In addition, I²CNER's researchers have made every effort to secure the sustainability of the Institute beyond the WPI period by writing proposals for external research funding, which resulted in 2 prestigious grants from JST-CREST/METI totaling ~280 million JPY/year for 5 years being approved in FY2015. These initiatives, as well as the commitment from KU, demonstrate the permanence of I²CNER and the path forward to sustainability of the Institute.

Organizational Reforms: In FY2015, building upon the organizational reforms that were implemented in FY2014, the I²CNER Director continued his regular face-to-face meetings with EVP Wakayama to discuss various issues related with I²CNER's integration with KU units, such as I²CNER's involvement in the coordination of energy research and education throughout KU. In the year since KU first instituted its university-wide merit-based salary system, which was conceived based upon the success of I²CNER's merit-based salary system, KU has begun paying a total of 261 faculty within the system (approximately 12.5% of its total faculty, with its final goal being 20%). After establishing the KU cross-appointment system in FY2014 based upon the success of Director Sofronis' cross appointment, which was the first ever at KU, President Kubo awarded I²CNER 1 tenure track assistant professor position jointly with IMI in the area of applied math for energy. The recruitment process for this position is underway, and I²CNER will soon have its first cross-appointment within KU.

- 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 308 journal publications in FY2015, of which, 14 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, 318, and 308 publications in FY 2011, 12, 13, 14, and 15, respectively). On a related note, since its inception, 124 of the Institute's publications have been cited between 10 and 19 times, 50 have been cited 20-29 times, 15 have been cited 30-39 times, 13 have been cited 40-49 times, and 19 have been cited 50 or more times. In addition, in FY2015, I²CNER researchers received 37 national and international awards (including best poster presentations) from various societies and institutions, including Prof. T. Kunitake's 2015 Kyoto Prize in Advanced Technology for "Pioneering Contributions to Materials Science"; Prof. Horita's Medal with Purple Ribbon; Prof. Tsuji's award from the Geological Society of Japan (last year, he received an award from the Seismological Society); Prof. Ida's award, Presto on Chemical Conversion of Light Energy, from the Japan Science and Technology Agency

(JST); and the most-cited award received by Profs. Edalati, Yamamoto, Horita, and Ishihara for their paper in *Scripta Materialia*. As an Institute, in FY2015, we realized 5 of the short-term and 2 of the mid-term milestones in our division roadmaps, made significant progress toward 7 milestones in other projects, and realized a NEDO Target in the Hydrogen Storage division. In FY2015, I²CNER filed for 18 patents and was granted 20 patents (some of which were applied for in or before FY2014). Moreover, I²CNER hosted 2 international symposia, and held 18 seminars in the Institute Interest Seminar Series (29 speakers) and 21 seminars (22 speakers, 19 non-Japanese) in the I²CNER Seminar Series. The Institute's researchers were responsible for organizing, co-organizing, or serving on the scientific committee for 13 international conferences, 23 international conference sessions/symposia or workshops, and 9 I²CNER international workshops. Our researchers have given 375 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 25 institutions around the world, and 52 internationally recognized researchers visited I²CNER for scientific interaction and exchange. Additionally, we are considering interactions with 4 internationally recognized research centers/universities, namely, the University of Edinburgh, the Helmholtz Institute Forschungszentrum Juelich, the Southwest Research Institute, and the University of New South Wales (UNSW). The agreement with UNSW is currently being negotiated. Lastly, we hold agreements with 4 internationally recognized research centers/universities (SINTEF/NTNU of Norway, Illinois, the California Air Resources Board (CARB), the National Fuel Cells Research Center (NFCRC) of the University of Irvine, and ECOSTORE, a consortium based in the European Union).

The research activities in FY2015 are as follows: Coupling chemical synthesis, atomic resolution microscopy, and first-principles modeling, Illinois Professor Ertekin and PI Ishihara demonstrated for the first time that isolated dopant atoms embedded into titania can function as co-catalysts for the photocatalytic production of hydrogen gas at rates that can be as much as ten times as large as undoped systems. To our knowledge, this is the first direct comparison of measured activity across a spectrum of dopant species to computational predictions. PI Adachi was the first to connect a critical degradation mechanism to traps in a most exciting novel photovoltaic technology (hybrid perovskite devices). Hole traps lying above the valence-band edge were shown to increase under solar illumination in the presence of humidity. Moisture-induced degradation is the primary concern in moving this technology to manufacturing. The "polymer-wrapped carbon" approach of PI Nakashima to covering the carbon catalyst support in polymer electrolyte fuel cells and Li-O₂ batteries with a protective thin layer dramatically stabilizes and strengthens the function of the carbon surface. This discovery provides a radically new technique for the manufacturing of long lifetime electrodes with high performance. PI Takata developed a new platform for the design of novel mixed-wettability boiling surfaces for enhanced efficiency and reliability in energy and water applications by confirming that nanobubbles form preferentially on hydrophobic regions adjacent to hydrophobic domains. Using novel Raman spectroscopy methods, PI Xing unlocked the fundamental physics governing charge and heat transport in suspended 2D nanomaterials. This increased fundamental understanding enables the easier integration of 2D materials in the semiconductor, electronics, battery energy, and composite materials industries. PI Akiba achieved hydrogen storage capacity of 9 wt% and on-set temperature of 90°C through amide/hydride composites, which satisfies a NEDO target for on-board hydrogen storage applications. Continuing their work on biomimetic catalysis, the group of PI Ogo succeeded in developing a new synthetic [NiFe]-based catalyst for O₂ reduction via an O₂ adduct. This is the first example worldwide of a side-on iron (IV) peroxo complex of an O₂-tolerant hydrogenase mimic. Targeting the economic viability of the process that converts CO₂ from power plants to fuels and using optimized gas diffusion electrodes, Illinois Prof. Kenis went beyond the current benchmark and achieved partial current densities for CO production as high as 280 mA cm⁻² at a cathode potential of -2.2 V vs. Ag/AgCl. Specifically, Prof. Kenis achieved enhancement in partial current density for CO up to 30% and this by using a dilute CO₂ feed. In an alternative collaborative approach, PI Yamauchi and Prof. Kenis utilized Cu catalysts with large surface roughness to achieve electroreduction of CO₂ to ethylene and ethanol at current densities 10 times larger than the levels reported prior to their work and at an overpotential (< 0.7 V) that is the smallest reported in the literature. Using innovative numerical and experimental methodologies, PI Tsuji and PI Christensen quantified the dynamics of CO₂ behavior in targeted reservoir rocks and

demonstrated that inertial effects govern dynamic CO₂ migration, and that CO₂ saturation is controlled by the flow capillary number and the viscosity ratio between CO₂ and water. These discoveries are transforming how we ascertain effective and safe CO₂ storage. In addition, PI Tsuji's new monitoring method (developed by fusing hydrology and geophysics) for the quantification of CO₂ saturation in reservoirs is currently deployed in an ongoing CO₂ sequestration project at a coal-fired power plant in Saskatchewan, Canada. A yield strength level of 600 MPa and acceptable hydrogen compatibility has been attained in the low-cost alloy Fe-16Cr-10Ni by PI Takaki. This result is extremely important as it shows that low cost metastable austenitic alloys can be manufactured with high strength and acceptable hydrogen compatibility by applying a commercially viable material-processing method. In his work related with the tensile and fatigue properties of hydrogen-exposed, coated specimens of a high-strength martensitic stainless steel (JIS-SUS630), WPI researcher Dr. Yamabe demonstrated that the relative reduction in area and the fatigue life of the coated steels were not degraded by hydrogen, in contrast to the non-coated specimens. These results demonstrate that barrier coatings may offer a viable pathway to deploying high-strength, low-cost steels for hydrogen service. Using geographic information system analysis, Prof. Itaoka of the Energy Analysis division and WPI Visiting Professor K. Hirose (Toyota Motor Corporation) investigated hydrogen station deployment and identified prospective areas for hydrogen station locations in order to meet the refueling demand that will be driven by fuel cell vehicles. Prof. Itaoka and Dr. Hirose identified the important metropolitan areas which are not covered by the existing/planned stations and which need to be serviced by new stations.

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 (57) of collaborative projects in which its researchers are involved with industry. A total of 22 projects resulted in technology transfer events. The following are representative examples for each division: i) Prof. Ishihara's transfer of dual carbon battery technology for energy recovery from automobiles to Ricoh Co. Ltd., ii) Prof. Matsumoto's discovery of optimum chemical compositions of proton-conducting electrolytes and electrodes specifically suitable for steam electrolysis has been transferred to Nippon Shokubai Co., Ltd. for the development of a steam electrolyzer operating at 600°C for mass production of hydrogen from solar energy, iii) Prof. Takata's group have provided the Mitsubishi Heavy Industries, Central Glass Corp with fundamental data on thermophysical and transport properties, and heat transfer characteristics of newly developed refrigerants for the design of commercial products of high temperature heat supply heat pump, iv) Prof. Akiba is working with IWATANI Co. Ltd to develop high performance hydrogen absorbing alloys suitable for stationary hydrogen storage; v) Prof. Yamauchi's synthetic method for the preparation of atomically well mixed Fe-Ni nanoalloys has been transferred to Daido Steel, vi) Prof. Fujikawa's functional nanomembrane technology for gas separation has been transferred to Nanomembrane Technology Inc. for upscale development, vii) Prof. Tsuji's innovative continuous CO₂ monitoring system in collaboration with the Japan Oil, Gas and Metals National Corporation (JOGMEC) has been transferred and deployed in the ongoing CO₂ sequestration project in Saskatchewan, Canada, viii) the high durability of coated, commercial Cr-Mo storage cylinders under high-pressure hydrogen gas has been demonstrated by the hydrogen-pressure cycle tests. This technology has been transferred to industry, and Toyota Tsusho Corporation is targeting the technology for prototypes of various hydrogen-components; ix) 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). Moreover, 10 additional projects (5 in the CO₂ Capture and Utilization division, 1 in the Hydrogen Storage division, 1 in the Electrochemical Energy Conversion Division, and 3 in the Hydrogen Materials Compatibility Division) in collaboration with industry may result in technology transfer.

In FY2015, I²CNER reviewed the structure and objectives of its former "Hydrogen Production" and "Fuel Cells" divisions. The review involved extensive interactions between all Japanese and international members of the divisions, discussion with the EAD and the Science Steering Committee, and input from the IPRC. It was decided that the two divisions should be eliminated so that the Institute could introduce in their place two new divisions: "Molecular Photoconversion Devices" and "Electrochemical Energy Conversion." The objectives of these new divisions, the associated research projects, and the new roadmaps have been defined by the members of the divisions in a way that ensures that the objectives best serve the mission of I²CNER for a carbon-neutral society

(CNS).

The project on monitoring leaked CO₂ from the sub-seabed has been terminated. The projects in the revised division roadmap are now as follows: (i) molecular-scale investigation of CO₂, (ii) pore-scale investigation of CO₂, (iii) field-scale investigation of CO₂. In addition to these 3 projects, we introduced a new project titled "linkage of multi-scale phenomena." In this, the objective is to study and identify upscaling mechanisms so that our model and experimental results from the molecular and pore levels inform our models and simulations at the field scale.

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

i) Molecular Photoconversion Devices: Using a thermally stimulated current technique, a critical degradation mechanism in the most exciting novel photovoltaic technology (hybrid perovskite devices) was demonstrated. In fact, it is for the first time that it was shown that hole traps lying above the valence-band edge increase under solar illumination in the presence of humidity. Moisture-induced degradation is the primary concern in moving this technology to manufacturing; In addition, using artificial photosynthesis based on a combination of an inorganic semiconductor and a biocatalyst, we demonstrated hydrogen production efficiency from 300 nm photons of 0.31 and 1.57% for whole cells and the enzyme modified catalyst, respectively.

ii) Electrochemical Energy Conversion: The main shortcoming of polymer electrolyte fuel cells and Li-O₂ batteries, which are key energy devices that are now in use and targeted for the future, is the degradation of electrodes that use carbon as the catalyst support. Our recent experimental results demonstrate a new approach to synthesizing an organic polymer that results in the formation of a protective thin layer at the surface, which dramatically stabilizes and strengthens the function of the carbon surface. This "polymer-wrapped carbon" approach of PI Nakashima's group is opening a new door to the discovery of long lifetime electrodes with high performance, to make these energy devices applicable to our daily lives.

iii) Thermal Science and Engineering: We confirmed that nanobubbles preferentially form on hydrophobic regions adjacent to hydrophobic domains. This finding represents a platform for the design of novel mixed-wettability boiling surfaces for enhanced efficiency and reliability in energy and water applications; Also, we have developed and validated two novel Raman spectroscopy methods (steady-state and transient laser flash) capable of measuring the thermal conductivity, thermal diffusivity, and interfacial thermal resistance of suspended 2D nanomaterials. We used these novel techniques in combination with the T-type method to characterize for the first time the (i) thermoelectric performance of an individual free-standing single crystal Bi₂S₃ nanowires and (ii) the in-situ heat transport in defect-engineered free-standing single-layer graphene sheets, unlocking the fundamental physics governing charge and heat transport.

iv) Hydrogen Storage: We achieved hydrogen storage capacity of 9 wt% and an on-set temperature of 90°C for on-board applications (amide/hydride composites), and obtained higher effectiveness of the high pressure torsion (HPT) approach to activation of TiFe-based alloys through the addition of Mn.

vi) Catalytic Materials Transformations: Current hydrogen fuel cells require precious platinum metal as anode and cathode catalysts. In 2013, we succeeded in synthesizing [NiFe]hydrogenase as an alternative and cheap model catalyst for the hydrogen splitting reaction. In FY2015, in continuation of our previous studies, we succeeded in developing a new synthetic [NiFe]-based catalyst for O₂ reduction via an O₂ adduct. This is the first example worldwide of a side-on iron (IV) peroxo complex of an O₂-tolerant hydrogenase mimic.

v) CO₂ Capture and Utilization: Compared to our current benchmark (250 mA cm⁻²), optimization of gas diffusion electrodes (GDEs) leads to partial current densities for CO production as high as 280 mA cm⁻² at a cathode potential of -2.2 V vs. Ag/AgCl. Also, due to the improved mass transport with the use of optimized GDEs, the same significant achievement was observed with a dilute feed (50-50 CO₂ and N₂). This achievement helps toward the economic viability of a process that converts CO₂ from power plants to fuels. Compared to the performance of state-of-the-art Ag catalysts on commercially available GDEs, use of Ag on our optimized GDEs led to an enhancement in partial current density for CO up to 30%, despite the use of a dilute CO₂ feed.

vii) CO₂ Storage: Using innovative numerical and experimental methodologies, we quantified the dynamics of CO₂ behavior in targeted reservoir rocks and demonstrated that inertial effects govern dynamic CO₂ migration, and that CO₂ saturation is controlled by the flow capillary number and the viscosity ratio between CO₂ and water. These discoveries change the way we ascertain effective and safe CO₂ storage.

viii) Hydrogen Materials Compatibility: A yield strength level of 600 MPa and acceptable hydrogen compatibility has been attained in the low-cost alloy Fe-16Cr-10Ni. This result is extremely important, as it shows that low cost metastable austenitic alloys can be manufactured with high strength and acceptable hydrogen compatibility by applying a commercially viable material-processing method. The tensile and fatigue properties of hydrogen-exposed, coated specimens of a high-strength martensitic stainless steel (JIS-SUS630) demonstrated that the relative reduction in area and the fatigue life of the coated steels were not degraded by hydrogen, in contrast to the non-coated specimens. These results demonstrate that barrier coatings may offer a viable pathway to deploying high-strength, low-cost steels for hydrogen service.

ix) Energy Analysis: Using geographic information system analysis, we investigated hydrogen station deployment and identified prospective areas for hydrogen station locations in order to meet the refueling demand that will be driven by fuel cell vehicles. We concluded that the most effective approach was to locate the hydrogen stations in a way that minimizes average distance between potential customers and the nearest hydrogen stations. Our analysis demonstrated that more hydrogen stations need to be located in internal city locations, especially in every prefectural capital. We also identified the important metropolitan areas which are not covered by the existing/planned stations and which need to be covered by new stations.

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

Molecular Photoconversion Devices (Lead Principal Investigator: Prof. Ishihara)

The objective of this division is to reduce carbon emissions through cost effective conversion of solar energy to electricity and hydrogen, and energy conservation through organic based lighting devices and development of new materials for surface molecular brushes for low friction technologies. The research projects include new organic materials to convert solar energy into electricity, novel inorganic, organic, and molecular photocatalysts to directly split water into oxygen and hydrogen, new concept molecules as organic light emitting diodes, and new molecules for low friction. The research efforts include unique techniques for the analysis of the interface structure of organic dye and inorganic semiconductors, synthesis of novel molecules for organic light emitters and photoelectrochemical and photovoltaic cells, device fabrication and testing, and theory-based materials development.

Hydrogen production using a biocatalyst hydrogenase

This achievement is related to Project 2-1 in the roadmap of the Division. In FY2015, we have been developing an artificial photosynthesis method based on a combination of an inorganic semiconductor and a biocatalyst. The study examined a hydrogenase biocatalyst produced by recombinant DNA methods using *Escheria Coli* BL21(DE3). A redox mediator, methylviologen, was used to promote electron transfer from the inorganic semiconductor to the hydrogenase. Two hydrogenase systems were characterized, one based on purified hydrogenase enzyme and the other based on whole cells. The latter simplifies handling and improves safety. The efficiency of H₂ production from 300 nm photons was 0.31 and 1.57% for whole cells and the enzyme modified catalyst, respectively. A schematic of the whole-cell approach and the experimental results are shown in Fig. 1.1, below. The 2020 milestone for this project is 1% efficiency. Therefore this system has achieved the milestone for 300 nm photons. The experiments were also significant because this is the first report using whole cell hydrogenase which demonstrates charge transport through the cell wall.

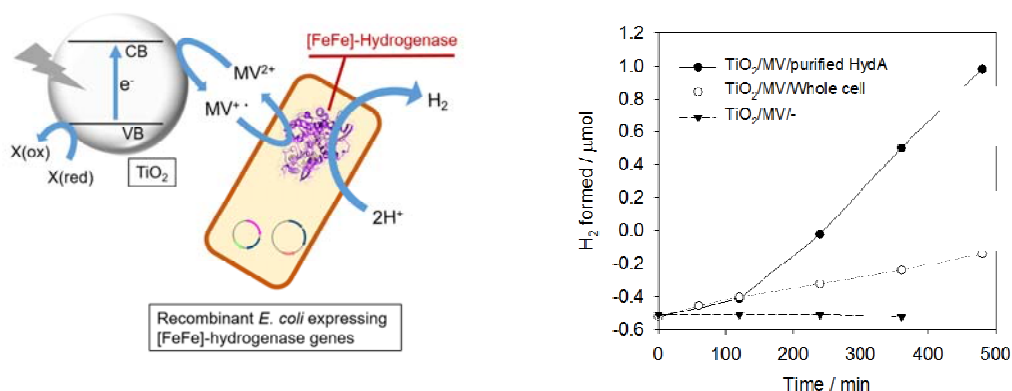


Fig. 1.1. (left) a schematic representation of the whole cell hydrogenase approach with the cell coupled to the TiO₂ absorber material and (right) the experimental results for the purified hydrogenase and whole-cell approach as a function of time.

Publication

Y. Honda, H. Hagiwara, S. Ida, and T. Ishihara, Application to Photocatalytic H₂ Production of a Whole-cell Reaction by Recombinant Escherichia coli Cells Expressing [FeFe]-Hydrogenase and Maturases Genes, *Angew. Chem. Int. Ed.* Accepted for publication.

Degradation mechanisms in hybrid perovskite photovoltaics

This achievement is related to Project 1 in the roadmap of the Division. Previously, we have investigated organic photovoltaic cells based on bulk heterojunctions. Recent results have demonstrated that the hybrid perovskite materials result in significantly improved efficiency but with low stability. This scientific achievement related to mechanisms of degradation of hybrid organic/inorganic CH₃NH₃PbI₃-based perovskite solar cells (PSCs).

We have shown that formation of hole traps is directly related to device stability. Prior work had only examined trap formation in fresh material before degradation. This study is the first to connect that degradation explicitly to traps. The devices studied here used PEDOT:PSS and PC₇₁BM as contacts to the CH₃NH₃PbI₃. The best device produced to date had a 16% solar conversion efficiency, exceeding the 11% short-term milestone value in the division roadmap for 2020. The device degradation was studied by analysis of the hysteresis between forward and reverse current-voltage scans. For low scan rates and as-fabricated devices there was virtually no hysteresis. The results were the same for devices fabricated in either dry N₂ or lab air. This was attributed to the highly dense materials formed. However, as the device was operated under light the devices fabricated in air showed increasing hysteresis, developing much more rapidly than the samples fabricated in dry N₂. This was attributed to humidity in the air. The behaviors are compared in Fig. 1.2. This was analyzed by the thermally stimulated current (TSC) technique in which charge is injected with a small forward bias and extracted under a reverse bias pulse as a function of temperature (similar to deep level transient spectroscopy). The results showed the development of two traps in the devices fabricated in air, while no traps were detected in films deposited in dry N₂ (Fig. 1.2). The degraded samples show changes in the x-ray diffraction pattern including formation of an amorphous background and additional peaks.

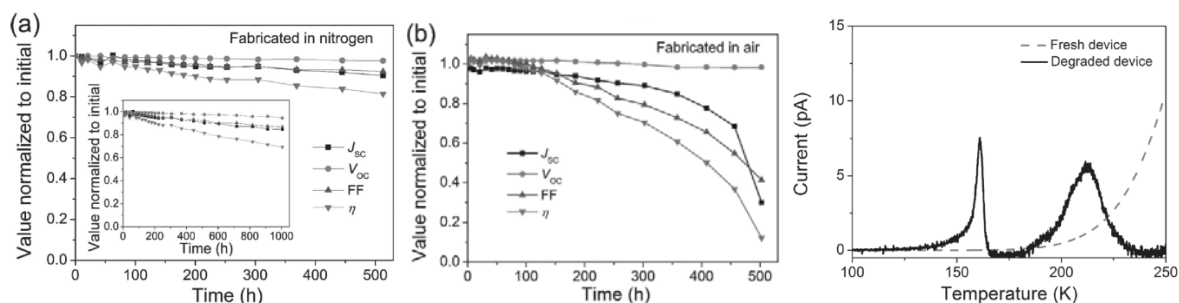


Fig. 1.2. Degradation of devices fabricated in dry N_2 (a) and in air (b) as a function of time under Xenon lamp illumination at 100 mW cm^{-2} (simulated AM1.5 solar spectrum) and the development of traps detected by the thermally stimulated current technique (c).

Publication

C. Qin, T. Matsushima, T. Fujihara, W. J. Potscavage Jr., C. Adachi, Degradation mechanisms of solution-processed planar perovskite solar cells: thermally stimulated current measurement for analysis of carrier traps, *Adv. Mat.*, 28, 446-471, 2016.

Electrochemical Energy Conversion (Lead Principal Investigator: Prof. Matsumoto)

Electrochemical processes are at the heart of efficient conversion between electrical and chemical energies. The objective of this division is to conduct scientific research and technological development for energy-efficient, low-cost, and robust electrochemical energy conversion, in systems including polymer electrolyte fuel cells (PEFC), solid oxide fuel cells (SOFC), and solid oxide electrolysis cells (SOEC). PEFC is the preferred solution for automotive fuel cell applications. Inefficiencies at low temperatures (ca. 80°C) are leading to a focus on higher temperature ($>100^\circ\text{C}$) hydrogen PEM fuel cells. Research addresses catalyst activity, support durability, and high temperature electrolyte identification and evaluation. SOFCs are utilized for stationary electricity generation at various scales. Research addresses developing a fundamental understanding of electrode and electrolyte materials and electrochemical events taking place in the SOFC, surface/interfacial catalytic processes on metal oxides, and electrode and electrolyte degradation. Electrolysis is used to produce hydrogen from electricity to respond the forthcoming demand of hydrogen fuel. SOEC and related devices are examined from the perspective of activity and durability of electrolyte and electrode components. Other relevant energy storage concepts, e.g. batteries, are also addressed in division activities.

Double polymer coated carbon nanotubes for high-durability fuel cells

Improvement of the durability of polymer electrolyte fuel cells (PEFC) is one of the most urgent targets of "Project 3-1 Polymer electrolyte cells" of this Division. PI Nakashima and Prof. Fujigaya developed a novel PEFC using polymer-wrapped carbon nanotubes (CNT) as the catalyst support material (CNT-based PEFC) showing a remarkably high durability (single cell test: $>400,000$ cycles, Fig. 1.3) at 80°C under humidified conditions. Such a remarkable durability has never been achieved so far: a conventional PEFC using carbon black (commercial PEFC) only withstands 5,000 cycles under the same operating conditions. The dramatic improvement was achieved by the use of the 'PBI-wrapping method,' in which PBI stands for polybenzimidazole, developed by Prof. Fujigaya and PI Nakashima. Owing to this achievement, the short-term milestone of the division roadmap, "PEC: Durable electrodes through novel design: 10^5 potential cycles" for Project 3 (electrodes) has been achieved.

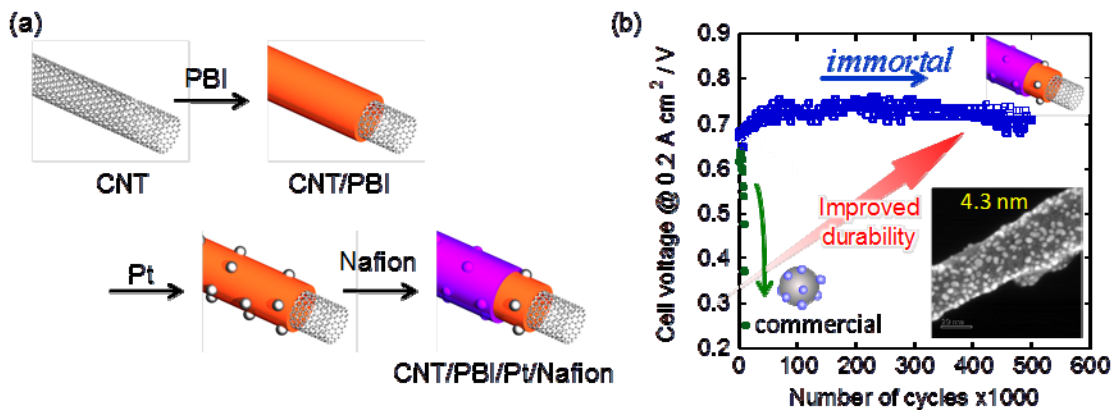


Fig. 1.3. (a) Schematic illustration of PBI-wrapping method. (b) Cell voltage at 200 mA·cm⁻² as a function of potential cycling numbers of the CNT-based PEFC (blue) and commercial PEFC (green).

Publication

M. R. Berber, I. H. Hafez, T. Fujigaya, N. Nakashima, A highly durable fuel cell electrocatalyst based on double-polymer-coated carbon nanotubes, *Sci. Rep.* 5, art. No.16711, 2015.

As a technological extension, the above mentioned polymer-wrapping method has been applied to lithium-oxygen (Li-O₂) secondary battery—related to the short term milestone “Novel battery: Proposal of new concept” of “Project 3-3 Energy storage”—to demonstrate a new approach to the design of ultimate rechargeable batteries due to their ultra-high capacity without the use of cobalt and other rare elements. At present, improvement of the cycle stability upon charging-discharging of rechargeable batteries is a crucial problem. Prof. Fujigaya and PI Nakashima found that the PBI-wrapping method dramatically enhances cycle stability. When charging-discharging was tested on carbon nanotubes (CNTs) and PBI-wrapped CNTs, cycle stability was improved from 3 cycles to 50 cycles (Fig. 1.4) due to the catalytic effect of PBI. In sum, the benefits of the PBI-wrapping method include simple processing, low-cost, and unprecedented durability in multiple cases. Elucidation of the mechanism, e.g., how the wrapped interfaces function as interfaces for reactions and catalyst support, is our next focus area.

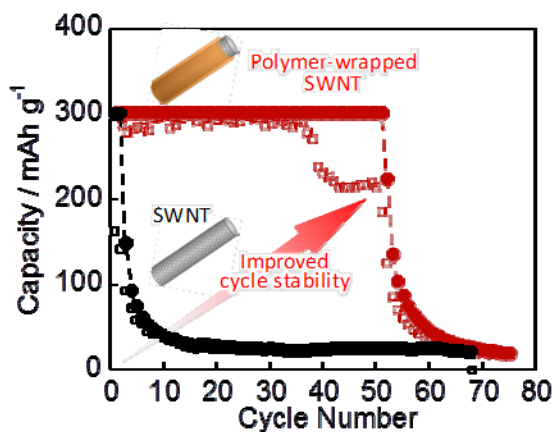


Fig. 1.4. Plots of the capacity on charge (open circle) and discharge (filled circle) cycles as a function of cycle number for the cells based on CNT (black) and PBI-wrapped CNT (red) between 2.0-4.5 V (vs. Li/Li⁺) at a current density of 0.1 mA cm⁻².

Publication

T. Fujigaya, S. Hirata, I-C. Jang, J. Morita, R. Kanamori, T. Ishihara, and N. Nakashima, *Adv. Energy Mater.*, submitted.

Surface and Interface Phenomena in Solid Oxide Cells

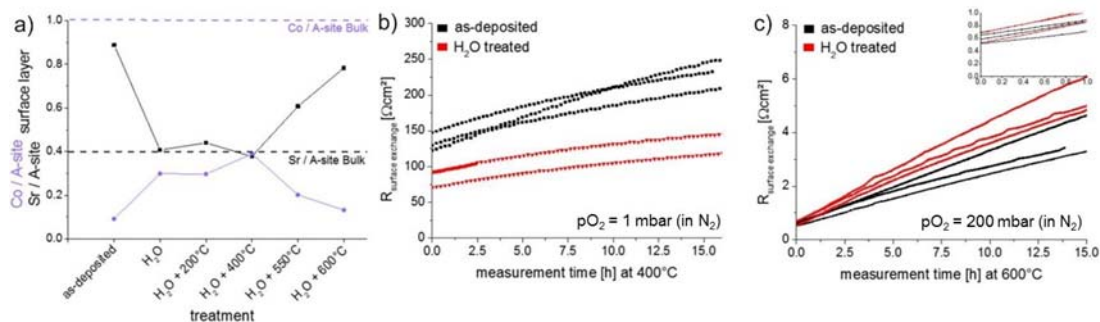


Fig. 1.5. (a) Cation fractions of water-rinsed surface of LSC thin films after annealing for 1 h at different temperatures as determined by LEIS; (b) and (c) Increase in the surface exchange resistance with time for as-deposited and H₂O treated thin film electrodes, measured at (b) 400°C in pO₂ = 1 mbar and (c) 600°C in pO₂ = 200 mbar.

Using leading-edge surface analysis techniques to measure both surface composition and the kinetics of oxygen exchange, the work of Professors Tellez and Druce and PI Kilner has revealed important features of the surface composition and kinetics of electrodes at lower temperatures (e.g. I²CNER's target temperature of 500°C for solid oxide cells). In particular, their investigations of the kinetics of strontium segregation and its effects on the electrochemical performance of La_{0.6}Sr_{0.4}CoO_{3-δ} (LSC) thin film model electrodes at 400–600 °C (*J. Mater. Chem. A*, 3, 22759–22769, 2015) which was carried out in collaboration with Prof. Fleig at the Vienna University of Technology, revealed a systematic change of the surface composition with respect to the annealing temperature on water-rinsed surfaces of LSC. This work demonstrates clearly that the SrO segregation rate markedly increases with temperature (Fig. 1.5a). Second, this study also determined that that electrode degradation takes place more rapidly with increasing temperature (Figs. 1.5b and c). These results show clear evidence that SrO segregation is a direct reason underlying electrode degradation. Sr is a general component in most of the electrode materials. This work builds on their previous suggestions of the significance of the SrO segregation and loss of transition metals on the electrode surface. The above accomplishment in FY 2015 now provides direct evidence for this phenomenon, and thus contributes to the understanding and tailoring of electrodes for solid oxide cells.

In a related accomplishment, since electrode surfaces were shown to be transition metal free, a joint computational and experimental work by Tellez, Druce, and Staykov has elucidated the mechanism of oxygen activation and dissociation on transition metal-free surfaces. Driven by experimental results obtained by LEIS on SrTiO₃ single crystals, a theoretical model for the electrocatalytic reaction has been developed in collaboration with computations conducted by Staykov of Molecular Photoconversion Devices Division (*Chemistry of Materials*, 27, 8273–8281, 2015). The study reveals that although Sr is not active, oxygen vacancies present at the SrO surface are catalytically active sites for oxygen reduction. The sub-surface transition metal cations help the procedure by mediating the electron transfer from lattice oxygen ions to the O₂ molecule. This study provides us a view on the mechanism of electrode catalysis takes place on the electrode surface where transition metals are missing on the first layer.

These accomplishments correspond to the short-term milestone "SOC: Highly active stable electrode" and the mid-term milestone "Quantitative and predictive theory of oxygen exchange in terms of composition and defect chemistry" for Project 1 "Electrodes".

Related Publications

G.M. Rupp, H. Téllez, J. Druce, A. Limbeck, T. Ishihara, J. Kilner, J. Fleig, Surface chemistry of $\text{La}_{0.6}\text{Sr}_{0.4}\text{CoO}_{3-\delta}$ thin films and its impact on the oxygen surface exchange resistance, *J. Mater. Chem. A*, 3, 22759-22769, 2015.

A. Staykov, H. Téllez, T. Akbay, J. Druce, T. Ishihara, J. Kilner, Oxygen activation and dissociation on transition metal free perovskite surfaces, *Chemistry of Materials*, 27, 8273-8281, 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 CO_2 emissions. Selected representative results are:

Nanobubble Stability Induced by Hydrophilic Domains on Bi-Philic Surfaces

Microscale gas bubbles residing at a liquid/solid interface are key for reducing the liquid-to-solid temperature difference required for the onset of nucleate boiling, an important goal in liquid-to-vapor phase change heat transfer (Division Project : HMT-1, Milestone : Development of boiling surface with onset of boiling at less than 2K in ΔT_{sat} .) To extend our recent study of nanobubble stability on highly oriented pyrolytic graphite, which used peak force quantitative nanomechanics (*Langmuir*, 31, 982–986, 2015), we fabricated a bi-philic surface (hydrophilic/hydrophobic) to explore the effects of wettability on nanobubble formation (Division Project: HMT-1, Milestone: Clear understanding of wettability effects in liquid-vapor phase change). We discovered that initially, a small number of nanobubbles are generated which rapidly decrease in size on the smooth and uniform hydrophobic surface. However, on the bi-philic surface (hydrophobic surface with hydrophilic domains), the hydrophilic domains significantly increase the generation and stability of nanobubbles, with bubbles remaining on the surface up to three days after immersion. The findings elucidated here provide guidelines for the development of mixed-wettability boiling surfaces for increased phase change system reliability and efficiency.

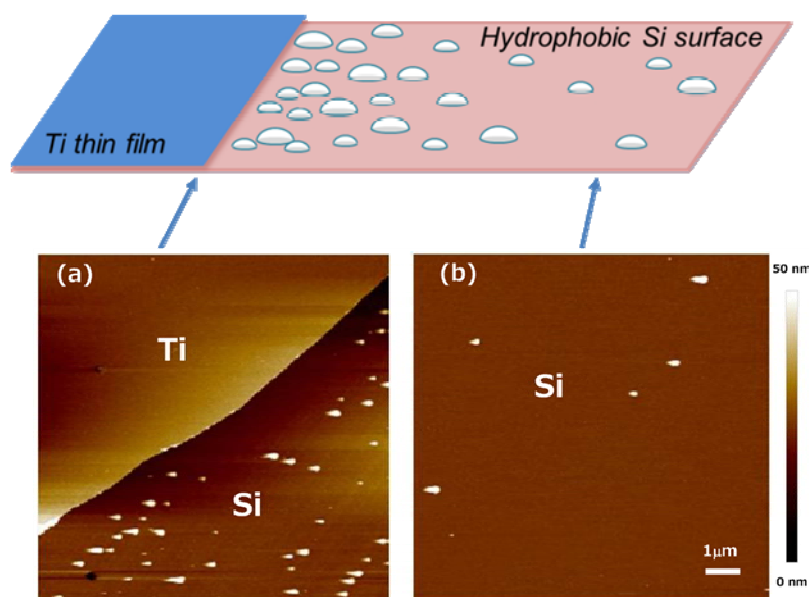


Fig. 1.6. (upper) Schematic of the enhanced nanobubble generation and stability adjacent to hydrophilic domains. (a) Close to the Ti/Si boundary, atomic force microscopy reveals many nanobubbles exist on the hydrophobic Si surface close to the hydrophilic edge, with (b) few nanobubbles on the uniform hydrophobic surface.

Publication

T. Nishiyama, K. Takahashi, T. Ikuta, Y. Yamada, and Y. Takata, Hydrophilic domains enhance nanobubble stability, *ChemPhysChem*, 17, 1-6, 2016.

Novel T-Type Method for the Thermal Characterization of Nanomaterials

Two dimensional (2D) materials have many potential applications in the electronics and energy industries. In this study, we develop and utilize a novel noncontact Raman spectroscopy technique to measure the thermal conductivity of suspended 2D materials including: graphene, MoS₂, and h-BN. Classical noncontact Raman spectroscopy works by laser heating the sample, measuring its Raman spectrum, and determining the local temperature based on the linear relationship between temperature and Raman band shifts. However, the heat flux, i.e. the absorbed laser power, needs to be theoretically estimated, causing large uncertainties. In this project, we have developed a novel steady-state Raman spectroscopy method in combination with a novel transient laser flash Raman spectroscopy method capable of measuring the thermal conductivity, thermal diffusivity, and interfacial thermal resistance of suspended 2D nanomaterials without prior knowledge of the laser absorption. We have shown our novel methods to be in excellent agreement with past studies, giving us confidence of the accuracy of the technique. The developed characterization approach represents a significant milestone in the nanoscale heat transfer community.

In addition to developing the novel thermal characterization technique, we used the T-type method, capable of measuring the thermophysical and thermoelectric properties of nanotubes, nanowires and nanoribbons, to (i) characterize the thermoelectric performance of an individual free-standing single crystal Bi₂S₃ nanowires and (ii) measure the in-situ heat transport in defect-engineered free-standing single-layer graphene. Specifically, the T-type method measurements yielded the following advances:

(i) The thermoelectric properties including the Seebeck coefficient, thermal conductivity and electrical conductivity were measured for the first time using the T-type method. The figure of merit was shown to be far less than the reported values of nanostructured bulk Bi₂S₃ samples. The fundamental mechanism of the discrepancy was investigated and found to stem from the Seebeck coefficient sign change at 320 K. Through this work the short-term milestone on "Development of measurement methods of physical properties of individual nanomaterials" in the division's roadmap for Project TP-3 has been realized.

(ii) Monolayer graphene ribbons were successfully suspended together with nanoscale hot films and milled using focus ion beam to create nanoscale defects and tune the heat transport. To characterize the effects of nanopores on heat transport, the in-situ thermal conductivity of the defect-engineered graphene was accurately measured using the T-type method. The nanopore defects were found to decrease the thermal conductivity by approximately 42%. The results of this work satisfy the mid-term milestone on "Clear understanding of nanoscale and interfacial thermal transport" in the division's roadmap for Project TP-3.

Publications

W. Ma, T. Miao, X. Zhang, K. Takahashi, T. Ikuta, B. Zhang, Z. Ge,, A T-type method for characterization of the thermoelectric performance of an individual free-standing single crystal Bi₂S₃ nanowire, *Nanoscale*, 8(5), 2704-2710, 2016.

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*, 117(6), 065102, 2015

H. Wang, K. Kurata, T. Fukunaga, H. Takamatsu, X. Zhang, T. Ikuta, L. Takahashi, T. Nishiyama, H. Ago, Y. Takata,, In-situ measurement of the heat transport in defect-engineered free-standing single-layer graphene, *Scientific Reports*, 6, 21823, 2016

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:

High performance hydrogen storage materials: Amide/hydride composites

In order to develop hydrogen storage materials with an appropriate hydrogen weight capacity for on board application, amide/hydride composites have been developed under a NEDO project in collaboration with the car industry. We have already reported the three-component amide/hydride composite, $\text{Mg}(\text{NH}_2)_2\text{-4LiH-LiNH}_2$; showed hydrogen release of 7.7 wt% and on-set hydrogen release temperature of 150°C , compared to the theoretical capacity of 9.0 wt%.

This fiscal year we intensively developed additives for improvement of hydrogen capacity, release temperature and cycleability (limited by formation of ammonia.) It was found that KH increases hydrogen capacity to the theoretical value of 9.0 wt%, reduces the hydrogen release temperature to 90°C , and prevents ammonia formation, as shown in Fig. 1.7. These achievements meet the targets set by NEDO and our Project 1 for on board hydrogen storage.

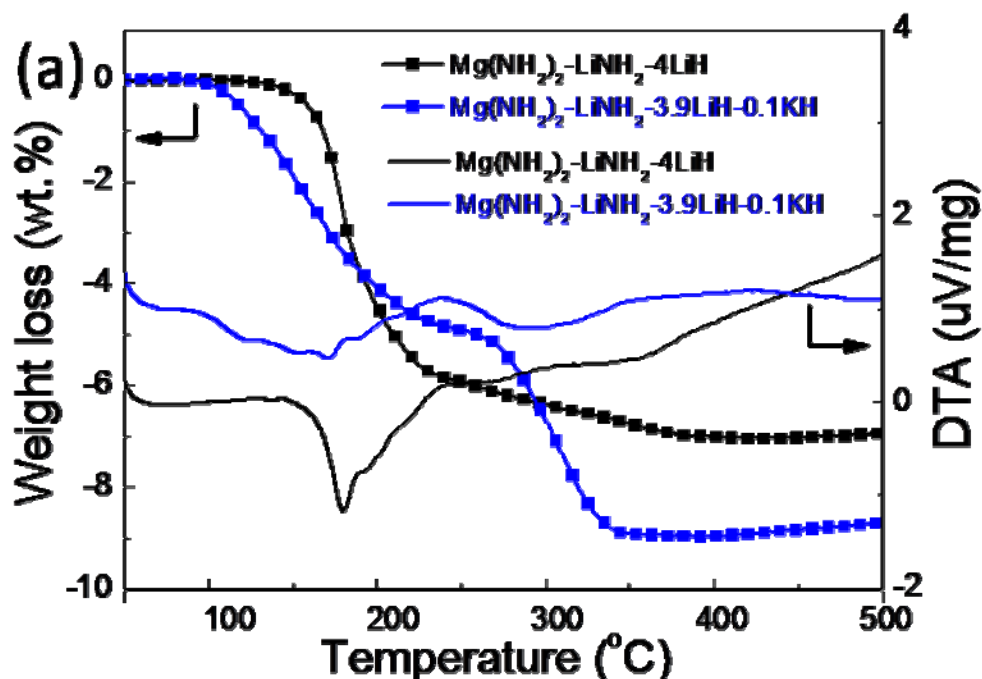


Fig. 1.7. Hydrogen capacity and on-set hydrogen release temperature of $\text{Mg}(\text{NH}_2)_2\text{-4LiH-LiNH}_2$ with and without KH addition

Publication

H.-J. Lin, H. -W. Li, B. Paik, J. Wang, E. Akiba, "KH-modified three-component $\text{Mg}(\text{NH}_2)_2\text{-LiNH}_2\text{-LiH}$ composites as promising hydrogen storage materials", Dalton Transactions, submitted.

Effect of lattice defects on hydrogen storage behavior of TiFe-based materials

The main drawbacks of TiFe- and Mg-based hydrides for hydrogen storage are difficult activation and high thermodynamic stability, respectively. Our earlier works showed that TiFe was activated by processing through the high-pressure torsion (HPT) method, but the activation

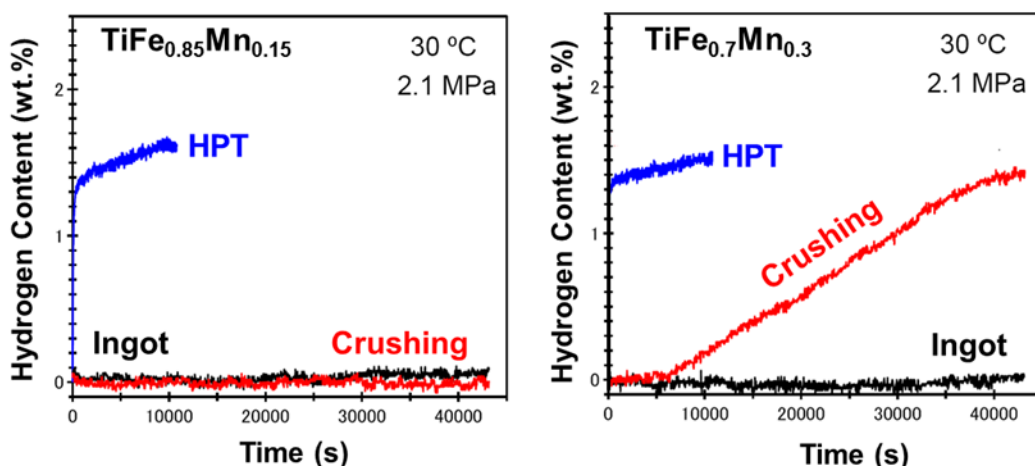


Fig. 1.8. Fast hydrogen storage at 30°C in TiFe-Mn intermetallics processed by High Pressure Torsion (HPT.)

pressure was as high as 10 MPa. We employed two strategies to activate TiFe at low pressures: (i) introduction of lattice defects by HPT processing for fast hydrogen diffusion; and (ii) enhancement of the thermodynamic stability of the hydride by the addition of Mn to TiFe. TiFe activated by these strategies absorbed hydrogen very fast at 30°C under pressures as low as 0.2-2 MPa. TiFe_{0.7}Mn_{0.3} could be activated even by crushing. This study provides important findings for the milestone of "Start commercialization of HPT-processed TiFe for stationary applications and HPT-processed Mg alloys for on board applications" in Project 3 of the Division.

Publications

K. Edalati, H. Emami, A. Staykov, D.J. Smith, E. Akiba, Z. Horita, Formation of metastable phases in magnesium-titanium system by high-pressure torsion and their hydrogen storage performance, *Acta Materialia*, 50, 150-156, 2015.

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

K. Edalati, H. Emami, Y. Ikeda, H. Iwaoka, I. Tanaka, E. Akiba, Z. Horita, New nanostructured phases with reversible hydrogen storage capability in immiscible magnesium-zirconium system produced by high-pressure torsion, *Acta Materialia*, in press, 2016.

H. Emami, K. Edalati, A. Staykov, T. Hongo, H. Iwaoka, Z. Horita, E. Akiba, Solid-state reactions and hydrogen storage in magnesium mixed with various elements by high-pressure torsion: experiments and first-principles calculations, *RCS Advances*, 6, 11665-11674, 2016.

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*, 92, 46-54, 2015.

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 CO₂ emissions in energy, power, or industrial production processes. Projects in the division address the development of: (i) novel biological and biomimetic catalysts for H₂, CO₂, and H₂O 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:

A High-Valent Iron(IV) Peroxo Core Derived from O₂

Continuing our previous studies of the first functional biomimetic iron-nickel hydrogen-splitting catalyst reported in *Science* (339, n6120, 682-684, 2013), we are pursuing the production of a catalyst for the complementary oxygen-splitting cathode side of the cell. Dioxygen-tolerant [NiFe] hydrogenases catalyze not only the conversion of H₂ into 2H⁺ and 2e⁻ but also the reduction of O₂ to H₂O. Chemists have sought to mimic such bifunctional catalysts with structurally simpler compounds to facilitate analysis and improvement. This year, we are reporting a new [NiFe]-based catalyst for O₂ reduction via an O₂ adduct. Such catalyst for O₂-activation is a model for studying O₂-tolerant [NiFe] hydrogenases. Structural investigations reveal the first example of a side-on iron (IV) peroxo complex. Our next step is to further modify the hydrogen and oxygen splitting catalysts so they can be used in a working fuel cell. Realization of such a fuel cell is a crucial step toward making fuel cells affordable enough for real world applications. These results satisfy the short-term milestone of H₂-activation "Isolation of new hydrogenase and its model complex" in Project 1 of the Division. In addition, this result is the benchmark of the first biomimetic model catalyst of O₂-tolerant [NiFe] hydrogenase, presenting the first example of a side-on iron (IV) peroxo complex.

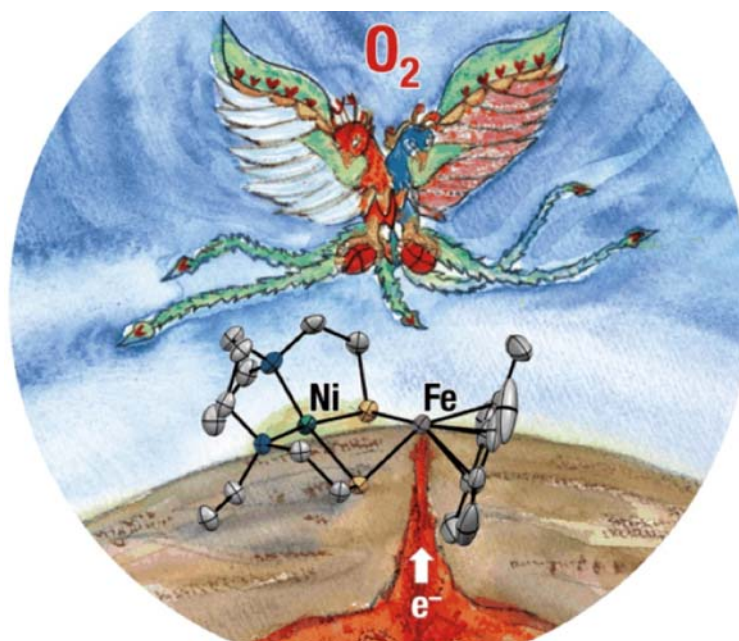


Fig. 1.9. A dioxygen-tolerant hydrogenase mimic to catalyze O₂ reduction. Selected for the back cover picture of *Angewandte Chemie International Edition (ACIE)*

Publication

T. Kishima, T. Matsumoto, H. Nakai, S. Hayami, T. Ohta, S. Ogo. *Angew. Chem. Int. Ed.*, 55(2), 724–727, 2016.

CO₂-free electric power generation via direct charge and discharge using the glycolic acid/oxalic acid redox couple

Efficient electric power generation from renewable-energy sources, such as through solar photovoltaics, wind turbines, and water waves, faces some difficult technological challenges due to the intermittent nature of these sources. Here, we demonstrate an electric power closed system technology that generates zero CO₂ emissions, and which is based on the glycolic acid (GC)/oxalic acid (OX) redox couple. Direct electric power storage in GC ensures considerable high energy density storage and good transportability through OX electroreduction with significantly high selectivity (>98%) using pure anatase-type titania (TiO₂) spheres under

mild conditions in the potential region of -0.5 to -0.7 V vs. the reversible hydrogen electrode (RHE) at 50 °C. The most desirable characteristic of this electroreduction is the suppression of hydrogen evolution even in acidic aqueous media (Faraday efficiency of 70–95%, pH 2.1). We successfully generated power without CO₂ emissions via selective electrooxidation of GC with an alkaline fuel cell.

Last year, we succeeded in generating power without CO₂ emissions using a direct ethylene glycol alkaline fuel cell, as reported in *Sci. Rep.* (4, 5620, 2014). This year, we managed to directly charge electric power into glycolic acid, an alcoholic compound to generate electric power using a direct glycolic acid alkaline fuel cell without CO₂ emissions, which is the first demonstration of CO₂-free power generation using a liquid energy carrier. This accomplishment is directly related to our long-term milestone "Power generation without CO₂ emissions" in the division's roadmap for Project 2.

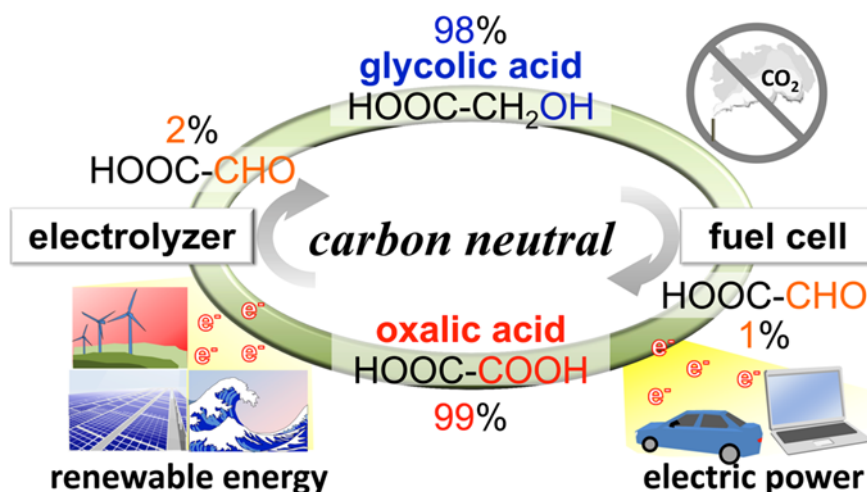


Fig. 1.10. Schematic of a carbon-neutral energy generation cycle by highly selective electrocatalysis using the glycolic acid/oxalic acid redox couple.

Publication

R. Watanabe, M. Yamauchi, M. Sadakiyo, R. Abe, T. Takeguchi, *Energy Environ. Sci.*, 8, 1456-1462, 2015.

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

The objective of this division is to develop: (i) highly efficient materials for CO₂ separation in power generation and industrial processes; and (ii) 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 CO₂ separation*, the objective is to develop novel membrane technology to separate CO₂ 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 CO₂ 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:

Optimizing the gas diffusion electrodes for electroreduction of CO₂ to CO

With the extensive research on the cathode catalysts, mass transport limitations are becoming a

challenge to high throughput electroreduction of CO₂ to CO. Gas diffusion electrodes (GDEs) -

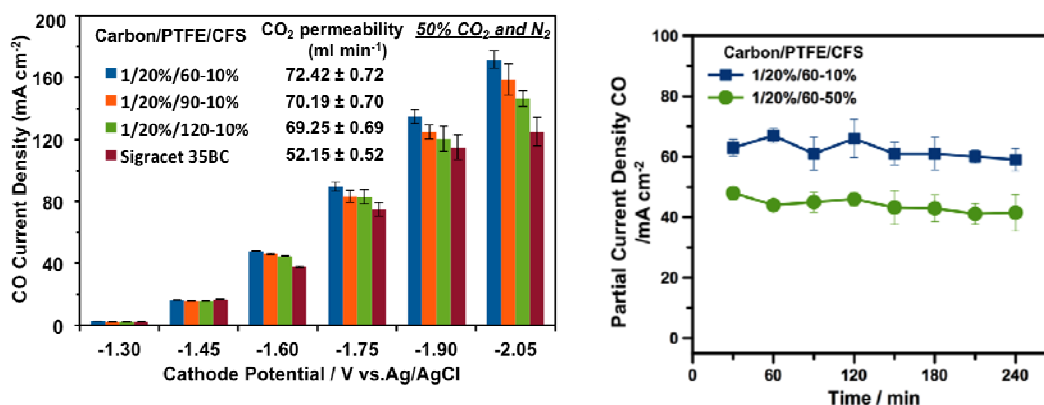


Fig. 1.11. (left) Partial current density for CO as a function of different potentials for GDEs with different thickness of CFSs with mixture of 50% CO₂/50% N₂ (left), and (right) partial current density for CO as a function of time when using GDEs with 10% and 50% wet proof level of CFSs over a total of 4h.

consisting of a carbon fiber substrate (CFS), a micro porous layer (MPL), and a catalyst layer (CL) have been used to improve mass transport of the reactants and products to and from the electrodes in electroreduction of CO₂. However, GDEs have not been optimized explicitly for the electroreduction of CO₂. In this project, we studied the effect of the MPL and CFS composition on cathode performance in electroreduction of CO₂ to CO. We determined that an optimum level of hydrophobicity of the MPL with 20 wt% polytetrafluoroethylene (PTFE), an optimum level of wet proof level of the CFS (10 wt% PTFE), and an optimum thickness of the CFS which is used as a commercial product of Toray-60 with a thickness of 190 μm. GDEs with this optimal composition lead to partial current densities for CO production as high as 280 mA cm⁻² at a cathode potential of -2.2 V and thus outperform commercially available GDEs. These optimized GDEs also exhibit no decay in performance during continuous operation for 4h. Furthermore, the enhanced cathode performance is more significant when using the dilute feed (50-50 CO₂ and N₂) due to improved CO₂ diffusion with the use of optimized GDEs. One of the short-term milestones in the division's roadmap for Project 2 is to improve "electrode structure for high current densities" for CO₂ reduction. This work demonstrates that in comparison to commercially available GDEs the optimized GDEs lead to an enhancement in cathode performance of up to 13% and 30% with the use of 100% CO₂ and dilute feed (50-50 CO₂ and N₂), respectively. In ongoing work, incorporation of carbon nanotubes (CNTs) into GDEs is being studied to improve electrode performance and durability. CNTs in CLs can lead to partial current density for CO as high as 350 mA cm⁻². Also, adding CNTs in MPLs helps to fabricate crack-free and PTFE-free MPLs.

Publication

B. Kim, F. Hillman, M. Ariyoshi, S. Fujikawa, and P. J. A. Kenis, Effects of composition of the micro porous layer and the substrate on performance in the electrochemical reduction of CO₂ to CO, Journal of Power Sources, 312, 192-198, 2016.

Development of CO₂ separation membranes over H₂

In pre-combustion CO₂ capture by membranes, the larger CO₂ molecule has to be separated from the smaller H₂ molecule. Our division targets in CO₂ separation over H₂ are shown in Table 1. Because the size of H₂ molecule is smaller than that of CO₂, a simple size-sieving separation membrane is not effective for CO₂/H₂ separation. Chemical interaction between CO₂ gas and membrane materials should be utilized for preferential CO₂ permeation across the membrane.

Table 1: Comparison of CO ₂ separation performance over H ₂			
	Permeance/GPU ¹	Selectivity	CO ₂ partial pressure [MPa]
Division Target	100	30	1.0
I²CNER (PAMAM in PEG²)	97	30	0.05

¹GPU = 7.5 × 10⁻¹² m³(STP)/(m² s Pa) (STP: Standard Temperature and Pressure)
²PEG: Polyethylene glycol

We have focused on amine compounds as CO₂-interacting agents to elevate the solubility in the membranes. Poly(amidoamine) (PAMAM) has been mainly used to prepare the CO₂ separation membranes by Prof. Taniguchi, and the CO₂ separation properties with a 330 nm in thickness at ambient conditions are listed in Table 1. Our current accomplishments on CO₂ permeance and selectivity are 97 and 30 respectively and these values are almost right on our division's roadmap targets, 100 for permeance and 30 selectivity. Our next target is to elevate the gas pressure because the real-world pressure for CO₂/H₂ separation, especially in the IGCC (Integrated Coal Gasification Combined Cycle) processes, is around 1MPa.

Publication

I. Taniguchi, T. Kai, S. Duan, S. Kazama, H. Jinnai, A compatible crosslinker for enhancement of CO₂ capture of poly(amidoamine) dendrimer-containing polymeric membranes, *Journal of Membrane Science*, 475, 175-183, 2015.

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 CO₂ to help ensure safe and permanent CO₂ 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 CO₂ injection in aquifer formations, and the requirement for long term monitoring of pressure variations near seismogenic faults. Selected representative results include:

On suitable reservoir conditions for effective and safe CO₂ storage

The CO₂ behavior and saturation in the storage reservoir is influenced by many reservoir parameters, including the viscosity and density of the fluids, interfacial tension, pore structure, and other porous medium characteristics (e.g., wettability and surface roughness). Therefore, it is a challenging task to identify suitable conditions for CO₂ storage.

To this end, we calculated non-wetting phase fluid (CO₂) displacements in 3D natural sandstone under various conditions using two-phase lattice Boltzmann (LB) simulations, and characterized the influence of reservoir conditions upon the non-wetting fluid (CO₂) - water flow behavior (Fig. 1.12a). The results of simulations under various reservoir conditions were used to classify the resulting two-phase flow behaviors into three typical fluid displacement patterns on the diagram of capillary number, $Ca = \mu_{nw} V_{nw} / \sigma$, and viscosity ratio, $M = \mu_{nw} / \mu_{water}$, where V_{nw} is the velocity of the non-wetting phase (CO₂), σ is the interface energy, and μ_{nw} and μ_{water} are the viscosities of the non-wetting phase and water, respectively. In addition, the non-wetting

phase saturation S_{nw} was calculated and mapped on the $Ca-M$ diagram (background color on the $Ca-M$ diagram). For CO_2 storage, we must consider the domain of $M < 1$ (or $\log M < 0$; red rectangle area in Fig. 1.12b), because the viscosity of CO_2 at reservoir-relevant conditions is lower than that of water. These results demonstrated that CO_2 saturation is controlled by both Ca and M , and the optimum CO_2 saturation scales with Ca and M (Fig. 1.12b). When we applied similar analysis to a simplified type of porous medium (2D homogeneous model in Fig. 1.12c), we found that CO_2 saturation and behavior are significantly different (Fig. 1.12d). These important differences between two-phase flow in 3D natural rock and in 2D homogeneous media could be due to the heterogeneity of pore geometry in the natural rock and differences in pore connectivity. By quantifying CO_2 behavior in the target reservoir rock under various conditions (i.e. saturation mapping on the $Ca-M$ diagram), our approach provides useful information for investigating suitable reservoir conditions for effective CO_2 storage (e.g., high CO_2 saturation).

This effort directly addresses the short- and mid-term milestones of Project 2 of the Division (Pore-scale CO_2 investigation), specifically the milestones: (i) Model injected CO_2 behavior (residual, solubility and mineral trapping; short-term); (ii) Increase storage capacity and security by enhanced residual and solubility trapping (mid-term). Lastly the work was done under international collaboration between Kyushu University and the University of Notre Dame.

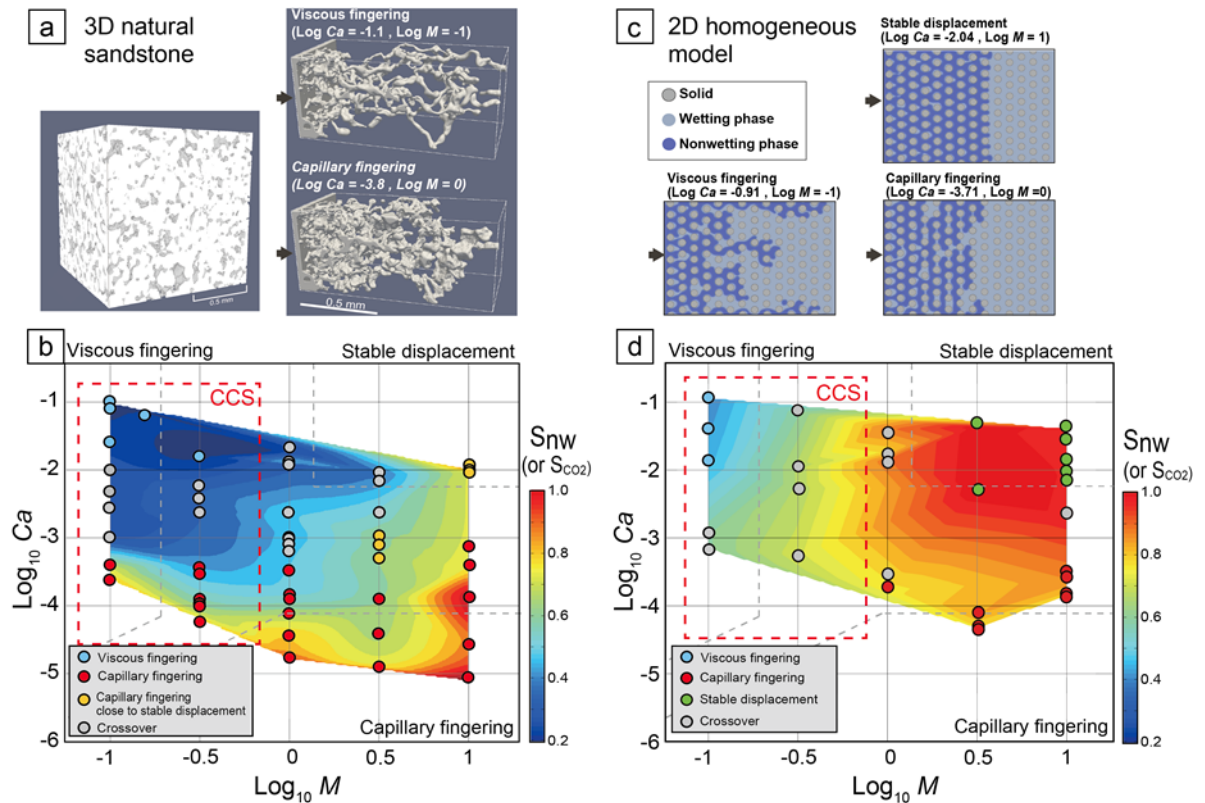


Fig. 1.12. (a) Left panel shows the 3D pore geometry (digital rock model) of a natural sandstone sample. Right panel shows two types of simulated behavior for the nonwetting phase (CO_2) in the 3D natural sandstone: viscous fingering and capillary fingering regimes; (b) Plot of the simulated displacement pattern (colored dots) and CO_2 saturation (background color) under various flow capillary numbers and viscosity ratios. The CO_2 infiltration behavior (i.e., that of the nonwetting phase) can be classified as primarily capillary fingering (red dots) or viscous fingering (blue dots), with little in the way of stable displacement. The gray dots indicate the crossover state, which cannot be classified as predominantly one of the 3 typical displacement patterns (meaning it is likely a combination of displacement patterns). The background color shows the saturation levels of the nonwetting, CO_2 phase S_{nw} (or S_{CO_2}). For CO_2 storage, the domain of interest is $M < 1$ (or $\log M < 0$; red-dashed rectangle); (c) Nonwetting phase behavior in a 2D homogeneous pore model at various flow conditions: viscous fingering, stable displacement, and capillary fingering regimes. (d) Plot of the displacement pattern and the nonwetting phase saturation for the 2D homogeneous model. Green dots indicate the stable displacement regime, which cannot be identified in the simulations for

the natural sandstone(Fig. b).

Publications

T. Tsuji, F. Jiang, K. T. Christensen, Characterization of immiscible fluid displacement processes with various capillary numbers and viscosity ratios in 3D natural sandstone, *Advances in Water Resources*, doi:10.1016/j.advwatres.2016.03.005, 2016.

F. Jiang and T. Tsuji, Numerical investigations on the effect of initial state CO₂ topology on capillary trapping efficiency, *International Journal of Greenhouse Gas Control*, 49, 179-191, 2016.

Y. Yamabe, T. Tsuji, Y. Liang, T. Matsuoka, T., Lattice Boltzmann simulations of supercritical CO₂-water drainage displacement in porous media: CO₂ saturation and displacement mechanism, *Environmental Science & Technology*, 49, 537–543, 2015.

Dynamics of CO₂ behavior in natural pore space

We have developed methodologies to overcome a lack of experimental data regarding the flow dynamics of CO₂ and water transport in porous media (i.e., rock), specifically at reservoir conditions (pressure and temperature) and in porous media that reflects the complexity of rock found in candidate geologic storage sites in Japan.

To assess the flow dynamics of CO₂ and water transport in heterogeneous porous media at reservoir conditions, we developed a unique high-pressure visualization measurement protocol using the microscopic particle image velocimetry (PIV) method in concert with fluorescent microscopy to quantify the flow of CO₂ and water in 2D porous micromodels. The micromodels are fabricated in silicon and placed in an overburden pressure cell that allows us to achieve reservoir-relevant conditions (>80 bar pressure and a range of temperatures) in the 2D porous micromodels. Optical access is provided to the porous flow through the pressure cell and a dual-camera system is used to acquire high-frame-rate imaging of both the water (seeded with fluorescent tracer particles) and CO₂ (tagged with a fluorescent dye) phases whereby spectral separation is used to isolate the two fluorescent signals and allow separate imaging on high-resolution image sensors. PIV methods are used to calculate the instantaneous water velocity fields from the movement of the tracer particles in the water phase (Fig. 1.13), while the instantaneous spatial configuration of the CO₂ is elucidated from the fluorescent emission of the CO₂ dye. We have made extensive measurements in homogeneous micromodels and are presently conducting experiments in heterogeneous micromodels that mimic the porous nature of rock relevant to geologic storage of CO₂. Our results highlight the unsteady and dynamic nature of flow within the rock pore structure, particularly dominant and preferential flow paths formed during bursting flow processes termed Haines jumps. During these events, we find the velocity of the CO₂ front to be more than 60 times larger than the bulk velocity, and thus the local Reynolds number well exceeds the applicability limits of Darcy's law. Furthermore, we observed individual CO₂ fingers with high velocity often displace water over a very large area of the micro model consisting of tens of pores. Thus, water flow driven by the CO₂ finger advancement is correlated across many neighboring pores. Conventional pore network models, for example, may not account for such effects. Lastly, this dynamic bursting phenomenon by which the CO₂ advances through the pore structure plays a defining role in how efficient the CO₂ infiltrates the rock and thus must be accounted for within pore-scale models in larger-scale numerical simulations.

This effort directly addresses the short- and mid-term milestones of Project 2 in the division's roadmap (Pore-scale CO₂ investigation), specifically the milestones: (i) Model injected CO₂ behavior (residual, solubility and mineral trapping; short-term); (ii) Increase storage capacity and security by enhanced residual and solubility trapping; mid-term).

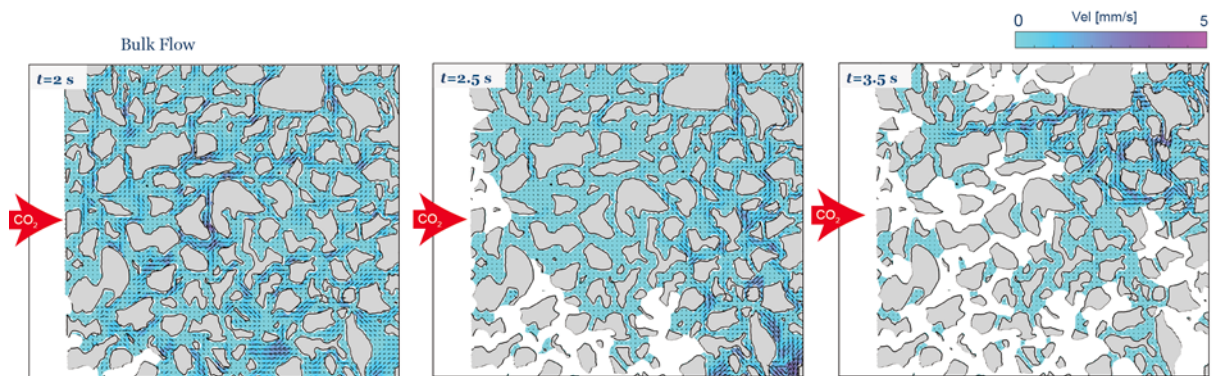


Fig. 1.13. CO₂ migration within a water-saturated micromodel. The micromodel is fabricated with a heterogeneous pore structure inspired by thin samples of a sandstone from the CCS injection site in Decatur, Illinois, USA. Color indicates the velocity magnitude of water movement (see color bar), the CO₂ is white and the porous grains of the micromodel are shown in gray.

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*, 18, 1391-1406, 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*, 51, 3017-3029, 2015.

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*, DOI: 10.1016/j.advwatres.2015.05.011, 2016.

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:

Next-generation high-strength, low-cost alloy for hydrogen service

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.

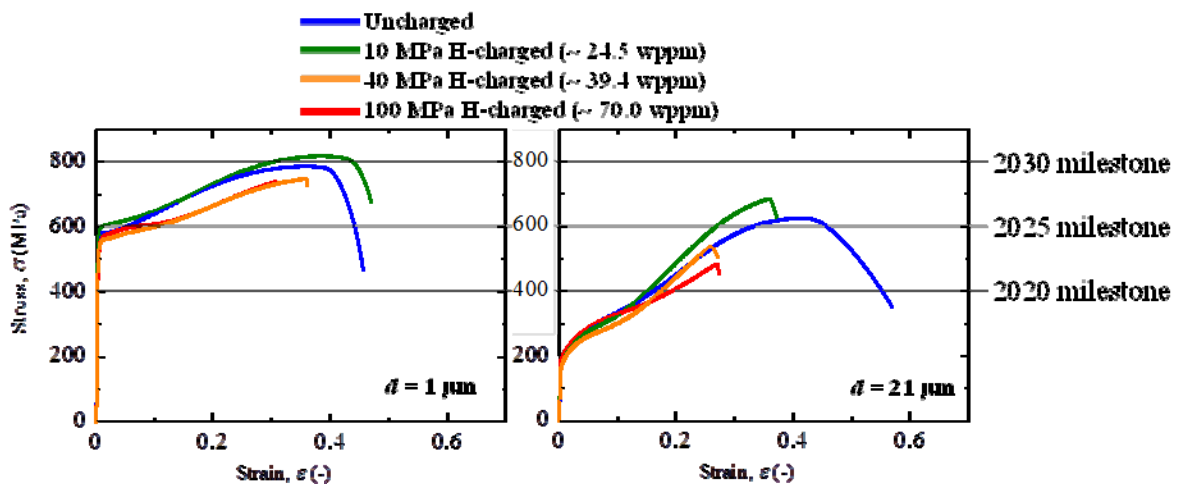


Fig.1.14. Tensile stress vs. strain data for the low-cost austenitic stainless steel Fe-16Cr-10Ni with ultra-fine grain size ($d = 1 \mu\text{m}$) and conventional grain size under hydrogen exposure conditions from 10 MPa to 100 MPa.

The achievements described below represent progress toward the ultimate target of commercially viable austenitic stainless steel with strength comparable to ferritic steels (e.g., 800 MPa), cost-competitive with alloy 304, and acceptable durability for fuel cell vehicles or fueling stations. This ultimate target is featured in Project 2: High-Strength, Low-Cost Stainless Steels for H_2 Service.

Through the process of synthesizing ultra-fine grains in austenitic stainless steel, a yield strength level of 600 MPa has been attained in the low-cost alloy Fe-16Cr-10Ni (Fig. 1.14), satisfying the mid-term milestone for Project 2. During this reporting period, the hydrogen compatibility of ultra-fine grained (UFG) Fe-16Cr-10Ni alloy was characterized by exposing tensile specimens to 100 MPa hydrogen gas (well above the pressure for actual hydrogen systems). Although this extreme hydrogen-exposure condition reduced the tensile ductility relative to the value in inert conditions, its absolute value (approximately 30%) is comparable to those for commercial alloys under hydrogen service conditions. Figure 1.14 shows the measured stress vs. strain data for a conventional grain size ($21 \mu\text{m}$) and ultra-fine grain size ($1 \mu\text{m}$) in the Fe-16Cr-10 Ni alloy with several hydrogen contents (no hydrogen as well as exposure to 10 MPa, 40 MPa and 100 MPa hydrogen gas). This result is extremely important as it shows that metastable austenitic alloys with cost similar to SUS304 can be manufactured with high strength and acceptable hydrogen compatibility by applying a commercially viable material-processing method.

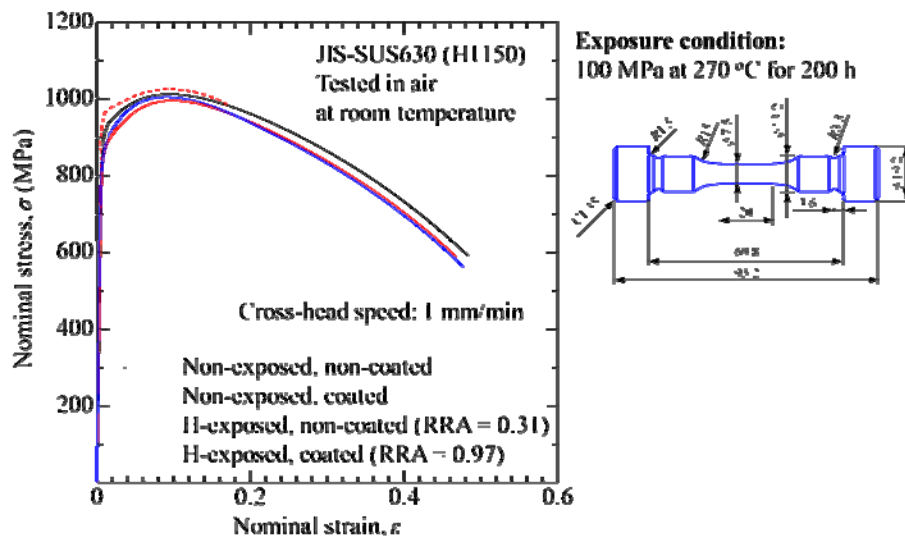
Based on previous experience applying UFG processing, the high yield strength of the UFG Fe-16Cr-10Ni alloy was expected, however the hydrogen compatibility of this metastable alloy was a relative surprise, since such metastable austenitic alloys (e.g. SUS304) are expected to suffer more from hydrogen-induced degradation than stable austenitic alloys (e.g. SUS316).

Publication

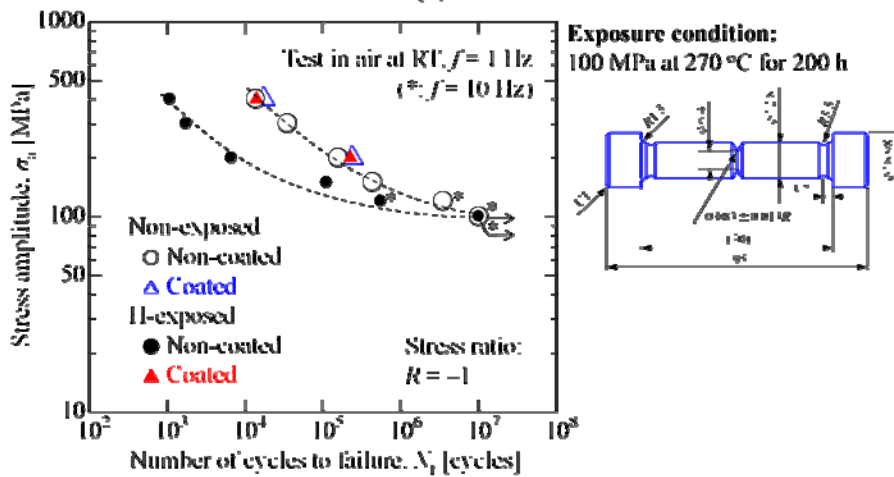
A. Macadre, N. Nakada, T. Tsuchiyama, and S. Takaki, Critical grain size to limit the hydrogen-induced ductility drop in a metastable austenitic steel, *International Journal of Hydrogen Energy*, 40, 10697-10703, 2015.

Barrier coatings: an alternative to synthesizing new alloys for hydrogen service

The achievements described below represent progress toward the milestone of develop and evaluate durable surface coating that resists hydrogen permeation at 100 MPa pressure. This short-term milestone is featured in Project 2: High-Strength, Low-Cost Stainless Steels for H_2 Service.



(a) Tensile test



(b) Fatigue-life test

Fig. 1.15. Tensile and fatigue-life tests of hydrogen-exposed and non-exposed specimens with and without the developed barrier coating (substrate: JIS-SUS630). The tensile and fatigue-life tests were performed in air at room temperature (RT). The specimens were exposed to high-pressure hydrogen gas at 100 MPa and 270 °C for 200 hours.

In addition to synthesizing new high-strength, low-cost alloys that are compatible with hydrogen, Project 2 focuses on technologies such as barrier coatings that inhibit hydrogen uptake into materials. These barrier coatings can be applied to improve the hydrogen compatibility of commercial steels, thus enabling a broader range of currently available high-strength, low-cost alloys to be considered for hydrogen service. Many studies have characterized barrier coatings in a low-pressure hydrogen gas environment (< 1 MPa), however coatings with high performance in high-pressure hydrogen gas (e.g. 100 MPa) have not been developed.

In previous reporting periods, an aluminum-based multilayer surface coating (consisting of alumina, aluminum and Fe-Al) with excellent resistance to hydrogen permeation was developed from investigations in 100 MPa hydrogen gas. It was also discovered that the hydrogen barrier characteristic of the developed coating was attributed to hydrogen trapping at the interface between the Al and Fe-Al layers based on analysis of local hydrogen concentrations by secondary ion mass spectroscopy (SIMS). This hydrogen-trapping function of layer interfaces

has not been reported in other studies of barrier coatings.

In this reporting period, tensile and fatigue properties of hydrogen-exposed, coated specimens were measured. A high-strength martensitic stainless steel (JIS-SUS630), which is known to suffer severe hydrogen-induced degradation, was used as a substrate. Surprisingly, tensile tests of smooth, round-bar specimens and fatigue-life tests of circumferential notched specimens clarified that the relative reduction in area and the fatigue life of the coated steels were not degraded by hydrogen, in contrast to the non-coated specimens (Fig.1.15). These results demonstrate that barrier coatings may offer a viable pathway to deploying high-strength, low-cost steels for hydrogen service.

Publication

J. Yamabe, T. Awane, and S. Matsuoka, Elucidating the hydrogen-entry-obstruction mechanism of a newly developed aluminum-based coating in high-pressure gaseous hydrogen, International Journal of Hydrogen Energy, 40, 10329–10339, 2015.

Energy Analysis (Acting Division Leader: Prof. Itaoka)

This division plays a critical role in I²CNER. It is responsible for providing carbon emission, energy efficiency, and cost analysis of current and emerging I²CNER and other energy processes, technology, and infrastructure. These analyses help ensure that I²CNER'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 I²CNER and other energy system analyses.

Probability analysis of I²CNER's scenarios

An approach to determining the accuracy of our predictions of the level of carbon emissions reduction in our scenarios is to consider the impact of the development of new technologies on meeting emissions goals. To quantitatively evaluate the probability at which new technology development and deployment will enable the targeted greenhouse gas (GHG) emissions reduction, we estimated probability distribution functions of GHG emissions reduction amounts in 2050 as follows: For each selected important technology, future development of key parameters are projected assuming that they would be developed as existing similar technologies. Probability distributions of key parameters varied depending on the technology category.

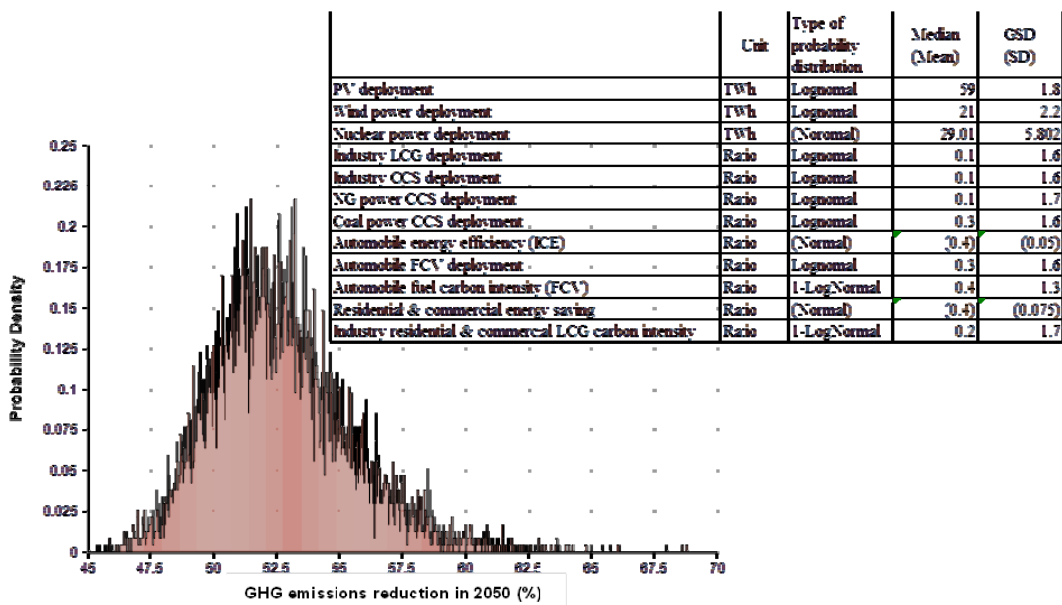


Fig. 1.16. Monte Carlo simulation results for the probability of GHG emissions reduction in 2050 under the assumption that development of important technologies takes place with probability distributions whose mid-values reflect continuation of current efforts. LCG denotes low carbon town gas containing low carbon methane and/or hydrogen produced from renewable energy--Power to Gas concept--and GSD and SD

denote geometric standard deviation and standard deviation, respectively. The term "Ratio" in the "unit" column denotes the percentage of technology penetration into the targeted application. It is remarkable that the probability density around 70% emissions reduction is very low implying an urgent need for technology breakthroughs.

For example, the increase of automobile fuel efficiency with an internal combustion engine is classified as a mature existing technology having a narrow range of parameter variation with an assumed normal probability distribution. On the other hand, wind power deployment is classified as a new technology whose deployment is having a wide range of parameter variation with a possibility of an extreme value, and it was thus assumed to have a lognormal probability distribution. Preliminary analysis on probability distribution of GHG emissions reduction in Japan by 2050 was conducted using Monte Carlo simulation (Fig. 1.16) followed by rank order correlation analyses (importance analyses) on the results of the Monte Carlo simulation (Fig. 1.17).

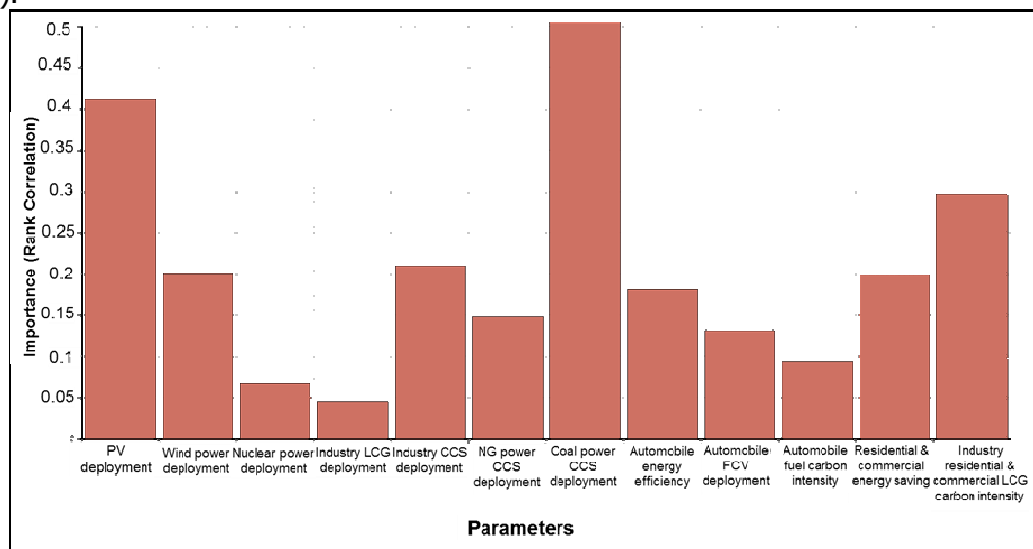


Fig. 1.17. Importance analysis of technology development: Rank order correlations of GHG emission reductions and technology development for the Monte Carlo simulations shown in Fig.1.16

Our results reveal that it is very unlikely that Japan will achieve 70-80% emissions reduction by 2050 by relying upon the current efforts that focus on gradual development of technologies that improve efficiency and lower carbon intensity in conjunction with gradual deployment of new technologies. I²CNER's scenarios can be interpreted as the cases of a combination of extreme values in the probability distribution of the key parameters. They must appear around the right end of the horizontal axis of Fig. 1.16. Breakthroughs in technology development, which I²CNER's scenarios assume, should realize the extreme values of the key parameters. In addition, our results revealed that technology development to accelerate deployment of CCS in coal power generation and PV is very important. This approach allows the identification of the impact of technology breakthroughs as well as the technologies which are most likely to contribute substantially to meeting the emission reduction goals.

Publication

K. Itaoka, S. Kimura, K. Okamura and A. Arai, Energy technology analyses for deep GHG emission reduction by 2050 in Japan, Paper presented at the Annual Conference 2014 of the Society for Environmental Economics and Policy Studies, Machida, Tokyo, Japan, Sep 13-14, 2014.

Investigation of optimum deployment of hydrogen refueling stations in Japan's metropolitan areas

The objective of this study was to develop an effective model for domestic hydrogen station deployment and identify prospective areas for hydrogen station locations in order to meet the refueling demand that will be driven by fuel cell vehicles. (FCV). Proper hydrogen station

placement is currently critical for stimulating the FCV demand in the market areas. We examined deployment models using GIS (geographic information system) analysis to consider user convenience and FCV penetration phases. To run the models, we assumed that potential FCV customers were current high-priced luxury car (over 5 million yen) owners. Based on our model results, we concluded that the most effective approach was to locate the hydrogen stations in a way that minimizes average distance between potential customers and nearest hydrogen stations. The respective model yielded the most suitable location of the refueling stations to serve potential customers (Fig. 1.18). Our modeling also identified the difference in location between the existing /planned hydrogen stations and the optimum layout by our study and suggested the most appropriate sites of the stations. The model demonstrated that more hydrogen stations need to be located in internal city locations especially in every prefectural capital. Our analysis also identified the important metropolitan areas which are not covered by the existing/planned stations and are in need to be covered by new stations.

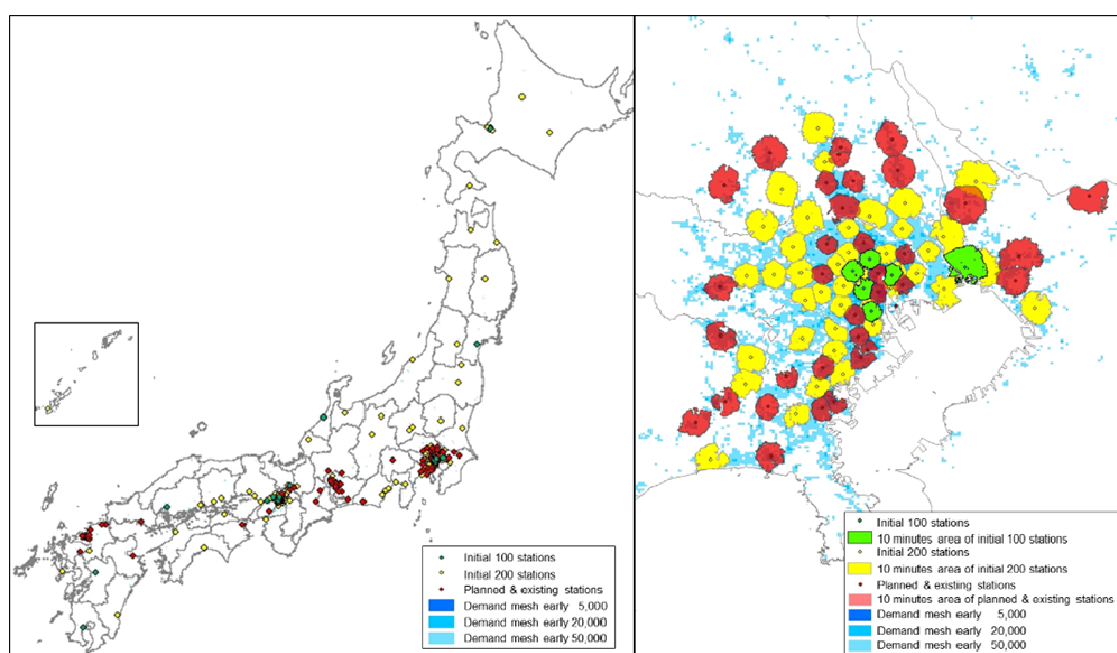


Fig. 1.18. Red dots and red areas show existing/planned station sites and their 10 minute driving radiuses. The additional stations that will be created, bringing the total of initial stations to 100, are indicated by green dots, and their 10 minute driving radiuses are indicated by green areas. The additional stations in the initial 100 to 200 stations and their 10 minute driving radiuses are indicated by yellow dots and yellow areas. The early 5000 customers are represented by blue areas. The additional 15000 customers, which will bring the total to 20000 early customers, are represented by light blue areas. Lastly, the additional 30000 customers, which will bring the total to 50000 early customers, are represented by pale blue areas.

Publications

K. Itaoka, Methodology development to find potential locations of hydrogen refueling station in Japan, Paper presented at the 6th World Hydrogen Technologies Convention (WHTC), Sydney, Australia, Oct 11-14, 2015.

K. Itaoka, S. Kimura, and A. Arai, Deployment analysis of hydrogen stations for FCEVs in Japan, submitted to International Journal of Hydrogen Energy.

2. Advancing fusion of various research fields

The Director has at his disposal the "I²CNER Competitive Funding" which is intended to foster and advance interdisciplinary research. The Director considers the overall progress and activities of each of I²CNER's full time researchers when making decisions about how to allocate these funds. 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 response to the recommendation by JSPS that I²CNER expand beyond engineering into different academic fields, such as mathematics or social sciences, in FY2015, the I²CNER Director decided to utilize the competitive fund to support the Institute's new initiative on Applied Math for Energy. The FY2015 competitive fund call for proposals was open to all faculty of Kyushu University, provided that they proposed a project which was relevant to the stated objectives of I²CNER's Applied Math Initiative. The Institute received several proposals in response to the call, including joint proposals between I²CNER-KU faculty and a few by KU faculty outside of I²CNER. After rigorous screening by the IPRC, 5 applications have been selected as "seed projects," the idea being to foster close, ongoing collaboration between I²CNER and other KU units, in particular, the Institute of Mathematics for Industry (IMI).

The applications that were awarded are:

- i) Prof. S. Managi, "Global energy economy modeling: welfare analysis considering environment," Department of Urban and Environmental Engineering.
- ii) Prof. J. Murata, "Design of Demand Response Programs Using Inverse Optimization," Department of Electrical Engineering.
- iii) Prof. T. Tsuji, "Characterization of heterogeneous rock pore structure using persistent homology: Insight into scale dependence of hydrological and elastic properties," I²CNER. (In collaboration with PI Christensen, University of Notre Dame).
- iv) Prof. D. Triadis, "Anomalous diffusion in realistic pore-scale simulations of two-phase flow for geologic CO₂ sequestration" IMI, Australia Branch, Trobe University.
- v) Prof. R. Nishii, "Statistical analysis of global gene expression data and applications to plant growth," IMI.

The progress of the interdisciplinary projects that were selected in FY2014 was assessed carefully in FY2015, including 1 progress presentation before all of I²CNER by each researcher who received funds, and 1 individual meeting with the Director. After careful consideration of the progress that was made in previously selected projects in FY2012-FY2014 (only 3 publications that were published as a result of these projects were truly interdisciplinary), it is the goal of the Director to award competitive funds only to those researchers who make a truly exceptional proposal, and to award the funds in slightly larger "chunks" to fund overall fewer projects per year on a moving forward basis. The FY2015 projects on Applied Math will be evaluated by the IPRC in FY2016.

A joint I²CNER-AIMR workshop was organized Associate Prof. A. Staykov at I²CNER on Sept. 2, 2015. The purpose of the workshop was to bring together researchers at the postdoctoral, assistant professor, and associate professor levels who are involved in top-level interdisciplinary research on carbon materials and nanographenes so that they could exchange information and experiences on the synthesis, application, catalysis, and development of novel experimental and theoretical techniques. The workshop addressed four thematic areas: synthesis of nanographene materials, presented by Associate Professor S. Lyth (I²CNER) and Assistant Professor P. Han (AIMR); organic chemistry, presented by Assistant Professor M. Watanabe (I²CNER) and Assistant Professor M. Nishihara (I²CNER); physical properties of carbon nanomaterials, presented by Dr. B. Cuning (I²CNER) and Dr. T. Bayer (I²CNER); theory of carbon nanomaterials, presented by Assistant Professor D. Packwood (AIMR) and Associate Professor A. Staykov (I²CNER). The workshop, which was attended by many researchers from I²CNER and Kyushu University, led to active and robust discussions and novel projects, among which were the successful KAKENHI grant application of Dr. Han (AIMR) and Dr. Watanabe (I²CNER) and the long-term theoretical collaboration between Dr. Packwood (AIMR) and Dr. Staykov (I²CNER).

At the moment, Dr. Staykov and Dr. Packwood are working on the organization of a similar workshop in 2016, which will include participants from I²CNER, AIMR, and iCeMS. This year's workshop will focus on the development of novel experimental and theoretical methods and

their application in materials science. The workshop will take place at I²CNER and will again target young researchers at the postdoctoral, assistant professor, and associate professor levels.

The 2016 I²CNER Annual Symposium, which was titled "Computational Solutions to Fundamental Problems in Carbon-Neutral Energy Research," was held in order to i) bring together experts from the computational and experimental community, and ii) discuss and converge upon the most critical needed advances in computation relevant to the mission of I²CNER, with the overarching goal being to accelerate the transition from basic science to orders of magnitude improvements in performance through coupling of computational modeling and key experiments (fusion). The workshop focused on 5 subthemes: "Molecule/Surface Interactions," "Transport of Ions Through Solids and High Temperature Modeling," "Molecule/Molecule Interactions – Charge Transfer and Chemical Reaction Dynamics," "Linking of Atomistic to Continuum Scales," and "Pore-scale Flow Processes." The deliverable of the symposium was a "Basic Needs" report on computation in I²CNER, which will be used to guide future initiatives/investments related with computation and how it can inform I²CNER's existing research themes.

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

- i) Molecular Photoconversion Devices: We demonstrated for the first time that isolated dopant atoms embedded into titania can function as co-catalysts for the photocatalytic production of hydrogen gas. This work uses an *integrated approach that couples chemical synthesis, atomic resolution microscopy, and first-principles modeling* to elucidate how isolated dopant atoms promote hydrogen production, yielding production rates that can be as much as ten times as large as undoped systems. In a collaborative effort, experiments at Kyushu University that were interpreted by modeling at the University of Illinois have demonstrated an improved photoelectrode design yielding water oxidation without an applied voltage and improved stability. The approach of coating Earth-abundant CaFe₂O₄ with a very thin layer of TiO₂ yields a photoelectrode sensitive to the highest intensity portion of the solar spectrum, potentially significantly enhancing artificial photosynthesis efficiency (*solid state physics, electronic behavior of materials, and electrochemistry*).
- ii) Electrochemical Energy Conversion: Understanding complex chemo-mechanical relationships is crucial for understanding and avoiding failures in any solid-oxide-cell-based electrochemical devices. The elucidation of the mechanism of how electronic conductivity is controlled and minimized mechanically in graphene oxide is the most outstanding demonstration of mechano-chemical effect accomplished this year (*electrochemomechanics*).
- iii) Thermal Science and Engineering: The Miljkovic and Takata research groups are unlocking the fundamental mechanisms of contaminating atmospheric hydrocarbon adsorption on solid surfaces through time resolved X-Ray Photoelectron Spectroscopy (XPS), Time of Flight Secondary Ion Mass Spectroscopy (TOF-SIMS), and Low Energy Ion Scattering (LEIS) in order to characterize the chemistry (molecules and structure) of the adsorbed hydrocarbons, which has not been done before (*Chemistry, electrochemistry, materials science, electrical engineering, physics, and mechanical engineering*).
- iv) Hydrogen Storage: A novel synthesis method of borohydrides has been developed and various dodecaborates with improved ionic conductivity were synthesized and successfully used as a solid-state super ionic conductor for an all-solid rechargeable battery (*Synthetic chemistry, crystallography, spectroscopy, hydrogen storage and electrochemistry*).
- v) Catalytic Materials Transformations: The investigation of the crystal structure of the type 2 [NiFe]-hydrogenase from *Citrobacter sp. S-77*, which has a novel functional mechanism having O₂-tolerant and high H₂-activation potential, by PI Ogo is the first in the world. Understanding the crystal structure of the naturally occurring enzyme that we found in the type 2 hydrogenase opens new pathways to the design of new synthetic model catalysts having both O₂ tolerance and high H₂-activation potential.
- vi) Catalytic Materials Transformations in collaboration with CO₂ Capture and Utilization: Use of Cu catalysts with large surface roughness resulted in a combined Faradaic efficiency (46%) for the electroreduction of CO₂ to ethylene and ethanol in combination with current densities of

$\sim 200 \text{ mA cm}^{-2}$. This is a 10-fold increase in performance relative to the levels reported prior to this work and is achieved at an overpotential ($< 0.7 \text{ V}$) that is the smallest reported in the literature (*Materials chemistry, electrochemistry, analytical chemistry, and chemical engineering*).

vii) CO₂ Storage: We have developed a novel monitoring method to quantify CO₂ saturation in reservoirs, based on hydrologic and elastic characteristics of the reservoir rock. The method, which relies on a continuous and controlled seismic source, relates the CO₂ saturation with monitoring-derived seismic velocity. This monitoring system is currently deployed in an ongoing CO₂ sequestration project at a coal-fired power plant in Saskatchewan, Canada. (*Earthquake science (seismology) and exploration geophysics*).

viii) Hydrogen Materials Compatibility: State of the art microstructural observations led to the realization that the hydrogen-induced quasi-cleavage fracture of the commercially available 304 austenitic stainless steel used in high-pressure hydrogen service is caused by a synergistic effect of hydrogen-enhanced localized plasticity and hydrogen-enhanced decohesion with the assistance of hydrogen release from α' -martensite at transformation (mechanical metallurgy and electron microscopy). Quantitative insights into chemomechanical effects on intergranular cracking were obtained through a thermodynamic treatment of new surface creation accompanying fracture. Closed solutions for the work of fracture for the nickel system were derived for brittle fracture and surface segregation of solutes in the limit of a mean field approach (*Materials physics, solid mechanics, mechanical metallurgy*).

ix) Energy Analysis in collaboration with Catalytic Materials Transformations: We investigated greenhouse gas emissions through a life-cycle assessment of the carbon neutral cycle (CN cycle), in which oxalic acid is converted into glycolic acid using electricity, assuming that the glycolic acid is produced by wind power in west Australia and transported by oil tanker to Japan. The results show that the CN cycle emits less than 50% of the level currently emitted by the power grid (579g-CO₂/kWh in FY2014) and those emissions can be further reduced by increasing the efficiency of the production of glycolic acid by a polymer electrolyte alcohol electrosynthesis cell (*catalytic materials, reaction systems, and life-cycle assessment*).

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

Molecular Photoconversion Devices (Lead Principal Investigator: Prof. Ishihara)

Integrated Experimental and Theoretical Approach to Improved Hydrogen Production Catalysts in Two-Dimensional, Doped Titania Nanosheets

(Experiments in photochemistry, transmission electron microscopy, and first-principles atomistic computer simulations)

In this achievement, our team combined nanoscale synthesis, high resolution transmission electron microscopy, and computational chemistry to demonstrate a new approach to photocatalytic hydrogen production assisted by single atom co-catalysts embedded as dopants in two-dimensional doped titania nanosheets. In contrast to typical co-catalysts which are clusters of particles, high resolution transmission electron microscopy and scanning tunneling microscopy revealed that isolated Rhodium atom dopants incorporated into the titania nanosheets serve as co-catalysts that act as active sites for water oxidation and reduction. At optimal doping concentrations, the hydrogen production rate is increased by a factor of ten in comparison to the undoped sheets. Alongside the experimental measurements, atomistic first-principles simulations based on density functional theory reveal the mechanisms by which the isolated Rh dopants induce changes to the water molecule adsorption and dissociation energy landscape on the nanosheets. Motivated by this achievement, we have extended this work to map the full reaction mechanism of the oxygen evolution reaction (OER) on these nanosheets, both pristine and those containing transition metal dopants. Based on these insights, we further assessed the full spectrum of 3d, 4d, and 5d transition metals as candidate dopants for the experimentally synthesized nanosheets. Our work directly combines atomistic

computational modeling with experiments in water splitting chemistry on two-dimensional doped titania nanosheets, and to our knowledge is the first direct comparison of measured activity across a spectrum of dopant species to computational predictions. This accomplishment targets the short-term milestone 1 (energy conversion efficiency > 1%) of Project 2-1 “Water splitting with organic and inorganic composite” in the division’s roadmap.

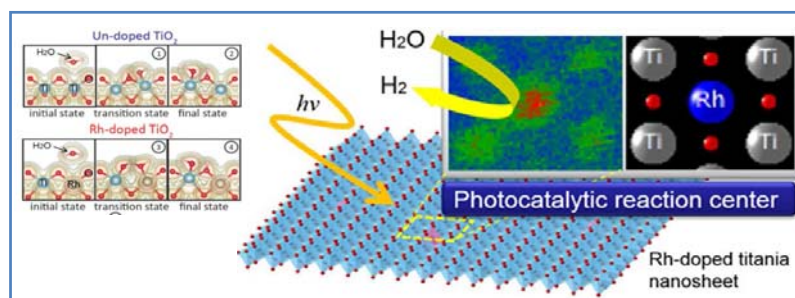


Fig. 2.1. Schematic of two-dimensional titania nanosheets with isolated Rh dopant atoms incorporated, and electronic charge density from simulations illustrating water molecule dissociation at the catalytic sites.

Publication

S. Ida, N. Kim, E. Ertekin, S. Takenaka, and T. Ishihara, Photocatalytic reaction centers in two-dimensional titanium oxide crystals, *Journal of the American Chemical Society*, 137(1), 239-244, 2015.

Combining modeling and experiment to improve photoelectrodes

(Solid state physics, electronic behavior of materials, and electrochemistry)

This achievement is related to Project 2-2 targeting the mid-term milestone “new concept” of Project 2 in the division’s roadmap. Earth-abundant materials such as CaFe₂O₄ (CFO) are attractive candidates for photoelectrodes because of their low cost and ease of handling. CFO is a p-type semiconductor that could serve as a photocathode for artificial photosynthesis but it suffers from two problems, it degrades during operation and the onset potential is too low to drive water oxidation. We have dramatically improved the performance of CFO photocathodes by coating the surface with TiO₂. This approach was developed based on a photoelectrochemical cell model developed at the University of Illinois and applied to the research being conducted at Kyushu University. Based on the simulation results from the Rockett group, researchers led by Shintaro Ida and Tatsumi Ishihara were able to dramatically improve the electrode performance. The TiO₂ coating protects the CFO surface while at the same time it reduces recombination of photogenerated carriers at the surface. The experiments showed reduced performance under UV photons that stimulated the TiO₂ but the model demonstrated that improved performance could result if longer wavelength photons excite only the CFO. This was shown experimentally. Thus the model showed how to operate the TiO₂-coated CFO photoelectrodes for best performance and the experiments validated the model and showed the improvement successfully. The resulting photoelectrodes produce a voltage sufficient to oxidize water without bias voltage.

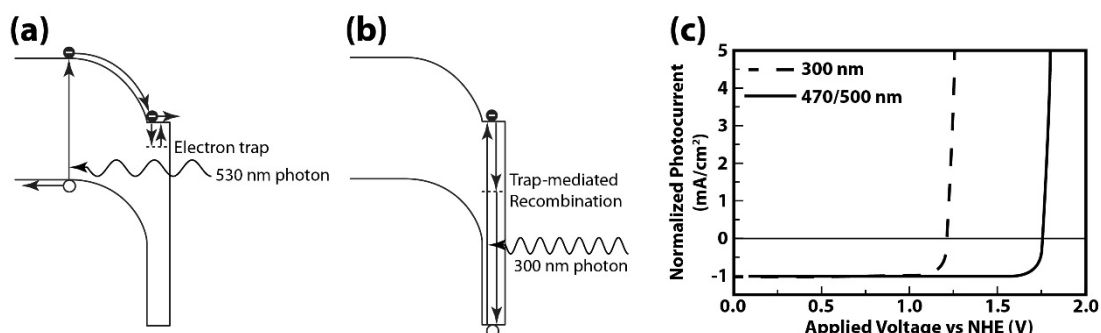


Fig. 2.2. Theoretical results simulating the effect of coating a CaFe₂O₄ photoelectrode with TiO₂ under (a) 530 nm photons and (b) 300 nm photons and the experimentally-determined performance (c) of the photoelectrode. The model showed how performance could be improved while the experiments demonstrated a photoelectrode capable of water oxidation without externally-applied bias.

Publication

S. Ida, K. Kearney, T. Futagami, H. Hagiwara, T. Sakai, M. Watanabe, A. Rockett and T. Ishihara "Photoelectrochemical H₂ evolution from CaFe₂O₄ photocathodes without an external applied voltage: experimental and modeling results, J. Am. Chem. Soc., submitted.

Electrochemical Energy Conversion (Lead Principal Investigator: Prof. Matsumoto)

Electro-chemo-mechanical phenomena in electrochemistry

Electro-chemo-mechanics (ECM) is an inherently interdisciplinary approach, linking electrical, chemical, and mechanical aspects of materials to understand and tailor properties for enhanced efficiency and durability. Electrode and electrolyte properties impacted by the interplay of these elements include ionic conductivity, surface reaction kinetics, and chemical expansion-induced mechanical failure; therefore, ECM is a theme cross-cutting several projects of the electrochemical energy conversion division. In FY 2015, Professors Perry, Bishop and PI Tuller have been combining their experimental electroceramic approaches with computational simulations and with low-dimensional carbon chemistry in an extended interdisciplinary approach to establish fundamental ECM relationships in fuel/electrolysis cell electrodes, as described below:

i) Mechano-electrical: To better understand the electrical properties of novel low dimensional carbon materials, as candidate membrane for low temperature fuel cells, Perry, Tuller, and Bishop have applied ceramics characterization approaches (ac-impedance spectroscopy, blocking electrode techniques) to graphene oxide (GO) paper synthesized by Professor Lyth's group (*ACS Applied Materials and Interfaces*, in press). This work targets obtaining excellent gas barrier properties in systems that can be fabricated in ultra-thin form to minimize resistance. The collaboration demonstrated for the first time the fraction of the conductivity that is protonic vs. electronic under different operating conditions. The humidity dependence of the electronic conductivity is attributed to a chemo-mechanical effect where water intercalation between GO layers pushes them further apart and obstructs the electronic pathway. This understanding is important for evaluating GO's potential as an electrolyte, related to the short-term milestone "Fundamentals of nanoconfined and surface proton conductivity mechanism in nanomaterials" for Project 2 in the division's roadmap.

ii) Chemo-mechanical: Perry, Tuller and Bishop carried out a comprehensive assessment of perovskite chemical expansion, which revealed significant differences with respect to fluorite-structured oxide behavior through the use of new empirical and computational atomistic models (collaboration with D. Marrocchelli, MIT) describing lattice distortions accompanying oxygen loss and the effective size of oxygen vacancies (*Phys. Chem. Chem. Phys.*, 17, 10028-10039, 2015) (Fig. 2.3). Chemical expansion, the lattice dilation accompanying small chemical changes, leads to device mechanical failure and must be minimized. Building on the prior experimental investigations of particular factors impacting chemical expansion in perovskites, this understanding directly corresponds to the division milestone "Factors

impacting chemical expansion in perovskites identified and understood" (Project 1) and relies on collaboration between experiment and computation, and is important for future design of more durable solid oxide fuel/electrolysis cell electrodes with lower chemical expansion.

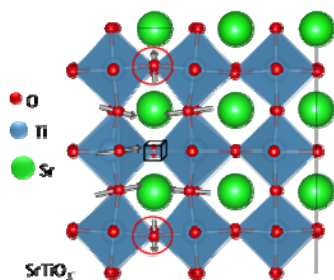


Fig. 2.3. Simulated distortions around an oxygen vacancy (black cube) in perovskite SrTiO_3 , related to understanding chemical expansion in this structure, taken from (*Phys. Chem. Chem. Phys.*, 17, 10028-10039, 2015).

iii) Electro-chemical: We developed an iterative experimental – computational approach in the search for “missing” materials within the earth-abundant Zn-Ti-O ternary phase space, leading to the discovery of a new, conductive, highly robust pseudobrookite phase (*Dalton Transactions*, 45, 1572-1581, 2016). Such design of earth-abundant, robust, electrically conductive oxides may serve in future electrodes for low temperature PEM fuel cells. This work is a collaboration with V. Stevanovic (Colorado School of Mines / National Renewable Energy Laboratory,) L.Y. Lim (Stanford University,) and T.O. Mason (Northwestern University.) The properties of this new phase may be promising for use as a low cost, low temperature electrode (*Dalton Transactions*, 45, 1572-1581, 2016). This work denotes progress against the mid-term milestone “Pt-free electrode: Negligible degradation, improved efficiency (<5% H_2O_2)” to address the stability challenge posed by carbon-based electrodes for polymer cells in “Project 1 Electrodes.”

Publications

T. Bayer, S.R. Bishop, N.H. Perry, K. Sasaki, S.M. Lyth, Mixed ionic / electronic conductivity and permittivity of graphene oxide paper, *ACS Applied Materials and Interfaces* (in press.)

D. Marrocchelli, N.H. Perry, and S.R. Bishop, Understanding chemical expansion in perovskite-structured oxides, *Phys. Chem. Chem. Phys.* 17, 10028-10039, 2015, DOI: 10.1039/C4CP05885B.

N.H. Perry, V. Stevanovic, L.Y. Lim, and T.O. Mason, Discovery of a ternary pseudobrookite phase in the earth-abundant Ti-Zn-O system, *Dalton Transactions*, 45, 1572-1581, 2016, DOI: 10.1039/C5DT04145G.

Additive-Controlled Electrodeposited Ni and NiFe Films for High-Activity Oxygen Evolution Reaction Catalysts

(Electrochemistry and thin film deposition technology)

As the energy demand continues to grow and natural energy resources to decrease, clean renewable energy sources (wind, solar) and efficient energy-storage systems are needed. One of the biggest challenges is how to store renewable energy into energy-rich molecules. H_2 with its high mass specific energy density has been considered to be a promising energy storage molecule that releases energy in fuel cells with only water as by product. The electrochemical splitting of water using electricity from renewable sources is an attractive way to produce carbon free source of H_2 . Thus, water electrolysis is dealt with in multiple milestones in the division roadmap. However, the efficiency of the overall reaction is limited primarily by the stability and the overpotential of the oxygen evolution reaction (OER) at the anode. The work of Gewirth has focused on obtaining stability and reasonable activity at high current density with nonprecious catalysts. He has developed a Pt-free anode synthesized by electrodeposition, a

technique commonly used in thin film deposition but that had not been previously applied to the preparation of electrocatalysts.

It should be mentioned that water electrolysis is the subject of multiple milestones in "Project 3-1 Polymer electrolyte cells" and more directly in "Project 3-3 Energy storage", i.e., short-term milestone "Water electrolysis: High efficiency >80% (HHV)" and long-term milestone "Pressurized, highly stable water electrolysis at 1.4 V" in Project 3-1 and the milestones "Reversible PEFC/PEEC operation at 120-150°C, roundtrip efficiency~50%" (short-term) and "Ditto>60%" (mid-term) of Project 3-3. However, the efficiency of the overall reaction is limited primarily by the stability and the overpotential of the oxygen evolution reaction (OER) at the anode. OER is additionally difficult with non-precious-metal catalysts set as the short-term milestone "Pt-free electrode: Elucidation of roles of C, N, Fe in active site" in Project 1 Electrodes. Stability and reasonable activity at high current density with nonprecious catalysts remain a challenge. What PI Gewirth has chosen for this challenge is the electrodeposition to prepare the Pt-free anode.

His recent results demonstrate that by simple electrodeposition method of Ni, Co, and NiFe in the presence of 3,5-diamino-1,2,4-triazole (DAT), fractal-like structures with nearly arbitrary large surface area can be fabricated. This method produces robust and highly efficient OER catalysts exhibiting at least 72 hour stability even in extremely harsh OER conditions (high pH, high potential, and vigorous gas evolution), in contrast to the poor stability of nanoparticle or precipitated-based catalysts.

NiFe electrodeposited by this additive-controlled electrodeposition exhibits very high OER activity with $j = 100 \text{ mA/cm}^2$, i.e. mass activity $\sim 1200 \text{ A/g}$ of catalyst at $\eta = 300 \text{ mV}$ (1.53 V vs RHE) in 1 M NaOH which is among the most active OER electrocatalysts in an alkaline electrolyte reported to date. Moreover, we can tune this current density to nearly any arbitrary value by altering the amount of NiFe electrodeposited, without any evidence of material or activity degradation due to the metallic nature of the initial deposit.

This additive-controlled electrodeposition method can be used to fabricate fractal-like nanoscale structure of almost all metals for several applications not only limited to water splitting. For example fractal-like Cu can be used as a high activity, high selectivity catalyst for CO_2 reduction reaction. Cu and Ag fractal structures could also be applied to improve the enhancement factor of surface enhanced Raman scattering (SERS), and thus prove useful in the development of SERS spectroscopy, SERS-based biosensors, or plasmon-based analytical devices

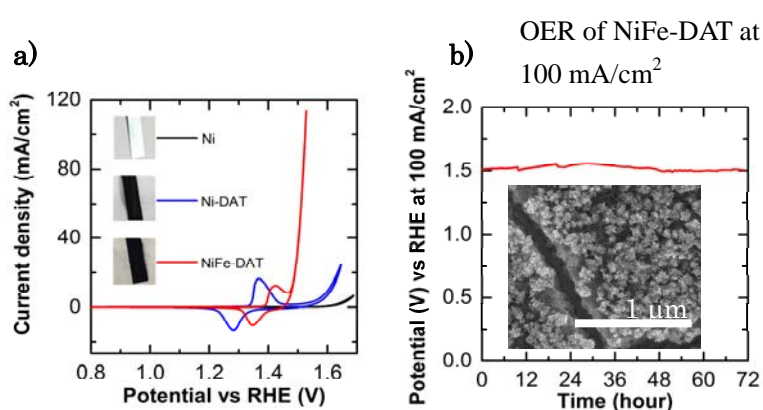


Fig. 2.4. (a) CV of Ni, Ni-DAT and NiFe-DAT in 1M NaOH solution; (b) Stability test of NiFe-DAT catalyst at 100 mA/cm^2 for 72 hours; inset shows SEM image of NiFe-DAT film.

Publication

T. T. H. Hoang, and A. A. Gewirth, High activity oxygen evolution reaction catalysts from additive-controlled electrodeposited Ni and NiFe films, *ACS Catal.*, 6(2) 1159–1164, 2016.

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

Spatial Control of Heterogeneous Nucleation using Focused Ion Beam Milling

(Supramolecular chemistry, material science, and thermal Science)

One of the key targets of the thermal science and engineering division is to provide a clear understanding of wettability affects liquid-to-vapor phase change (Division Project : HMT-1, Phase change heat transfer). To help achieve this aim, we conducted an experimental study to develop submicron-scale bi-philic surfaces with nanoscale bi-philicity. To develop the bi-philic surfaces, samples coated with hydrophobic self-assembled monolayers (SAMs) were irradiated using focused ion beam (FIB) to create arrays of hydrophilic spots. The surface of the irradiated regions became more hydrophilic with increased FIB ion dosage. Submicron scale bi-philic surfaces were developed with ≈ 110 nm diameter hydrophilic dots. The wettability difference was confirmed by condensation and evaporation experiments of pure water, where condensed droplets with ~ 300 nm diameters nucleated preferentially on the hydrophilic dots (Fig. 2.5) whereas pinned droplets remained on the hydrophilic dots after evaporation, respectively. These results improve our understanding of the basic science of heat and mass transfer to develop more efficient thermal systems and offer a surface design platform to rationally engineer the spatial location of nucleation sites. (Division Project HMT-1, short-term milestone "clear understanding of wettability effects in liquid-vapor phase change.")

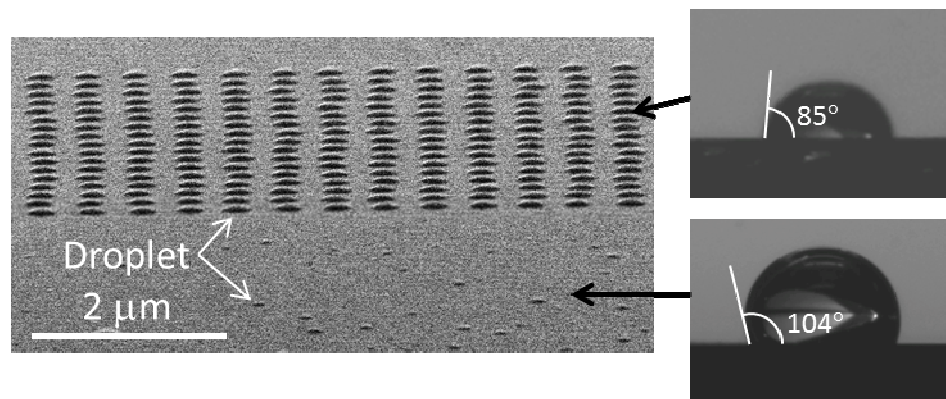


Fig. 2.5. (left) SEM image of spatial control of condensation nucleation of water droplets on a bi-philic (hydrophobic background, hydrophilic dots) surface fabricated by SAM deposition and FIB irradiation. (right images) Macroscopic characterization of the advancing contact angle on the hydrophilic and hydrophobic areas.

Publication

Y. Yamada, K. Takahashi, T. Ikuta, T. Nishiyama, Y. Takata, W. Ma, A. Takahara, Tuning surface wettability at the submicron-scale: Effect of focused ion beam irradiation on a self-assembled monolayer, *J. Phys. Chem. C*, 120 (1), 274-280, 2016.

Fundamental Studies of Hydrocarbon Adsorption on Solid Interfaces

(Chemistry, electrochemistry, materials science, electrical engineering, physics, and mechanical engineering)

Professor Miljkovic's research group at Illinois and PI Takata's research laboratory at Kyushu have been collaborating on a very fundamental and interdisciplinary problem related to the effects of surface alteration (wettability) due to hydrocarbon adsorption from the atmosphere. Better fundamental understanding of this process has the potential to fundamentally alter the field of interfacial science, which has importance to both the thermal science division, in addition to the catalysis and electrochemistry divisions of I²CNER. We aim to answer what

governs the kinetics of adsorption, what molecules are adsorbing, what is the surface coverage and effect on wettability.

We have been studying the surface chemistry of clean metallic and semiconducting solid interfaces as they are exposed to laboratory air, and allowed to contaminate with hydrocarbons in the atmosphere. To quantify the process, we have been using time resolved X-Ray Photoelectron Spectroscopy (XPS) and Time of Flight Secondary Ion Mass Spectroscopy (TOF-SIMS). We are currently studying the interface using Low Energy Ion Scattering in order to characterize the chemistry of the first surface adsorbed layer, which has not been done before. The fundamental understanding elucidated from this work help achieve the long-term milestone of understanding phase change heat transfer from the nano to macro scales (HMT-1).

Publication

Y. Yokoyama, H. Cha, T. Imazeki, D. Orejon, Y. Takata, N. Miljkovic, Effect of atmospheric hydrocarbon adsorption on the solid-vapor interface, In preparation.

Hydrogen Storage (Lead Principal Investigator: Prof. Akiba)

Borohydrides for energy storage

(Synthetic chemistry, crystallography, spectroscopy, hydrogen storage and electrochemistry)

De-/Re-hydrogenation reactions of metal borohydrides $M(BH_4)_n$ with a high gravimetric hydrogen density of 10 mass% require the diffusion of constituent elements especially for the cation M^{n+} . Investigation of the diffusion behavior of M^{n+} is of great importance for understanding the kinetics and the exploration of new solid ionic conductor. For the first time we have successfully synthesized the bimetallic dodecaborate, $LiNaB_{12}H_{12}$ containing no crystal water. $LiNaB_{12}H_{12}$ exhibits a lower phase transition temperature, smaller hysteresis, and significantly higher ionic conductivity than its monometallic counterparts, i.e., $Li_2B_{12}H_{12}$ and $Na_2B_{12}H_{12}$. The ionic conductivity of $LiNaB_{12}H_{12}$ reaches a value of 0.79 S/cm at 550 K, which is approximately 8 times higher than that of $Na_2B_{12}H_{12}$ and 11 times higher than that of $Li_2B_{12}H_{12}$. These interesting results demonstrate our strategy of employing bimetallic dodecaborates to be effective in improving the ionic conductivity. This work is related to Project 2 in our division's roadmap. Fundamental understanding of intermediates is essential to achieve the division's targets. At least, the mid-term milestone for hydrogen storage capacity over 10 wt% has been reached and we now focus on how to reduce the hydrogen release temperature.

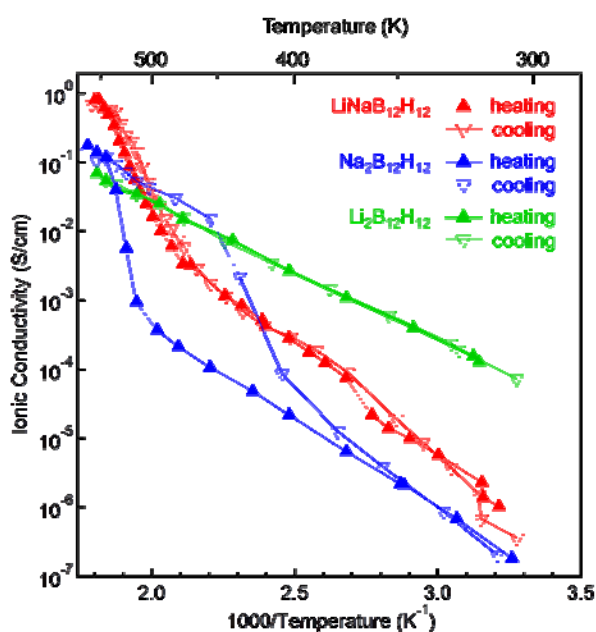


Fig. 2.6. Ionic conductivity measurements for $LiNaB_{12}H_{12}$, $Na_2B_{12}H_{12}$, and $Li_2B_{12}H_{12}$ as a function of

temperature.

Publication

L. He, H.-W. Li, H. Nakajima, N. Tumanov, Y. Filinchuk, S.-J. Hwang, M. Sharma, H. Hagemann, E. Akiba, Synthesis of a bimetallic dodecaborate $\text{LiNaB}_{12}\text{H}_{12}$ with outstanding superionic conductivity, *Chemistry of Materials*, 27, 5483–5486, 2015.

Development of new Mg-based hydrogen storage materials by binding-energy engineering (Computational science, materials science and metallurgy)

The main drawback of Mg-based hydrides for mobile hydrogen storage applications is their high thermodynamic stability and high dehydrogenation temperature. We established the concept of binding-energy engineering to design new Mg-based phases which can desorb hydrogen at ambient temperature. First-principles binding energy calculations were employed to design the materials. Since the elements in most of the designed materials were thermodynamically immiscible, the HPT method was used for atomic-scale mixing of the elements.

New phases with the bcc, hcp and fcc crystal structures could be synthesized in the immiscible Mg-Zr system which exhibited reversible hydrogen storage at room temperature. They absorbed ~ 1 wt.% of hydrogen in ~ 20 s and fully desorbed the hydrogen in the air. A new Mg_4NiPd phase with the B2-type structure was also designed which exhibited 0.6 wt.% reversible hydrogen storage at room temperature.

Although the amount of reversible hydrogen storage is still low in these materials, the current study introduces a new approach to produce new materials with low-temperature hydrogen storage capability. This study constitutes significant progress toward the short-term milestone of “HPT-processed Mg alloys for on board application” in Project 3 in the division’s roadmap.

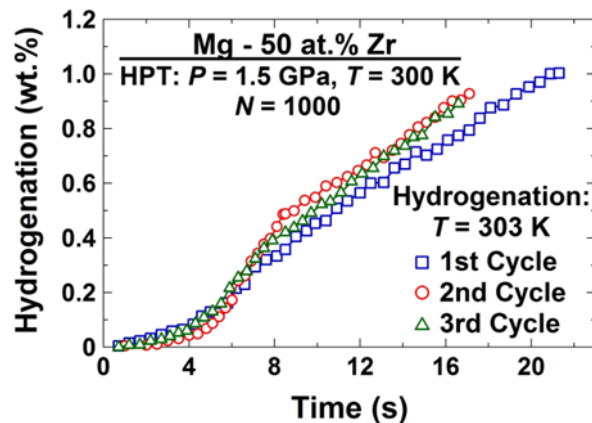


Fig. 2.7. Formation of new phases in immiscible Mg-Zr system with fast hydrogen storage capability at room temperature.

Publications

K. Edalati, H. Emami, Y. Ikeda, H. Iwaoka, I. Tanaka, E. Akiba, Z. Horita, New nanostructured phases with reversible hydrogen storage capability in immiscible magnesium-zirconium system produced by high-pressure torsion, *Acta Materialia*, In press.

H. Emami, K. Edalati, A. Staykov, T. Hongo, H. Iwaoka, Z. Horita, E. Akiba, Solid-state reactions and hydrogen storage in magnesium mixed with various elements by high-pressure torsion: experiments and first-principles calculations, *RCS Advances*, 6, 11665-11674, 2016.

K. Edalati, H. Emami, A. Staykov, D.J. Smith, E. Akiba, Z. Horita, Formation of metastable phases in magnesium-titanium system by high-pressure torsion and their hydrogen storage performance, *Acta Materialia*, 50, 150-156, 2015.

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

Improved purification, crystallization and crystallographic study of Hyd-2-type [NiFe]-hydrogenase from Citrobacter sp. S-77

(Microbiology, biochemistry, and structural biology)

The [NiFe]-hydrogenase isolated from *Citrobacter* sp. S-77 (HYD2-s77) has been reported to be type 2 hydrogenase. Type 2 [NiFe]-hydrogenases have been reported to be sensitive to O₂, but biochemical electrochemical studies indicate that the type 2 HYD2-s77 has high oxygen stability and a 637-fold higher mass activity than Pt at 50 mV in a hydrogen half-cell. Crystallization and preliminary X-ray diffraction analysis indicate that this new enzyme exhibits potential tolerance to O₂. Since no structural information on the type 2 [NiFe]-hydrogenases has yet been reported, complete identification of the crystal structure of HYD2-s77 will provide a more detailed structural comparison with the other types of [NiFe]-hydrogenases and structural evidence for its high specific activity and possible O₂ tolerance.

The results of this work along with those from our previous biochemical studies published in *Angew. Chem. Int. Ed* in 2014, constitute significant progress toward realizing the mid-term milestone “practical H₂-catalyst and crystal structure of hydrogenase” for hydrogen activation of Project 1 in the division’s roadmap. This interdisciplinary work was conducted in collaboration with the University of Hyogo.

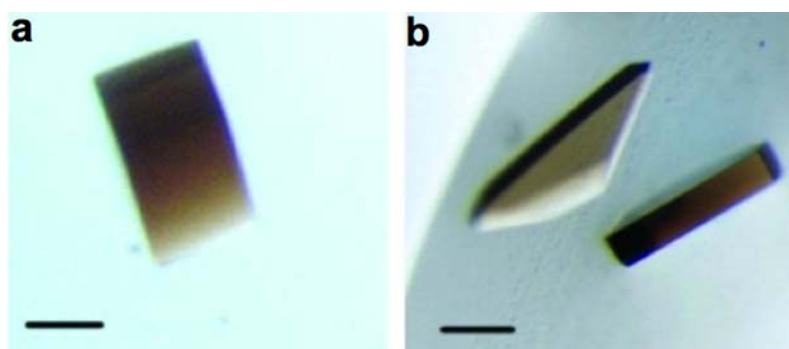


Fig. 2.8. Crystals of the hydrogenase unit of the [NiFe] hydrogenase from *Citrobacter* sp. S-77. (a) A crystal obtained from the protein sample with trypsin treatment, (b) Crystals obtained from the protein sample without trypsin treatment (the scale bar is 0.05 mm in length).

Publication

N. D. M. Noor, K. Nishikawa, H. Nishihara, K-S. Yoon, S. Ogo, Y. Higuchi. Improved purification, crystallization and crystallographic study of Hyd-2-type [NiFe]-hydrogenase from *Citrobacter* sp. S-77, *Acta Crystallogr. F (Struct. Biol. Commun.)* 72, 53-58, 2016.

Catalytic Materials Transformation in collaboration with CO₂ Capture and Utilization (Lead Principal Investigators: Profs. Ogo and Fujikawa)

Active Cu nanoparticle catalysts for the one-step electrosynthesis of ethylene and ethanol from CO₂ in an alkaline electrolyzer

(Materials chemistry, electrochemistry, analytical chemistry, and chemical engineering)

In this collaborative project with the Yamauchi Group in the Catalytic Material Transformation Division, we combined the expertise of Prof. Yamauchi (chemistry) in synthesizing and characterizing active metal nanoparticle catalysts and the expertise of Prof. Kenis (chemical engineering) in optimizing the process for the electrochemical conversion of CO₂. Specifically, the Yamauchi group synthesized and characterized active Cu nanoparticles with different morphologies. The Kenis group formulated these catalysts into ink and deposited the catalysts on gas diffusion electrodes, which are further assembled in an electrochemical flow reactor to

measure the activity of the catalysts. We found that the use of catalysts with large surface roughness results in a combined Faradaic efficiency (46%) for the electroreduction of CO₂ to ethylene and ethanol in combination with current densities of $\sim 200 \text{ mA cm}^{-2}$, a 10-fold increase in performance achieved at much lower overpotential (only $< 0.7 \text{ V}$) compared to prior work. This study shows that the efficient conversion of CO₂ to C₂ hydrocarbons is possible, which is one step further to accelerate the transition to a low-carbon society. This is a new effort related to our division's efforts to develop "catalysts for efficient CO₂ conversion (here to C₂ products) and to produce other chemicals (e.g., alcohols, hydrocarbons.) In addition, this work reports that more than 100 mV less overpotential is required to produce ethylene and ethanol compared to values reported in the literature, which will lead to significant improvements in energy efficiency for this process. We do not have target numbers for Faradaic efficiency and current density at this stage because we do not yet have an economic analysis for these products. We expect that further developing bimetallic Cu-based catalysts will help achieving high Faradaic efficiencies for ethylene and ethanol. In addition to improving the catalyst performance, Yamauchi and Kenis along in collaboration with the EAD will also determine what performance will be needed for economic viability. The work targets the short-term milestone "Catalysts for efficient CO₂ conversion" in the division's Project 2 "Electrochemical conversion."

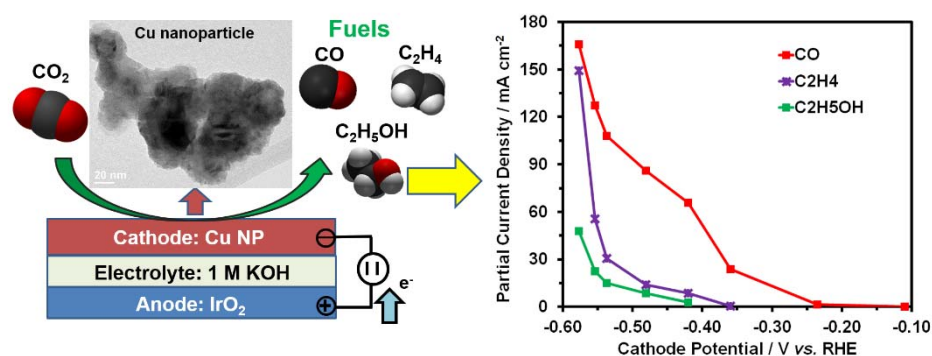


Fig 2.9. Partial current density for CO, ethylene, and ethanol as a function of cathode potential when using Cu nanoparticles as the catalyst in an electrolyzer operated with 1M KOH as the electrolyte.

Publication

S. Ma, M. Sadakiyo, R. Luo, M. Heima, M. Yamauchi, P. J. K. Kenis. J., One-step electrosynthesis of ethylene and ethanol from CO₂ in an alkaline electrolyzer, *Power Source*, 301, 219-228, 2016.

CO₂ Capture and Utilization in collaboration with Electrochemical Energy Conversion (Lead Principal Investigators: Prof. Fujikawa and Prof. Matsumoto)

Alkaline anion exchange membranes based on KOH-treated multilayer graphene oxide (Engineering, materials chemistry, gas permeability vs. ion conductivity)

Mixed ionic-electronic conductors have been studied for application in many electrochemical systems such as fuel cells, chemical sensors, and membranes for gas separation. Graphene oxide (GO) with ions is considered as low dimensional ionomer and electro-conductive material and has the potential for a mixed ionic-electric conducting membrane for fuel cells.

We have developed novel ion exchange membranes via cation exchange of pure graphene oxide (GO) dispersions, followed by simple vacuum filtration. The maximum conductivity was 6.1 mS/cm at 70 °C, approaching that of commercially available anion conducting membranes with OH⁻ confirmed as the dominant charge carrier. A demonstration with an alkaline fuel cell utilizing a GOKOH membrane has been done. The initial open circuit voltage (OCV) was 0.94V, and the maximum power density was $\sim 1 \text{ mW/cm}^2$. Importantly, hydrogen gas permeation through the membranes was several orders of magnitude below that of conventional polymers. Current accomplishment is an original and important proof-of-concept for the application of pure graphene-oxide based ion exchange membranes with high gas barriers in electrochemical devices. The work targets the "New polymer electrolytes: 10^{-2} S/cm at 0-120°C (RH=30%)"

and "Fundamentals of nanoconfined and surface proton conductivity mechanism in nanomaterials" short-term milestones of the Electrochemical-Energy-Conversion division's Project 2 "Electrolytes."

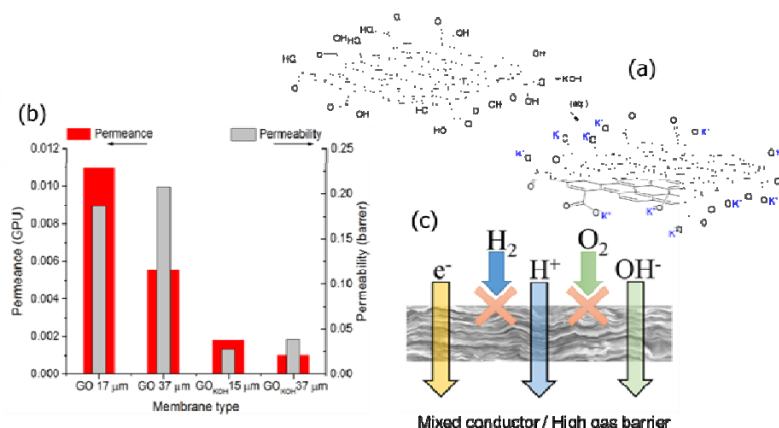


Fig. 2.10. (a) Schematic representation of the KOH treated graphene oxide sheet, (b) Hydrogen permeability of the pristine and KOH treated GO membranes, (c) Schematic representation of the KOH treated membrane possessing conductivity with OH⁻ as a dominant carrier and few orders higher gas barrier compared to conventional membranes.

Publication

T. Bayer, B. V. Cuning, R. Selyanchyn, T. Daio, M. Nishihara, S. Fujikawa, K. Sasaki, and S. Lyth, Alkaline anion exchange membranes based on KOH-treated multilayer graphene oxide, *J. Memb. Sci.*, 508 51–61, 2016.

CO₂ Storage (Lead Principal Investigator: Prof. Tsuji)

Continuous and accurate monitoring of injected CO₂

(Earthquake science (seismology) and exploration geophysics)

In carbon capture and storage (CCS,) the monitoring of injected CO₂ is crucial for (i) predicting the risk of CO₂ leakage from storage reservoirs, (ii) increasing the efficiency of CO₂ injection and reducing the cost, and (iii) reducing the risk of injection-induced seismicity. As a monitoring method, time-lapse seismic surveys have been used to determine the spatial distribution of injected CO₂. In the conventional seismic monitoring method, however, the interval of the time-lapse surveys is usually long due to their high cost, and it is difficult to continuously monitor the injected CO₂. Obviously, continuous monitoring of dynamic CO₂ behavior is critical for detecting accidental incidents associated with CO₂ injection (e.g., leakage.)

We developed a novel monitoring method for injected CO₂ using a continuous and controlled seismic source (Figure 2.11a). The continuous source system was originally developed for earthquake or volcano monitoring. To apply this system for injected CO₂ monitoring, we employed a higher frequency range as a source signal. We further improved the temporal resolution and accuracy of the monitoring by using surface waves. Our monitoring system is cost-effective, with high temporal resolution and high accuracy, compared to conventional monitoring. Our field experiments show that hourly-variation of surface-wave velocity can be monitored with better than 1 % accuracy (Figure 2.11b). This temporal stability allows the possibility to detect changes in seismic velocities associated with CO₂ leakage through the fault zone. The present monitoring technique is used in the ongoing Aquistore CCS project in Canada which is managed by SaskPower and the Petroleum Technology Research Centre (PTRC) and is the world's first commercial-scale, post-combustion CO₂ carbon sequestration project at a coal-fired power plant.

This effort directly addresses the short-term milestone "Develop effective monitoring system" in the division's roadmap for Project 3 (Field-scale CO₂ investigation).

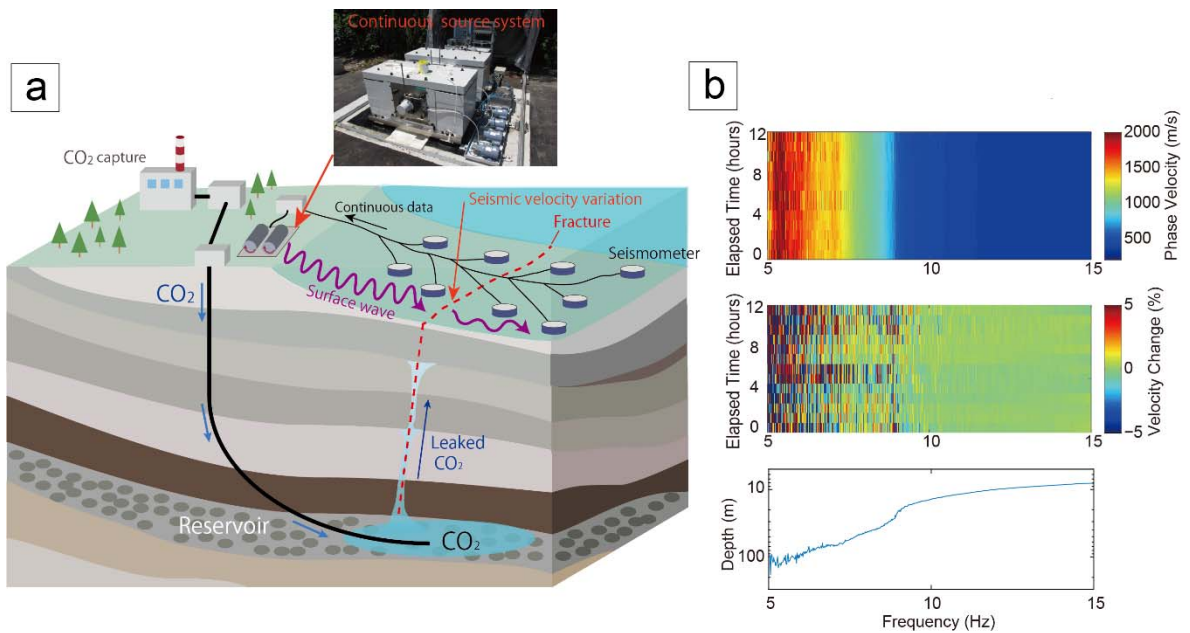


Fig. 2.11. (a) Continuous seismic monitoring of injected CO₂ and detection of leaked CO₂. The upper photo shows the monitoring device, which generates a continuous and repeatable source signal. (b) Hourly-variation of the surface-wave velocity (upper) and relative velocity (middle). Lower panel shows the frequency dependence of the surface waves on depth. Seismic velocity at higher frequency indicates the velocity at shallower formation. This monitoring system is currently deployed in an ongoing CCS project at a coal-fired power plant in Saskatchewan, Canada.

Publications

T. Ikeda, T. Tsuji, T. Watanabe, K. Yamaoka, Development of surface-wave monitoring system for leaked CO₂ using a continuous and controlled seismic source, *International Journal of Greenhouse Gas Control*, 45, 94-105, 2016.

T. Tsuji, T. Ikeda, T. A. Johansen, B. O. Ruud, Passive seismic interferometry for fluid injection monitoring: Elucidating time variations of shallow formation and its impact on the deep reservoir monitoring, (being revised after the first review).

On the relationship between CO₂ saturation and seismic velocity (Hydrology and geophysics)

Time-lapse seismic surveys are suitable for monitoring CO₂ distributions within reservoirs, but it is difficult to quantify the amount of subsurface CO₂ (i.e., CO₂ saturation) from this seismic data (i.e., through the measured seismic velocity.) To estimate CO₂ saturation from the measured seismic velocity, the relationship between CO₂ saturation and seismic velocity must be determined. This relationship is difficult to be quantified because the response of the seismic velocity to CO₂ saturation is not unique, and is also influenced by the CO₂ distribution in the pore spaces of rock. Therefore, quantitative monitoring requires knowledge of hydrology (CO₂ behavior or hydrologic properties) tightly coupled to geophysics (elastic properties).

This study evaluated the influence of CO₂ within rock pores on the relationship between seismic velocity and CO₂ saturation (Fig. 2.12a). We conducted two computational studies with different injection pressures, using (i) a two-phase lattice Boltzmann method for CO₂ injection simulation (i.e., hydrologic simulation) and (ii) wave propagation simulation with a finite difference approach for the evaluation of seismic velocity (i.e., elastic simulation). The change of capillary number associated with various injection pressures affected the CO₂ displacement patterns (Fig. 2.12b.) Viscous fingering was typical at high capillary numbers, whereas both viscous and capillary fingering were observed at low capillary numbers. These differences in CO₂ behavior can influence the seismic velocity. We identified a difference in the relationship between seismic velocity and CO₂ saturation in a few cases; i.e., lower seismic velocity was observed in the high capillary number case compared to a low capillary number case with exactly the same

saturation (Fig. 2.12a.) It was found that the difference in the elastic velocity response to CO₂ saturation is controlled by CO₂ distribution features. The capillary numbers vary with distance from the injection well (Fig. 2.12b), with low capillary numbers expected far from the injection well and high numbers near the well. This study demonstrates that the capillary number at each reservoir location (e.g., distance from injection well) should be considered to accurately estimate CO₂ saturation from measured seismic velocity derived from monitoring data. This effort directly addresses the mid-term milestone “Laboratory and theoretical studies for quantitative monitoring” in Project 3 in the division’s roadmap (Field-scale CO₂ investigation).

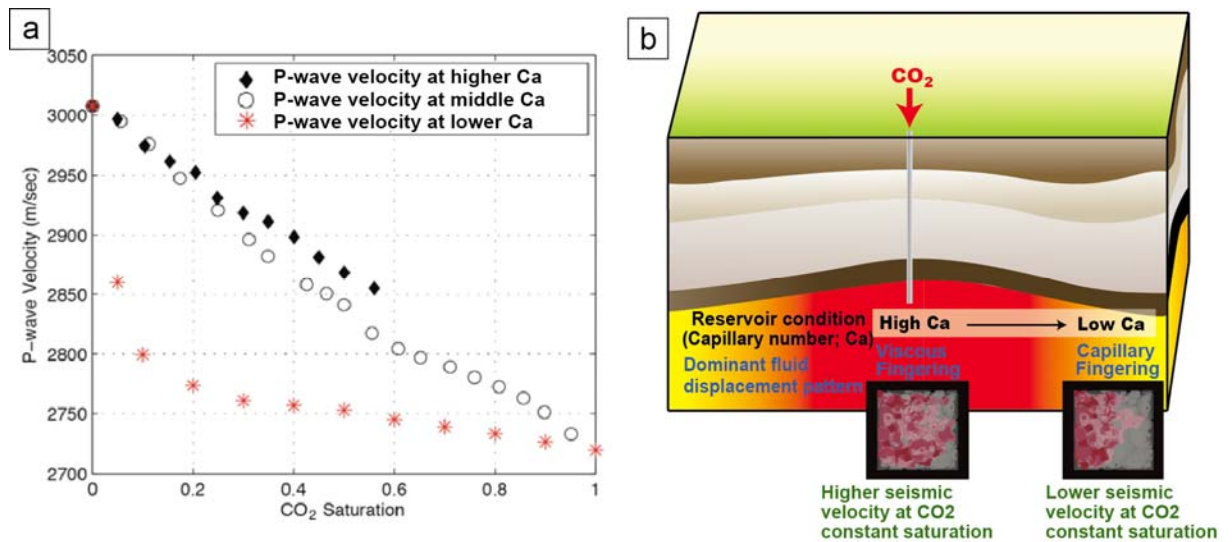


Figure 2.12. (a) Relationship between seismic (P-wave) velocity and CO₂ saturation at various capillary numbers Ca calculated by lattice Boltzmann fluid flow simulations and dynamic wave propagation simulations. (b) Injected CO₂ behavior at different reservoir flow conditions (capillary number). For accurate geophysical (seismic) monitoring the relationship between seismic velocity and CO₂ saturation should be accounted for.

Publications

H. Yamabe, T. Tsuji, Y. Liang, T. Matsuoka, Influence of fluid displacement patterns on seismic velocity during supercritical CO₂ injection: Simulation study for evaluation of the relationship between seismic velocity and CO₂ saturation, *International Journal of Greenhouse Gas Control*, 46, 197-204, 2015.

T. Tsuji, T. Ikeda, F. Jiang, Evolution of hydrologic and elastic properties of natural rock due to mineral precipitation: Use of Vp/Vs ratio for permeability prediction, Submitted.

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

Mechanistic interplay between hydrogen and deformation microstructure in stainless steel (Mechanical metallurgy and electron microscopy)

The interdisciplinary achievement described below represents progress toward the milestone of identify mechanisms for hydrogen-induced fracture mode transition in ferritic and austenitic alloys, considering role of hydrogen-induced microstructure evolution. This short-term milestone is featured in Project 1: Physical Descriptions of Hydrogen-Materials Interactions.

It is well recognized that the resistance of austenitic stainless steels to hydrogen embrittlement (HE) depends on the stability of austenite: transformation of austenite to martensite during deformation generally results in higher HE susceptibility. However, the mechanism to cause a lower ductility or higher fatigue-crack growth rate of austenitic stainless steels in the presence

of hydrogen has not been well understood and consequently the application of conventional stainless steels in high-pressure hydrogen service is limited. In an effort to clarify the mechanistic interplay between hydrogen and deformation microstructure in austenitic stainless steels, two alloys with different austenite stabilities were featured: 316L (higher stability) and 304 (lower stability).

During this reporting period, non-charged (4 mass ppm of H) and H-charged (104 mass ppm of H) specimens were subjected to slow strain rate tensile and fatigue-crack growth tests, and the effect of hydrogen on microstructure evolution immediately beneath the fracture surfaces was examined using a combination of a focused-ion beam (FIB) lift-out technique and transmission electron microscopy (TEM). The results obtained from the uniaxial tensile test using type 304 stainless steel are summarized here. The fracture surface of type 304 showed ductile dimples in the non-charged state, whereas the hydrogen-induced fracture surface consisted of "flat" and "quasi-cleavage (QC)" features; the "QC" feature is shown in Fig. 2.13c. Figures 2.13a and 2.13b present the microstructure developed immediately beneath the hydrogen-induced "QC" fracture surface and a diffraction pattern. From this detailed microstructural observation, it was proposed that "QC" fracture is caused by a synergistic effect of hydrogen-enhanced localized plasticity and hydrogen-enhanced decohesion with the assistance of hydrogen release from α' -martensite at transformation. This interdisciplinary study combining mechanical metallurgy and electron microscopy will enable determination of alloy composition and microstructure that optimizes cost and performance in austenitic stainless steels.

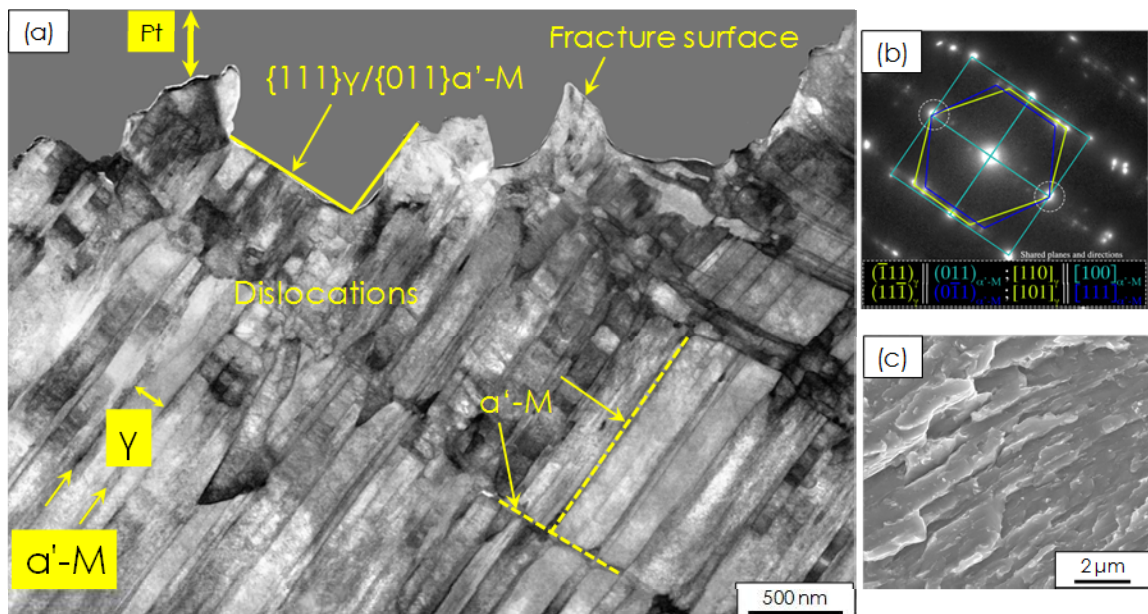


Fig.2.13. Hydrogen-induced "quasi-cleavage" failure caused by uniaxial tension of type 304 austenitic stainless steel: (a) microstructure immediately beneath fracture surface revealed by FIB-TEM; (b) diffraction pattern of (a); (c) SEM image of "quasi-cleavage" fracture surface.

Publication

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

Advancing thermodynamics-based modeling of hydrogen-assisted intergranular cracking (Materials physics, solid mechanics, mechanical metallurgy)

The interdisciplinary achievement described below represents progress toward the milestone of identify mechanisms for hydrogen-induced fracture mode transition in ferritic and austenitic alloys. This short-term milestone is featured in Project 1: Physical Descriptions of Hydrogen-Materials Interactions.

During this reporting period, the modeling of hydrogen-assisted intergranular cracking was advanced through a thermodynamic treatment of new surface creation accompanying fracture. This thermodynamic approach focuses on the composition of the newly formed surfaces, which depends on the chemical potential of the components of a material and their mobility. Modeling surface composition is the foundation of the thermodynamic approach to fracture, since composition is connected to surface energy which in turn is an element of the work to fracture. In this approach, the work to fracture representing the mechanical aspect was combined with the Gibbs adsorption isotherm covering the chemical aspect. Compared to previous models, the present one provides a more generalized but also simpler and quantitative insight into chemomechanical effects on intergranular cracking. The model demonstrates that in extreme cases separation of lattice planes or separation of two crystals with a common interface occurs without applied external forces. Closed solutions for the work of fracture are derived for brittle fracture and surface segregation of solutes in the limit of a mean field approach. The results obtained for the nickel system are shown in Fig. 2.14. This interdisciplinary modeling effort combines material physics, solid mechanics, and mechanical metallurgy.

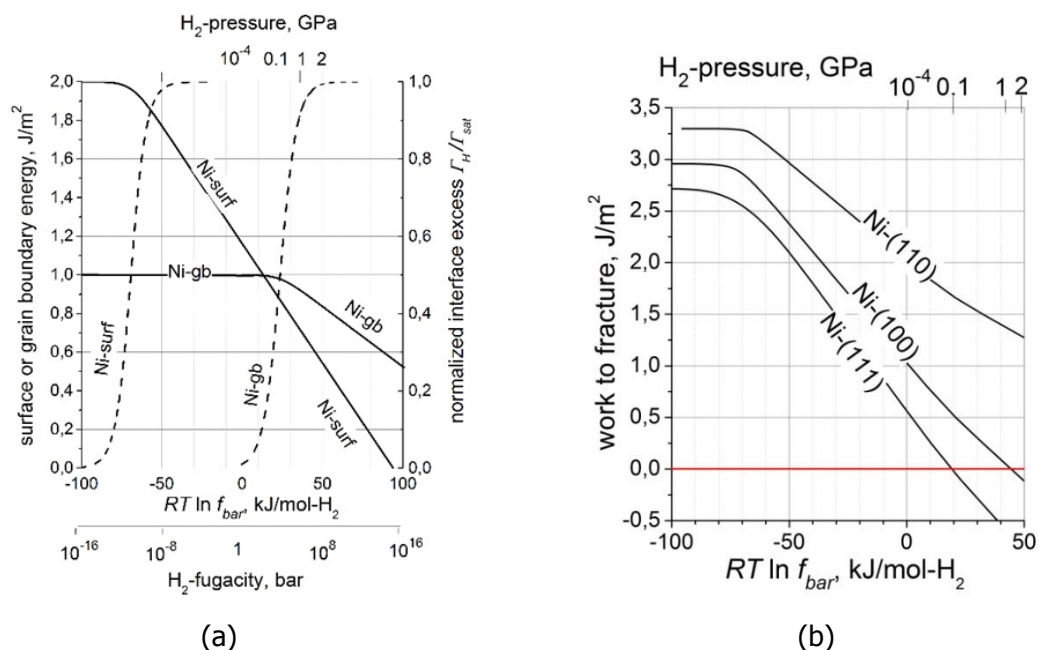


Fig. 2.14. (a) A quantitative example of surface energy and grain boundary energy changes in nickel (solid lines) as a function of hydrogen fugacity (lower abscissa) or corresponding hydrogen pressure (upper abscissa). The changes are due to hydrogen occupying the interfaces with increasing hydrogen fugacity (right ordinate, dashed lines). (b) Hydrogen-induced changes of the ideal work to fracture. It is interesting to note that cracks separating (111)-interfaces of Ni can form without external forces, if hydrogen pressures exceed 0.1 GPa.

Energy Analysis (Acting Division Leader: Prof. Itaoka)

Green House Gas (GHG) analysis of low carbon fuel import (Catalytic materials, reaction systems and life-cycle assessment)

One important consideration for the reduction of carbon emissions in Japan is to import carbon-neutral energy sources from outside Japan. There is a possibility to import low carbon fuel based on renewable energy from abroad where renewable energy sources are more abundant or carbon capture and storage (CCS) is more feasible consistent with the conditions of the locations' natural environments. This approach would result in an overall reduction in carbon emissions, not merely shift the emissions to another location. In addition to the availability of renewable energies or the feasibility of CCS, it is important to examine types of fuel sources as useful energy carriers. This requires an analysis of the feasibility and applicability of the entire production, supply chain and use of the low-carbon emission energy carriers. As a part of the feasibility study, we investigated (GHG) emissions carrying out the life-cycle assessment (LCA)

of three different energy sources and import pathways: (i) glycolic acid produced using wind power in the west Australia and transported by oil tanker; (ii) Bio diesel fuel (BDF) produced from Jatropha plantations in Indonesia and transported by oil tanker; and (iii) liquefied hydrogen produced from brown coal by gasification in conjunction with CCS in the east Australia and transported by tanker.

The first technology uses the carbon neutral cycle (CN cycle) being developed in I²CNER, whereby oxalic acid is converted into glycolic acid by electricity. The second technology utilizes Jatropha plants. This technology was selected for assessment of the feasibility of biofuel import based on a literature survey that looked into bio fuel crops to be raised in marginal soil with high yield but not suitable for edible crops. The third technology is being developed by Kawasaki Heavy Industries, Ltd. We carry out the analyses based on data from Kawasaki which are open literature. We chose one kWh electricity generation as a functional unit for comparison assuming original fuel cell using oxalic acid for the first technology, diesel engine for the second technology, and SOFC for the third technology as a power generator. Although the complete set of the relevant energy pathways is not yet available, we carried out the GHG analyses based on currently available data of the relevant components in each pathway. For wind power generation and Jatropha plantations, we used typical values from the LCA literature. We also conducted sensitivity analyses assuming levels of technology development for the key parts in each of the pathways.

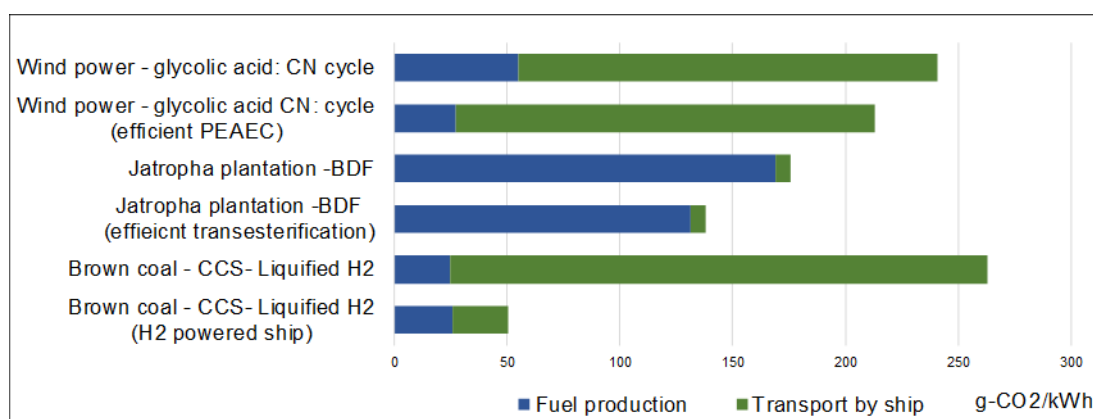


Fig. 2.15. GHG emissions in the three pathways of low carbon fuel import (g-CO₂/kWh.) The average GHG emissions from power grid electricity in FY 2014 was 579g-CO₂/kWh.

The results which are summarized in Fig. 2.15 show that all three pathways emit less than 50% of the level currently emitted by the power grid (579g-CO₂ /kWh in FY2014). The wind power - glycolic acid (CN cycle) pathway can be improved by increasing the efficiency of the production of glycolic acid by a polymer electrolyte alcohol electrosynthesis cell (PEAEC). However, a relatively large amount of CO₂ emissions still occurs upon transportation to Japan by regular tankers due to the relatively low energy density of glycolic acid and the use of diesel engines in the tankers. For the Jatropha plants – BDF pathway, energy inputs to produce Jatropha and BDF constitute a large emission source. Lastly, large CO₂ emissions due to the low energy density of the energy carrier also occurs for the brown coal – liquefied hydrogen pathway. These emissions can be substantially reduced by using the boil off hydrogen loss from the containment tanks as fuel to run the tanker. We are currently investigating the cost of the three pathways.

Regional techno-economic model for hydrogen from renewable energy
(Systems engineering and financial economics)

Use of hydrogen energy storage technology to smooth out the output fluctuations of renewable energy power generation is viewed as an effective means to optimize the utilization of Japan’s high-potential renewable energy sources. We developed a relevant regional techno-economic model (Fig. 2.16) in collaboration with HyGrid (an industry research group instituted in 2012 and focused on utilization of renewable energy and hydrogen. I²CNER is a founding member of

HyGrid). Wind power's detailed power generation data were used to conduct economic analyses addressing selling electricity and producing hydrogen simultaneously. The hydrogen is intended to power fuel cell vehicles and be used for cogeneration systems in a given region. The model considered two options: one placing priority to selling electricity and the other placing priority to producing hydrogen. These results were compared to a model which considered simply selling electricity generated from wind power to the grid.

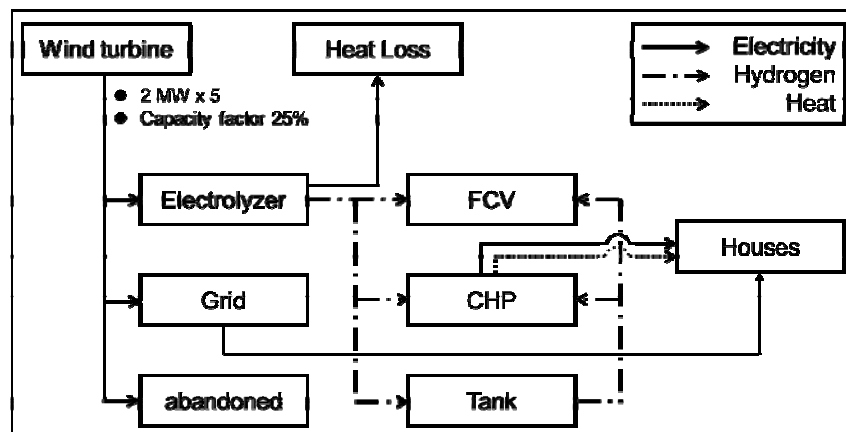


Fig. 2.16. Schematic model for regional hydrogen supply and utilization

The results of economic evaluation using net present value (NPV) and internal rate of return (IRR) show the significant influence of the hydrogen-related facility cost (Fig. 2.17). The revenue stream from electricity sales decreases substantially due to the impact of the hydrogen facility costs (CAPEX: capital expenditure). However, in times of low electricity prices, the value of the hydrogen and thus the value of the hydrogen production facility are positive. Since the returns on the internal rate of return from hydrogen production are lower than the direct electric grid option with no hydrogen production capability, improvements of durability of hydrogen production and storage are necessary to make them truly competitive.

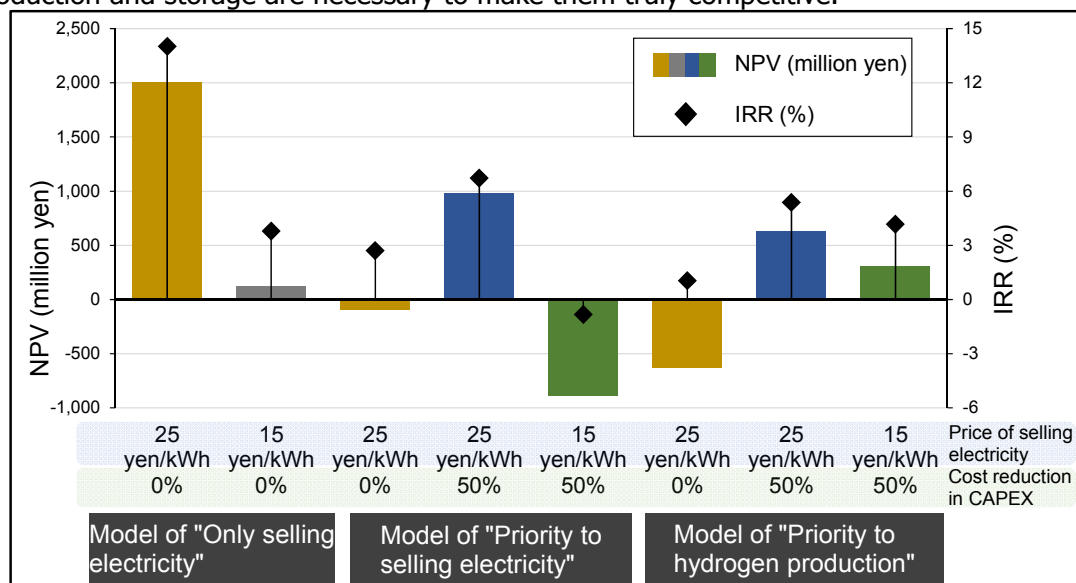


Fig. 2.17. Net present value (NPV) and internal rate of return (IRR) of sensitivity analyses of the three models. The term CAPEX denotes capital expenditure.

Publication

K. Hirose, K. Itaoka, T. Fukuda, and S. Kimura, Study of regional economic model with hydrogen from renewable energy, Proceedings of the 32nd Energy Systems, Economics and

Environment Conference, Feb 2-3, 2016, Tokyo, Japan.

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 initiated the process of advancing interactions with the Helmholtz Institute Forschungszentrum Juelich, Germany; the University of New South Wales (UNSW), Australia; the University of Edinburgh, Scotland; and the Southwest Research Institute (SwRI), USA in FY2015. As of March 31, 2016, I²CNER has a total of 26 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). Specific highlights of our globalization efforts include visits by the KU Executive Vice President in Charge of Research and Industrial Collaboration, Prof. Masato Wakayama, and the KU Executive Vice President in Charge of International Affairs, IP, and Promotion of Gender Equality, Prof. Reiko Aoki, to the UIUC Satellite; visits by the UIUC Vice Provost for International Affairs and Global Strategies, Prof. Reitumetse Mabokela, and the UIUC Dean of the College of Engineering, Prof. Andreas Cangelaris, to KU; the exchange visit of 1 student from the KU School of Letters to UIUC for 3.5 months under the KU-UIUC exchange program; the exchange visit of 6 KU undergraduates, including 2 female students, to UIUC for about 1 month; and the visits of 3 KU researchers to the UIUC Satellite under the I²CNER Collaborative Foreign Exchange Program.

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 52 distinguished visitors to Kyushu University from the United States, Canada, Korea, China, Indonesia, Australia, Finland, Scotland, Germany, France, Italy, Denmark, Japan, and England. The Institute's researchers were responsible for organizing, co-organizing, or serving on the scientific committee for 13 international conferences, 23 international conference sessions/symposia or workshops, and 9 I²CNER international workshops. In addition, our researchers have joint publications with researchers from 25 institutions around the world.

I²CNER Promotional Video at the MRS Annual Meeting

In FY2015, I²CNER partnered with WebsEdge, the company in charge of all the video programming of the MRS Society, to produce a promotional video for the Institute which was featured at the 2016 MRS Spring Meeting March 28-April 1, 2016 in Phoenix, AZ USA. In addition, the video will remain on the MRS website throughout FY2016 in order to increase its visibility. On average, these videos receive about 60,000 hits. I²CNER owns all the rights to the video, so it can also be used to promote the Institute in different ways in the future.

(<http://www.mrs.org/mrs-tv/>)

(https://www.youtube.com/watch?v=xkM6rys_SYM&feature=youtu.be&list=PLGv6BxyFHNv7PX5TGEqaiEhSE9JEzyNg)

Partnerships for International Research and Education (PIRE)

The PIRE program, a cooperative program between NSF and JSPS, is one of the most prestigious and competitive awards amongst the international programs of NSF. PIRE provides funding for international joint research carried out between US universities and their counterparts in Japan in order to generate new knowledge and discoveries; promote a diverse, globally engaged U.S./Japan workforce; and build the institutional capacity of U.S./Japan institutions to engage in productive international collaborations. The joint PIRE award to UIUC

and I²CNER, "Integrated Computational Materials Engineering for Active Materials and Interfaces in Chemical Fuel Production," is a result of I²CNER's successful fusion of computational science with experiment, and was awarded beginning in FY2015 for a total of 5 years. In addition, this is the first PIRE award ever awarded to Kyushu University. The project brings together researchers from Illinois, Kyushu, Northwestern University, Imperial College London, and the University of California at Berkeley. This project is a demonstrable example of the synergistic capabilities of the KU-UIUC partnership, i.e., with the help of the National Center for Supercomputing Applications (NCSA) at UIUC, the PIRE project may be the first in the world in which computations will be carried out using the petascale computing facilities at the University of Illinois concurrently with the experiments being carried out on KU's state of the art equipment at I²CNER, all in an interactive mode. The PIRE Kick-off Meeting took place at UIUC on December 7, 2015, in which Japanese and American researchers planned the research directions for the next year of the project. In FY2015, the framework for the 2-month PIRE exchange program, "x-FU(s)ION," which enables American students to travel to Kyushu, was established and 6 American exchange students are scheduled to visit Kyushu June 1-July 31, 2016.

Air Resources Board of the State of California (CARB)

In October 2015, I²CNER received from CARB a report assessing the Institute's potential for impacting technology. After having reviewed the report, I²CNER's Division Lead PIs have worked with the Energy Analysis Division to compile the Institute's official report. In February 2016, Director Sofronis visited CARB to explore the possibility of initiating closer interactions in the areas of structural materials for refueling stations and catalysis in energy systems. During his visit, Director Sofronis gave 2 technical presentations, 1 each on the aforementioned topics before technical associates of the agency, and 1 general presentation on I²CNER. In addition, Director Sofronis met with Mr. Richard Corey, the Executive Officer of CARB, and Ms. Catherine Dunwoody, the Chief of the Fuel Cells Program of the Agency. I²CNER and CARB agreed during the visit that CARB will continue reviewing our roadmaps and explore further interactions on materials reliability and life prediction, and fuel cells and implementation of hydrogen infrastructure technology. Finally, preliminary plans are in place to hold an annual I²CNER/CARB workshop to enrich our future collaborations.

Interactions with the US Department of Energy (DOE)

- In FY2015, Dr. Somerday, the Division Lead PI of the Hydrogen Materials Compatibility Division, led 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 was responsible for establishing and managing expectations for project objectives, milestones, and work progress through direct communication with the TDMs. Fundamental science that is relevant to a number of these projects is carried out at I²CNER. At the end of FY2015, Dr. Somerday accepted a new position at the Southwest Research Institute (SwRI) in San Antonio, TX. He will continue leading the Hydrogen Materials Compatibility Division from his new post.
- 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.
- On June 23, 2015, I²CNER hosted Dr. Erika Sutherland (Technology Manager at DOE) and Dr. Amgad Elgowainy (Argonne National Laboratory) at Kyushu University. Dr. Sutherland visited I²CNER to explore mutual interests between DOE and I²CNER and the hydrogen testing capabilities that are available at Kyushu University/I²CNER. Dr. Elgowainy shared his experiences with conducting research that is intended to directly influence governmental

policy. In addition to giving presentations, Drs. Sutherland and Elgowainy participated in meetings with I²CNER researchers and were given tours of various Kyushu laboratories, including I²CNER's.

National Fuel Cell Research Center (NFCRC)

NFCRC of the University of California at Irvine and I²CNER collaborate on challenges related to implementation of SOFCs operating in low and high pressure applications at both a systems and catalytic materials level. In particular, research collaboration on cathode and SOFCs/SOECs using proton conducting oxides is under consideration. In order to strengthen the collaborative framework between I²CNER and NFCRC, Prof. Jack Brouwer, the Associate Director of NFCRC, was appointed as a WPI Visiting Professor in FY 2015.

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 unite senior and junior scientists from within and outside of Europe around the goal of promoting education about hydrogen storage. International exchange of young researchers is also a priority of the ECOSTORE. I²CNER PI Etsuo Akiba (Hydrogen Storage Division Lead Principal Investigator) serves as an Associated Partner on the project. In conjunction with the 2-day ECOSTORE workshop that was hosted at KU in March 2015, I²CNER hosted master course student Sascha Dietzel, Helmholtz-Zentrum Geesthacht, Germany from February-September 2015. In addition, Dr. Le Thi Thu, Helmholtz-Zentrum Geesthacht, Germany visited I²CNER from August 20 to September 20, 2015 for her second round of training under the supervision of Prof. Etsuo Akiba.

Helmholtz Institute Forschungszentrum Juelich

I²CNER's interactions with the Helmholtz Institute Forschungszentrum Juelich in Germany were initiated in FY 2015. An initial visit to I²CNER/Kyushu University by a delegation led by Prof. Harald Bolt, a renowned researcher and senior member of the Board of Directors of Helmholtz, took place on July 13, 2015. The Juelich visitors spent a full day at I²CNER, taking extensive lab/facility tours, meeting with KU EVP Wakayama, and video-conferencing with Director Sofronis. Subsequently, I²CNER sent a delegation led by Director Sofronis to Juelich on September 17-18, 2015, and during the visit, the I²CNER team gave presentations at a mini-workshop, and discussed a MoU and plans for pursuing joint funding for graduate student and post-doc exchanges. Since these visits took place, I²CNER and the Helmholtz institute have produced a document that describes potential thematic research areas for future collaboration, which include proton conducting ceramic materials (PCCM) and membranes, oxygen transport membranes, low temperature solid oxide fuel cells and electrolyzers, solid-state batteries, materials for future heat exchangers, and characterization of point defect chemistry and dynamics in non-stoichiometric oxides. The Institutes are in the process of applying for funding, Juelich to the German Ministry of Education, and I²CNER to JSPS, in order to financially support their collaborative activities on faculty and postdoc exchanges.

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.

University of New South Wales (UNSW)

I²CNER's interactions with the University of New South Wales in Australia were initiated in FY2015 as mediated by I²CNER's connection with the Australian Consul in Fukuoka, Mr. Tom Yates. A UNSW delegation, which included the Pro-Vice Chancellor, Fiona Docherty; the Director of International Development, Chris McKenna; the Director of Studies of the Institute of Languages, Adele Pitkeathly; the Australian Consul-General and Trade Commissioner, Tom Yates; and the Australian Consulate-General Business Development Manager, Fumihito Matsumoto; visited I²CNER on June 24, 2015. An additional Australian delegation visited I²CNER on August 7, 2015, including the Chairman of WHTC 2015, Dr. Attilio Pigneri; the Toyota Motor

Corporation Australia Limited Manager of Government and Affairs and Advanced Planning Manager, Andrew Willis and Mario Filipovic, respectively; the Consul-General and Trade Commissioner, Tom Yates; and the Australian Consulate General Business Development Manager, Hirohisa Kato. I²CNER was also visited by the Parliamentary Secretary to the Premier for Western Sydney, Ray Williams, and the Commissioner-Japan in charge of Trade and Investment for New South Wales, Geoff Walker, on October 6, 2015. As part of the Institute's greater efforts to expand its productive collaborations on all continents, I²CNER PIs Hiroshige Matsumoto, Electrochemical Energy Conversion Division, and Etsuo Akiba, Hydrogen Storage Division, represented I²CNER at the World Hydrogen Technologies Convention 2015 (WHTC 2015) October 11-14 in Sydney, Australia, including giving presentations on their I²CNER work. Prof. Akiba also visited UNSW to discuss possible terms for a MOU during the same trip. In addition, 2 UNSW researchers, Profs. Francois Kondo Aguey-Zinsou and Youn Ng gave presentations at the joint I²CNER/UNSW International Workshop at Kyushu University on February 4, 2016. Negotiations for an agreement between Kyushu University and UNSW are currently underway. To advance and seal these collaborations, Director Sofronis and EVP Wakayama plan to visit UNSW in FY2016.

JFE Steel Corporation

I²CNER is collaborating with JFE on fundamental science problems that are related with hydrogen effects on the mechanical behavior of materials. Dr. Akihide Nagao of JFE is a WPI Visiting Scholar of I²CNER in the Hydrogen Materials Compatibility Division. The visit to JFE by Director Sofronis in November 2015 further strengthened this collaboration.

Visit of Dr. Robert Huang

In FY2015, I²CNER was visited by Dr. Robert T. Huang, the Founder of Synnex Corporation and the "Robert T. Huang Entrepreneurship Center (QREC)" of Kyushu University, and an Honorary Doctor of KU. Dr. Huang made his investment in QREC in 2010 in order to develop future entrepreneurial leaders who will make their mark on the international business landscape and by extension, contribute to the overall internationalization of Kyushu University. On January 25, 2016, Dr. Huang visited I²CNER in order to explore our research and familiarize himself with the best work that we are doing. During his visit, he took extensive lab tours, and had a meeting with Director Sofronis and Administrative Director Masuda in order to discuss with them the general I²CNER framework and how I²CNER's permanent position within KU enhances the internationalization of KU from the engineering perspective.

Influence on National and International Policy

PI Etsuo Akiba is playing an important role in an international network for research and development of hydrogen storage materials as an expert adviser of Task 32 for the Hydrogen Implementing Agreement in the International Energy Agency.

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

PI Takeshi Tsuji is a member of the committee of RITE (or the Ministry of Economy, Trade, and Industry), which influences operations standards. In addition, Prof. Tsuji participates in the committee of the Ministry of the Environment that will promote offshore CCS projects around the Japanese Islands. Prof. Tsuji is also a member of the JAMSTEC (or MEXT) committee which promotes the international ocean drilling project. Finally, Prof. Tsuji is a member of the committee on the "International Ocean Discovery Program" (US NSF).

Enhancing I²CNER's Global Perspectives through Personnel

In an effort to further strengthen the EAD's capability to analyze projects related with the societal aspects of generation and utilization of renewable energy on an international scale, the Institute is to hire an outstanding Australian researcher as an Assistant Professor in FY2016. Dr. Andrew Chapman, who will receive his Ph.D. in socio-environmental energy science from Kyoto University, also has previous experience working as a senior policy officer for the government of Australia, with a specific focus on renewable energy policy and infrastructure projects.

Collaborative Foreign Exchange Program

I²CNER's "Collaborative Foreign Exchange Program" is in place in order to encourage young researchers, especially Japanese, to visit our overseas collaborating institutions. The program requires that interested researchers submit a 2-page proposal for review 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 2015, 3 researchers (2 Japanese, 1 non-Japanese) had their proposals to visit the Illinois Satellite approved.

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

One of the most important goals of the I²CNER Seminar Series is to engage key members of the international community from academia, national laboratories, industry, and government agencies (policy makers). In FY2015, the Institute hosted a total of 22 speakers (19 non-Japanese) in 21 I²CNER Seminars. In view of input the Director received from the young faculty on how to improve the accessibility of the series, the Administration implemented a "sign-up sheet" system in FY2015, through which any I²CNER researcher can have a meeting with visiting seminar speakers. The quality of the seminar speakers is exemplified by the following speakers: Prof. Gerard Marriott, University of California, Berkeley, USA; Prof. Olivier Guillon, Director, Institute of Energy and Climate Research, Forschungszentrum Julich GmbH, Germany; Dr. Monterey Gardiner, Liaison Manager (Hydrogen Technology and Homologation), BMW Group Japan; Dr. Valeriy Maisotsenko, Professor Emeritus, Chief Scientist and Founder, Coolerado Corp. and Idalex, Inc., USA; and Dr. Eniya Listiani Dewi, Deputy Chairperson of Technology for Agriindustrial and Biotechnology, BPPT, Indonesia.

Institute Interest Seminar Series (IISS)

In order to advance interdisciplinary research collaborations amongst young researchers, the Institute regularly hosts the "Institute Interest Seminar Series (IISS)." A total of 29 speakers presented at 18 Institute Interest Seminars in FY2015. In response to input from the young faculty, the following changes have been made to the series in FY2015 to try to improve the overall atmosphere:

- An open invitation has been extended to non-I²CNER young faculty within KU to participate in this seminar series in order to expand opportunities for collaboration for our young faculty.
- Additional efforts to advertise the seminar series throughout KU in order to encourage wider participation have also been made, including posting a digital flyer on the I²CNER website, posting physical flyers on all notice boards in the I²CNER buildings, and sending email blasts to the PIs, I²CNER members, the Department of Engineering, the Department of Science,

- and main office of Ito campus via the public relations group.
- There is no longer a time limit for the seminars. Instead, the chairperson is expected to administer the seminar in a way that will encourage more discussion and debate.
- Speakers are 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.
- A monthly lunch hour seminar has been planned beginning in FY2016. The advantage of the lunch hour seminars is that they will allow the researchers to spend more time on the discussion portion of the seminar.
- More general research topics are to be featured, including social sciences, research ethics, etc.

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, 2016, there are 9 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 a retiree from the University of Illinois. In addition, there are 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 (WPI Principal Investigator), and 2) Prof. Ken Christensen, University of Notre Dame (WPI Principal Investigator).

Agreement on Academic Cooperation

The "Agreement on Academic Cooperation" between Kyushu University and UIUC helps the two universities to promote mutual understanding and strengthen their relationship.

EVP Wakayama's Visit to UIUC

May 21-22, 2015, KU EVP Wakayama visited UIUC to familiarize himself with the campus and to begin discussions with the Illinois administration on how to add breadth and depth to the overall engagement between Kyushu and UIUC beyond engineering. EVP Wakayama met with the Provost, Prof. Ilesanmi Adesida; the Vice Provost for International Affairs and Global Strategies, Prof. Reitumetse Mabokela; the Vice Chancellor for Research, Prof. Peter Schiffer; the Associate Chancellor for International and Corporate Relations, Prof. Pradeep Khanna; the College of Engineering Associate Dean for Research, Prof. Jennifer Bernhard; the Director of the Office of Technology Management, Ms. Lesley Millar-Nicholson; the Director of the National Center for Supercomputing Applications, Prof. Ed Seidel; the Director of the Institute for Genomic Biology, Prof. Gene Robinson; the Head of the Industrial & Enterprise Systems Engineering Department, Prof. Rakesh Nagi; the Head of the Math Department, Prof. Matt Ando; and the Director of iSEE, Prof. Evan DeLucia; among others.

Vice Provost Mabokela's Visit to Kyushu University

Continuing the string of visits by high-level Illinois administrators, Prof. Reitumetse Mabokela, UIUC's Vice Provost for International Affairs and Global Strategies, visited KU on June 22, 2015 to explore areas of strategic engagement between Illinois and Kyushu. During her visit to KU,

Prof. Mabokela took I²CNER lab tours, had discussions with our young researchers, and attended meetings with KU EVPs, the Dean of Engineering, the Dean of Languages and Cultures, the Dean of Mathematics, and the Director of the University Library.

Dean Cangellaris' Visit to Kyushu University

In order to explore the possibility of a more comprehensive cooperation between the UIUC College of Engineering and the KU Faculty of Engineering, Prof. Andreas Cangellaris, the Dean of the College of Engineering at UIUC, visited KU on June 30, 2015. During his visit, the Dean toured extensively I²CNER labs and related facilities including HYDROGENIUS, and met with KU EVPs Wakayama and Aoki, and the Dean and Vice Dean of Engineering. On July 1, Prof. Cangellaris traveled to Tokyo to meet with Mr. Tokiwa, the Director-General for the Research Promotion Bureau at MEXT; Dr. Kuroki, the WPI Program Director; and Dr. Asashima, the Executive Director of JSPS. Dean Cangellaris, EVP Wakayama, and Director Sofronis also had discussions with JST technology managers to explore potential interest of JST in the Applied Math for Energy initiative that KU and Illinois are planning.

EVP Aoki's Visit to UIUC

EVP Aoki traveled to Illinois at the invitation of Vice Provost Mabokela to participate in the EducationUSA Leadership Institute July 28-August 9, 2015. For more information on the ongoing EducationUSA initiative between Illinois and Kyushu, please see Section 6 *Kyushu-Illinois Synergy Beyond I²CNER* (EducationUSA).

Tim Barnes' Visit to Kyushu

The UIUC Director of Illinois Strategic International Partnerships, Mr. Tim Barnes, visited I²CNER December 10, 2015. During his visit, Mr. Barnes was given an overview of I²CNER and the WPI Program, took I²CNER lab tours, and had a general discussion with the International Affairs Department at KU Headquarters about the upcoming student and researcher exchange through the PIRE program. Mr. Barnes' trip was catalyzed by the broader EducationUSA initiative. For more details, please see Section 6 *Kyushu-Illinois Synergy Beyond I²CNER* (EducationUSA).

Planned Open Innovation Summit

In cooperation with the UIUC College of Engineering, the I²CNER Satellite is planning an Open Innovation Summit, which has been tentatively scheduled for Spring 2017. The Summit at UIUC will be the first of 2 summits, with the second summit being held in Japan following the initial event. The goal of the Summit is to explore embedding of industry liaisons in I²CNER who could work on potential unrestricted exploratory research projects and technology transfer, and the possible seeding of projects within I²CNER that will serve the long term interests of the company. Discussions on the strategy for the Summit are underway and the Summit Steering Committee has been formed. The Steering Committee will begin meeting in April 2016. Involvement/participation of the US Department of Energy is planned.

Biomimetic Energy Processing (KU-UIUC Joint Proposal)

A joint proposal between Kyushu and Illinois has been written by Profs. Seiji Ogo (KU) and Tom Rauchfuss (Illinois) on a "Biomimetic Energy Processing Initiative." This effort has the strong endorsement of the UIUC Dean of the College of Engineering and the support of the US Embassy to Japan. I²CNER is currently exploring avenues for submitting the proposal to foundations who are known to have interest high risk high return energy research.

US-Japan Institute for Applied Math for Energy (US-Japan IAME)

A joint proposal was developed between Kyushu and Illinois on an Institute for Applied Math for Energy (IAME), specifically on the mathematics of the power grid and mathematical data analysis. The proposal involved researchers from the Illinois Department of Mechanical Science and Engineering, the Illinois Department of Electrical and Computer Engineering, the Illinois Department of Math, and Kyushu University's Institute for Mathematics for Industry. The proposal was developed under the oversight of EVP Wakayama. The proposal was submitted to

the SIMONS Foundation, but was not awarded. Plans are in place and discussions have begun on how to advance and realize initial activities for IAME. Prof. Juliy Baryshnikov, UIUC Electrical and Computer Engineering, will travel to Fukuoka May 21-27, 2016 in order to meet with KU researchers and develop more concrete plans in this regard.

Revised Satellite Agreement

The Kyushu-Illinois Satellite Agreement was renewed and went into effect as of December 1, 2015. The Agreement, which addresses primarily administrative issues, includes a "Master Research Agreement (MRA)" as an attachment, which was written specifically to address how joint research between UIUC and KU is to be administered, including issues related with IP ownership, "Research Project Agreements" (RPAs), etc. The MRA requires all Illinois faculty members to sign RPAs, which outline specific deliverables in a "Statement of Work (SOW)." The spirit of the MRA/RPAs is to unite all Illinois research projects under the same terms and strongly encourage collaboration between Illinois and Kyushu, including mutual exchange, writing of joint papers, use of the I²CNER affiliation in publications, etc. We believe that the signing of the MRA can serve as a model for the entire WPI Program.

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 and UIUC, even beyond engineering. In FY2015, one student from KU's School of Letters visited UIUC for 3.5 months under this program.

3rd Group of Undergraduate Exchange Students hosted at Illinois

From February 24-March 24, 2016, 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. FY2015 was a milestone year for this program because the first 2 female students visited UIUC in this year's group. 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, including weekly lunches with American undergraduate student "buddies." At the end of their stay, the FY2015 group gave presentations on their research and cultural experiences at UIUC in a mini-workshop that involved the I²CNER Director and UIUC graduate students. Due to the success of the mini-workshop, this activity will be added to the program for all future groups of undergraduate exchange students from KU.

Fostering Young Researchers and Advancing their Career Paths

Evaluation of Young Investigators

The research progress of all young faculty members is reviewed by the Director, Associate Directors, and the corresponding Division Lead PI on a regular basis, including an individual face-to-face interview with the Director and Associate Directors near the end of each fiscal year.

Distribution of Funding to Young Faculty

The Director has at his disposal the "I²CNER Competitive Funding," which is intended to foster and advance interdisciplinary research. The Director considers the overall progress and activities of each of I²CNER's full time researchers when making decisions about how to allocate these funds. 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.

In response to the recommendation by JSPS that I²CNER expand beyond engineering into different academic fields, such as mathematics or social sciences, in FY2015, the I²CNER Director decided to utilize the competitive fund to support the Institute's new initiative on Applied Math for Energy. The FY2015 competitive fund call for proposals was open to all faculty of Kyushu University, provided that they proposed a project which was relevant to the stated objectives of I²CNER's Applied Math Initiative. The Institute received several proposals in response to the call, including joint proposals between I²CNER-KU faculty and a few by KU faculty outside of I²CNER. After rigorous screening by the IPRC, 5 applications have been selected as "seed projects," the idea being to foster close, ongoing collaboration between I²CNER and other KU units, in particular, the Institute of Mathematics for Industry (IMI).

The progress of the interdisciplinary projects that were selected in FY2014 was assessed carefully in FY2015, including 1 progress presentation by each researcher who received funds before all of I²CNER, and 1 individual meeting with the Director. After careful consideration of the progress that was made in previously selected projects (FY2012-FY2014), it is the goal of the Director that on a moving forward basis, competitive funds will be awarded only to those researchers who make a truly exceptional proposal, and that the funds will be distributed in slightly larger "chunks" to fund overall fewer projects per year. The FY2015 projects on Applied Math will be evaluated by the IPRC in FY2016.

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 2015.

I²CNER Peer Mentoring: Grant Writing Skills

Historically, the Institute has held special seminars for young researchers on a regular basis to help them improve their proposal-writing skills. In FY 2015, grant-writing skill building was administered on an individual basis to try to increase the Institute's overall success in winning external research funding. More specifically, I²CNER's full-time researchers with a proven track record of winning KAKENHI provided advice/consultation to three young researchers who are newer to the process.

Post-I²CNER Appointments of Young Researchers

In FY2015, many of I²CNER's young researchers leveraged their I²CNER appointments to advance their careers. Some examples are:

- Dr. Kevin White (postdoctoral researcher) accepted a position at Akron Ascent Innovations, USA.
- Dr. Wei Ma (postdoctoral researcher) accepted a position at Wenzhou Institute of Biomaterials and Engineering, China.
- Dr. Alexander Parent (postdoctoral researcher) accepted a position at North Dakota State University, USA.
- Dr. Limin Guo (postdoctoral researcher) accepted a position at Huazhong University of Science and Technology, China.
- Prof. Kiminori Shitashima (Associate Professor) accepted a position at the Tokyo University of Marine Science and Technology, Japan.
- Dr. Fei Jiang (postdoctoral researcher) accepted a position at Yamaguchi University, Japan.
- Dr. Yutaka Yamada (postdoctoral researcher) accepted a position at Okayama University, 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. 4 total students visited KU in FY 2015, including 2 from UIUC and 1 each from Helmholtz-Zentrum Geesthacht, Germany and Institut Teknologi Bandung, Indonesia.

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 fora which 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.

The 2016 I²CNER Annual Symposium, which was titled "Computational Solutions to Fundamental Problems in Carbon-Neutral Energy Research," was held on February 1-2, 2016 and was attended by more than 250 scientists. The vision for this 2-day workshop was to i) bring together experts from the computational and experimental community, and ii) discuss and converge upon the most critical needed advances in computation relevant to the mission of I²CNER. The workshop included 5 sessions, which were organized based on 5 subthemes ("Molecule/Surface Interactions," "Transport of Ions Through Solids and High Temperature Modeling," "Molecule/Molecule Interactions – Charge Transfer and Chemical Reaction Dynamics," "Linking of Atomistic to Continuum Scales," and "Pore-scale Flow Processes"). Attendees broke into small groups in order to discuss/debate issues related with each respective subtheme. Each subtheme group was responsible for writing a report on the outcomes of their discussions. The subtheme reports will be compiled into a "Basic Needs" report on computation in I²CNER, which will be used to guide future initiatives/investments in the area of computation.

On the evening of February 1, a special dinner lecture entitled "Trends in Scientific Computing and Data" was given by Prof. Edward Seidel, the Director of National Center for Supercomputing Applications (NCSA) at UIUC. NCSA plays a key role in the above-mentioned PIRE Program.

- Organization of the 2016 I²CNER in Tokyo symposium is underway in cooperation with the US Embassy. A possible focus of the symposium is how I²CNER can expand its research portfolio, specifically in relation to the fusion of disciplines.
- The 11th Japan-France Workshop on Nanomaterials was held in Rennes, France in May 2015, and 4 WPI institutes (AIMR, MANA, iCeMS and I²CNER) participated. I²CNER was represented by Director Sofronis and Professors Yamauchi and Fujikawa, who all gave presentations at the workshop.
- Director Sofronis and Dr. Somerday are in the midst of planning the 2016 International Hydrogen Conference, which will be held in Jackson Hole, Wyoming (USA) September 11-14, 2016. The International Hydrogen Conference is the premier topical meeting on hydrogen effects in materials.
- Associate Director Takata was the co-chair of the Organizing Committee for the 9th International Conference on Boiling and Condensation Heat Transfer held in Boulder, CO USA April 26-29, 2015.

- Associate Director Takata was the conference chair of the First Pacific Rim Thermal Engineering Conference held in Hawaii, USA March 13-17, 2016.

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.

- *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.
- *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. 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, the Faculty of Pharmaceutical Science, the Institute of Mathematics for Industry (IMI), and the Center for Asia-Pacific Future Studies have already utilized this system. 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.
- *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 3 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.
- *I²CNER 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 in cutting-edge research. The teaching load for I²CNER's young faculty 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 3 years in the framework of the TGU program. This college will encompass both natural sciences and social sciences. We envision that 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.

- *I²CNER's Role in Internationalizing Kyushu University: Effects on Administrative Culture*
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 with the improvement of 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.
- *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 March 1, 2016, 261 Kyushu University faculty (about 12.5%) will be paid within this system. Kyushu University's long-term goal is to pay approximately 20% of its faculty within this system.
- *Travel Expenses for Inviting Researchers from Overseas*
Under the 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 Faculty of Mathematics, and the Faculty of Information Science and Electrical Engineering have all issued increased per diem payments to world-renowned visiting researchers in FY 2015.

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)

○ *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 developed an energy-related plan centered on I²CNER. In addition, KU will "proactively advance collaboration and cooperation between I²CNER and other diverse fields/domains, such as natural science (especially theory), mathematics, humanities, and social sciences, etc., and will further improve its research system by leveraging the experience of the Kyushu University Administration."

○ *I²CNER'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, which will inform and support 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 the very concept of the faculty council system in Japan.

○ *President Kubo's Vision*

I²CNER is 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 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 can consider hosting Faculty Fellows at the PI level.

○ *I²CNER Synergy with Kyushu University*

Under the advisement of the KU President, meetings are underway with other Kyushu University units and the Executive Vice President for Research and Industry Collaboration 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.

○ *Securing and Filling I²CNER Tenured Faculty Positions*

Kyushu University implements the "University Reform Revitalization Program (URRP)" 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. In FY2015, the KU Administration structured its call for the URRP program strategically in order to prioritize different units of KU, including I²CNER. Specifically, Track 1 of the call was focused on the creation of an intra-university center on energy (please see *ONGERE* below), I²CNER, and cybersecurity and relevant education aspects.

In general, the Institute has been successful at winning and filling positions through this program. By the end of FY2015, I²CNER had filled a total of 4 Associate Professor and 2 Full Professor positions, with 2.283 points (approximately 3 positions) left to fill. In addition, the Institute won 1.79 additional points (1 Full Professor position and 1 Associate Professor position) to fill in FY2016 as a result of the proposal that was submitted at the end FY2015. One additional assistant professor position was awarded to I²CNER as a result of a joint IMI-I²CNER proposal to Kyushu University (please see *IMI-I²CNER Tenure-Track Positions on Applied Math for Energy* below for details). In sum, I²CNER has filled 6 tenured positions and has the potential to hire up to 6 more tenured faculty with the points that it has been awarded so far. The Kyushu University administration has stipulated that at least 2 of the tenured positions that I²CNER fills must be occupied by foreign PIs (1 of these positions has already been filled in FY2015).

Specifically, in FY2015, 1 tenured foreign PI position and 1 tenured Associate Professor Position were filled. The Institute appointed Prof. Bidyut Saha as a permanent-staying foreign PI with tenure as of January 1, 2016. Prof. Saha is a pioneer in the field of adsorption science and technology with seminal contributions in the development of processes, devices, systems and technologies for the application of adsorption principles for heat and mass transfer, waste heat recovery and storage for stationary and mobile applications, thermally driven refrigeration and air-conditioning, clean water harvesting, and solar thermal energy utilization. In view of the fact that energy efficiency increase is part of the foundation of the research roadmap of I²CNER, Prof. Saha's expertise on exploiting low grade thermal energy is a solid addition to I²CNER's team, and he will undoubtedly make significant contributions to the Institute's research mission. The strong external evaluation

letters we received in support of Prof. Saha's appointment are further proof of the outstanding quality of Prof. Saha's research accomplishments and potential to facilitate transformative change across I²CNER's research divisions.

The Institute also promoted Prof. Aleksandar Staykov, one of our most promising young foreign faculty members, to the position of the Associate Professor with tenure in the Molecular Photoconversion Devices Division as of January 1, 2016. Dr. Staykov, who is I²CNER's chief computational analyst, will help I²CNER build and expand strong computational capabilities across division boundaries.

- *IMI-I²CNER Tenure-Track Positions on Applied Math for Energy*
As was mentioned above, the Institute of Mathematics-for-Industry (IMI) and I²CNER worked together to submit a joint proposal to KU's newly initiated tenure-track faculty program, which resulted in 2 tenure-track assistant professor positions being awarded (1 each for IMI and I²CNER). The IMI-I²CNER proposal was selected from among 24 applicants at the final screening, which was held in March 2016. There will be a 5-year probation period for each position, which will be followed by promotion of the hired researcher to a tenured associate professor position if all criteria are met by the end of the probationary period.
- *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 are viewed as prestigious positions in Kyushu University. By way of example, I²CNER was recently awarded a tenured position for a mathematician through its joint proposal with IMI (please see above *IMI-I²CNER Tenure-Track Positions on Applied Math for Energy*).
- *Leveraging I²CNER infrastructure and international visibility to compete for research funding*
With regard to securing revenue, I²CNER researchers leverage the established infrastructure, research culture, and international visibility of the Institute to aggressively pursue funding. By way of example, three new major I²CNER research programs are: i) The JST-CREST Grant awarded to Profs. M. Yamauchi and N. Nakashima at a level of ~ 180 million JPY for the next five years; ii) the Research Center for Next Generation Refrigerant Properties (Next-RP) awarded to Profs. Y. Takata and S. Koyama at a level of 100 million JPY/year for 5 years beginning in FY2017 (METI has not yet made a decision on the proposal); iii) the joint PIRE program awarded by the US NSF and JSPS to researchers at Illinois and Kyushu at a level of ~ 495 million JPY over the next 5 years (4.5 million USD at an exchange rate of 110 JPY). Additional current and planned research center activities within I²CNER are: i) the Center for Small Molecule Energy (CSME) directed by Prof. Ogo and ii) the "International Research Center of Giant Straining for Advanced Materials (IRC-GSAM) that Prof. Horita is planning. 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 tenured faculty members whose research is impactful to the corporation's operations (e.g. Air Liquide's support of Prof. Alex Staykov). Further, as stated above, if the planned Open Innovation Summits are successful, I²CNER may establish a number of open innovation relationships with companies wherein the company may fund tenured position(s) in I²CNER or the company may pay for one of its employees to be immersed in I²CNER laboratories (for more details, please see *Open Innovation Summit* under the Role of the University of Illinois at Urbana-Champaign (UIUC) Satellite in Section 3). It is the vision of the Director that the main source of funding for the sustainability of I²CNER will be embedded centers that will be established by leveraging the ongoing and new initiatives of major sponsors, such as the government or large corporations. Not only will this allow I²CNER to sustain itself, but it will also provide the opportunity for I²CNER to evolve and accommodate breakthroughs in carbon-neutral energy technology and/or shifting priorities of the international scientific community and

the funding agencies. In other words, the Director's vision is that I²CNER will remain strong and agile by developing a core of embedded centers that will last beyond the WPI funding period.

○ *Options for long-term funding of I²CNER*

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

1. 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. For example, Kyushu University and the University of Illinois were awarded a joint NSF Partnerships for International Research and Education (PIRE) grant in FY 2015. In addition, Profs. Stephen Lyth (KU), Paul Kenis (UIUC), Andy Gewirth (UIUC), and Hong Yang (UIUC) applied to the WPI Progress 100 program in FY 2015.
2. 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.
3. 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).
4. Resources from technology transfer or patent sales. The Academic Research and Industrial Collaboration Management Office of Kyushu University (AiRIMaQ), which is under the direction of the Executive Vice President for Research and Industry Collaboration, is expected to play an active role in this development.
5. 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.
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. For more details, please see *Open Innovation Summit* under the Role of the University of Illinois at Urbana-Champaign (UIUC) Satellite in Section 3.

○ *Sustainability of I²CNER through 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, and 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 Academic Research and Industrial Collaboration Management Office of Kyushu University (AiRIMaQ) and the Office of Technology Management (OTM) of the University of Illinois has already started. AiRIMaQ and OTM agreed upon the IP management terms that are laid out in the revised I²CNER Satellite Agreement that went into effect on December 1, 2015.

○ *Maintaining the International Standard of I²CNER*

To attract leading researchers from overseas universities and research institutes to I²CNER, new initiatives, such as 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.

○ *I²CNER Director's Authority and Access to the KU President*

The Institute Director, Prof. Sofronis, has direct access to the Office of the President and the Office of the Executive Vice President (EVP) in charge of Research and Industry Collaboration. Regular meetings are held between the Director and the EVP in charge of Research and Industry Collaboration. Advice and counsel from the President is given as needed. 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. With regard to matters relating to the promotion of university-industry collaboration, the EVP in charge of Research and Industry Collaboration provides 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. 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 EVP in Charge of Research and Industry Collaboration is working to further strengthen awareness and support of I²CNER amongst the other Vice Presidents.

○ *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 FY 2014. I²CNER is the only permanent research institute at Kyushu University that has its own support office.

○ *Support from KU's Office for Strategic Research Planning*

The Office for Strategic Research Planning and other related offices of Kyushu University 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. Examples are the recently established Centers within I²CNER led by Profs. Yamauchi and Nakashima, and Takata and Koyama. In addition, the Office will continue to assist I²CNER in its efforts to compete for research funds from the local government and industries in related areas.

○ *I²CNER 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.

- *Organization for Energy Research and Education (ONGERE)*
In order to integrate research efforts and education on energy across its various units, KU established the "Organization for Energy Research and Education" (ONGERE) as of April 1, 2016. I²CNER is expected to play a central role in this new organization by helping to promote and advance a wide range of collaborations on energy research with other units of Kyushu University, thus capitalizing on potential opportunities to broaden and enrich its energy portfolio.

- *I²CNER's Place in Kyushu University Infrastructure*
Both I²CNER Buildings 1 & 2 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. The KU Administration is located at Shiiki Hall, which is adjacent to the I²CNER Buildings. Also in the same vicinity are KU's Center of Innovation (COI) project, the Center for Co-Evolutional Social Systems (CESS), and the new central library, which is under construction with a planned completion date in FY 2018. In short, the I²CNER buildings are placed very strategically amongst the newest infrastructure at Kyushu University.

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.

Director's Physical Presence

In FY 2015, the Director made 11 trips and spent a total of 113 days of his time in Japan (50.4%).

External Advisory Committee (EAC)

The membership of I²CNER's External Advisory Committee was further expanded and diversified in FY 2015 to better align with all aspects of the Institute's research. In April 2015, Prof. Michael Celia, Princeton University, expert on CO₂ storage and 2007 Nobel Laureate, specifically on pore scale behavior and upscaling to reservoir behavior, officially accepted our invitation to serve on the EAC. Prof. Celia made his first visit to I²CNER on January 29, 2016 and spent the day taking lab tours, attending presentations and engaging in discussion with members of the CO₂ Storage Division, and giving a seminar in the I²CNER Seminar Series, which was filmed and presented again on February 2 as part of the pore scale flow processes subtheme session of the 2016 I²CNER Annual Symposium.

Mr. Mark Paster, a former US DOE Energy Analyst, resigned his post on the EAC in February 2016. Upon Mr. Paster's resignation and subsequent recommendation, Dr. Monterey Gardiner, BMW Japan, was invited to serve on the EAC and give input specifically on technoeconomics of energy and any other area to which he wishes to contribute. Dr. Gardiner, who is a former Technology Manager for the US DOE and current Liaison Manager for BMW, officially accepted our invitation as of February 29, 2016.

The Institute's 4th EAC Retreat was held at UIUC on March 9-10, 2016, and involved 8 of the 10 members of the EAC (Prof. Adrian and Prof. Armstrong were unavailable to attend). The purpose of the retreat was to assess the current status and progress of I²CNER projects, and actions we can take to position ourselves strategically for a third term beyond 2020. The EAC offered constructive feedback on all aspects of the Institute, including the Institute's structure,

technical issues, and administrative matters. As of April 1, the EAC is working on finalizing its retreat report. The Director expects to receive the final report by the end of May 2016. Already, the input from the EAC has been distributed to all the Division Lead PIs in the form of a Powerpoint presentation.

The full list of members as of April 1, 2016 is as follows:

- Prof. Ronald J. Adrian (Chair), Arizona State University, USA, *National Academy of Engineering (NAE)*
- Dr. Deborah Myers (Co-Chair), Argonne National Laboratory, USA
- Dr. Robert J. Finley, Illinois State Geological Survey, USA
- Prof. Reiner Kirchheim, University of Göttingen, Germany
- Prof. Robert McMeeking, University of California, USA, *National Academy of Engineering (NAE)*
- 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)*
- Prof. Michael Celia, Princeton University, USA, *Nobel Laureate*
- Dr. Monterey Gardiner, BMW Japan (formerly with DOE), Japan

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) was revisited in order to make it more efficient, so as to enable it to reach more concrete and evaluative conclusions (e.g. more critical assessments of underperforming research efforts). The IPRC completed a "deep dive" review of all individual research efforts in the Institute in FY2015 and the Director is in the process of assessing "next steps" based upon this input from the IPRC. In addition, the IPRC is currently carrying out a "deep dive" review of all individual division projects in order to ensure the relevance of the I²CNER roadmaps to the I²CNER mission. The review will be completed and acted upon in FY2016.

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.

FY2015 Recruitment Campaigns

In FY2015, the Institute ran 1 open recruitment campaign for foreign PIs out of which we received 15 applications and made 1 hire. Similarly, the Institute ran 1 open recruitment campaign for faculty positions out of which we received 26 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 3 recruitment campaigns specifically for researchers for the Energy Analysis Division which resulted in 15 applications for faculty positions and 10 applications for postdoc positions, and 1 hire is expected to be made in FY2016.

NEXT-RP (Center for Next Generation Refrigerant Properties)

Profs. Y. Takata and S. Koyama have proposed the Center for Next Generation Refrigerant Properties (NEXT-RP) at a funding level of 100 million JPY/year for 5 years. If awarded, the project will begin in FY2017. The project will be funded by the New Energy and Industrial Technology Development Organization (NEDO), which is part of the Manufacturing Industries Bureau of METI. The objectives of the center will be: accurate evaluation of thermophysical properties and fundamental performance of heat exchange and air conditioning and refrigeration (ACR) cycle for zero-ODP and low-GWP refrigerants; organizing the R&D national research group led by Kyushu University; development of base knowledge and technology for thermophysical properties, performance of heat exchange, and the fundamentals of the ACR cycle; technology transfer and assistance to ACR industrial sectors; and contributions to Japanese ACR industries to make them more competitive in the global market. Other I²CNER researchers involved in the project are PI B.B. Saha and WPI Professor M. Kohno.

Asian Pacific Innovation Conference

In FY2015, I²CNER researchers worked cooperatively with the office of KU EVP Aoki on planning the 7th Asian-Pacific Innovation Conference (APIC), which will be held in Fukuoka on November 18-20, 2016. The event will be co-hosted by I²CNER and the Center for Science, Technology and Innovation Policy Studies (CSTIPS) of Kyushu University. This initiative is one example of I²CNER's effort to broaden our engagement with KU and will further strengthen our ties.

Kyudai Asian Studies Seminars

Director Sofronis has been invited to give a talk in the "Kyudai Asian Studies Seminars," which is an inter-disciplinary series of open seminars on the Asia-Pacific region and Japan. The series was initiated by the Department of Education, Faculty of Human-Environment Studies of Kyushu University. The seminar talks are conducted in English for a general audience on a variety of Asia-related (including Japan-related) topics, and provide an opportunity to hear general research presentations from all academic disciplines. Director Sofronis' seminar is planned during FY2016.

Director's Involvement in Teaching/Education at Kyushu University

Director Sofronis engages in KU education at every opportunity, and has given 2 lectures (1 each in FY 2013 and 2015) to the "Global 30" students of the School of Engineering ("Advanced Engineering A"). On February 5, 2016, Director Sofronis' lecture addressed general issues of materials response in chemomechanical environments.

Faculty Promotion Process

I²CNER's promotion process is based upon the process used at Illinois, which adheres to the high standards that are typical at top US universities. The process, which involves a confidential assessment by world-leading scientists from the international community in the candidate's area of expertise, is carried out by a promotion committee involving senior faculty members from both KU and Illinois. Following this process, 6 of I²CNER's young researchers were promoted in FY 2015 (5 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, 2016 (1 from Postdoctoral Researcher to Assistant Professor and 1 from Assistant Professor to Associate Professor).

Satellite Advisory Committee

The I²CNER Satellite Advisory Committee has been in place since the inception of the Institute. The committee members are Andrew Gewirth of UIUC and Ken Christensen of the University of Notre Dame. 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. The Director meets with all or part of the Committee on an ad-hoc basis.

Kyushu-Illinois Synergy Beyond I²CNER

EducationUSA

Following the visit of UIUC Vice Provost for International Affairs, Prof. Reitu Mabokela, to Kyushu University in June 2015, KU Executive Vice President Reiko Aoki was invited to visit UIUC in July 2015 to participate in the EducationUSA Leadership Institute at Urbana-Champaign, which was administered by Vice Provost Mabokela's office. EVP Aoki also participated in the 2 follow-on virtual trainings that were held in September 2015. As a result of these interactions and the efforts of Vice Provost Mabokela and EVP Aoki, Kyushu University, Nagoya University, and Hitotsubashi School of Social Sciences in Tokyo have been awarded an EducationUSA Leadership Institute follow-on grant from the US Department of State in order to found an Institute which will focus on developing strategic partnerships and sustaining inter-university relationships. As part of this project, the Director of Illinois Strategic International Partnerships, Mr. Tim Barnes, spoke at workshops in Japan in 2015. In July of 2016, the UIUC Director of Global Education and Training, Mr. Matt Rosenstein, and the UIUC Assistant Director for International Safety and Security, Ms. Andrea Bordeau, are scheduled to attend further training workshops in Japan.

NASA Astrobiology Institute Joint PhD student

In addition, there is a broader engagement beyond I²CNER between Kyushu University and the University of Illinois. By way of example, Ms. Miyako Shiraishi, a PhD student in the area of DNA replication and repair in the NASA Astrobiology Institute, which is part of the Institute for Universal Biology and the larger Institute for Genomic Biology at Illinois, is at Illinois working toward her PhD under the co-supervision of Dr. Isaak K. O. Cahn (UIUC) and Yoshizumi Ishino (KU). Ms. Shiraishi is scheduled to complete her PhD within 3 years.

Inroads for KU-UIUC Collaboration on Agriculture

The KU Faculty of Agriculture is in the process of launching a collaborative project called the "Establishment of a gateway for the inbound education program of agriculture." The primary objective of the program is to create opportunities to invite foreign students to KU, with the first exchanges taking place in 2018. Initial primary research topics in the program include bio-agriculture, functional food, and smart farming, though the scope of the program is expected to broaden as it matures. Though no academic degree can be conferred through the program, it will be accredited. The program will be funded at a level of ~2 million USD for the first four years. KU is in discussions with several major universities, including UIUC, about using this program as a framework for future collaboration in the area of agriculture.

7. Center's response to the site-visit report

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

1. More basic scientists such as mathematicians, theoreticians and perhaps social scientists should be invited soon.

In Kyushu University's Mid-term Plan, it is specifically mentioned that one of KU's goals is to "enhance research in the area of carbon-neutral energy, by collaborating with other fields such as theory, mathematics, humanities and social sciences, and by reinforcing and envisioning its international research capabilities in every aspect." Specific efforts that were made by I²CNER in this regard in FY2015 include:

1. The Competitive Fund was used to fund projects on Applied Mathematics for Energy (for more details, please see Section 3, *Distribution of Funding to Young Faculty*).
2. I²CNER won 1 joint tenured position with the Institute of Mathematics for Industry (IMI) and hiring efforts are ongoing (for more details, please see Section 5, *IMI-I²CNER Tenure-Track Positions on Applied Math for Energy*).

3. KU and UIUC researchers submitted a joint proposal to the Simons Foundation on Applied Math for Energy (for more details, please see Section 3, *US-Japan Institute for Applied Math for Energy (US-Japan IAME)*).
 4. I²CNER has been given two tenured positions that are earmarked for a computational scientist and an expert on the smart power grid (applied math, renewable integration to the grid). Recruitment efforts are in progress (the previous recruitment call closed on March 31, 2016).
2. At this stage, it is important to ensure sustainability of the center following the end of WPI funding.
Please see Section 5, *Options for long-term funding of I²CNER*.
3. A study should be advance on societal needs to include experts in environment, sociology and mathematics.
Please see the above response to 7.1.
4. The theme "environment" embodies a concrete domain of research, whose advancement can be expected to contribute to society. In this context, collaboration with industry is extremely important. Some of the technologies regarded as matured should be transferred to industry. A Technology Transfer plan should be considered.
I²CNER has been involved in "open innovation" interactions and collaborative projects with industry from the time of its inception. FY2015 was a landmark year with regard to technology transfer. Evidence of our success in promoting technology transfer in FY2015 can be seen in the following examples: I²CNER researchers are involved with industry through 57 collaborative research projects; a total of 22 of these projects resulted in technology transfer events and 9 such representative events (one from each division) are listed in Section 1; 8 additional collaborative projects with industry (5 in the CO₂ Capture and Utilization division, 1 in the Hydrogen Storage division, and 2 in the Electrochemical Conversion Division) may also result in technology transfer. These technology transfer activities constitute dramatic improvement relative to those in FY2014, in which 4 transfer events were reported.
In cooperation with the UIUC College of Engineering, the I²CNER Satellite is planning an Open Innovation Summit, which has been tentatively scheduled for Spring 2017. The Summit at UIUC will be the first of 2 summits, with the second summit being held in Japan following the initial event. The goal of the Summit is to explore the embedding of industry liaisons (preferably from companies with operations both in Japan and the US) in I²CNER who could work on potential unrestricted exploratory research projects and technology transfer, and the possible seeding of projects within I²CNER that will serve the long term interests of the company. Discussions on the strategy for the Summit are underway and the Summit Steering Committee has been formed. The Steering Committee will begin meeting in April 2016. Involvement/participation of the US Department of Energy is planned.
5. The increase of full-time researchers at I²CNER is highly appraised, but the number of foreign researchers still needs to be increased.
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. In FY2015, I²CNER hired Prof. Bidyut Saha as a tenured foreign PI in the Institute. I²CNER also gave tenure to a foreign associate professor, Prof. Alex Staykov. It should be noted that in principle, we shall never compromise our standards for I²CNER's established research culture in our pursuit of foreign PIs. Recruitment efforts are in progress (the previous recruitment call closed on March 31, 2016).

List of Center's Research Results and Main Awards

A. Refereed Papers

List only the Center's papers published in 2015. (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 2015, 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 .csv 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 2015.
 - 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 articles
 5. Articles written in other than English

Note: This list includes the refereed papers published in the calendar year 2015 either online or in print whichever comes first.

No.	Description
	A. WPI papers
	A.1. Original articles
1	Chouwatat, P., Nojima, S., Higaki, Y., Kojio, K., Hirai, T., Kotaki, M. and Takahara, A. (2016), An effect of surface segregation of polyhedral oligomeric silsesquioxanes on surface physical properties of acrylic hard coating materials, <i>Polymer</i> , 84, 81-88.
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668	Shi, Y., Garbayo, I. and Rupp, J.L.M. (2015), Role of lattice strain vs. solid solution doping on atomistic near order and oxygen ionic transport for ceria-based micro-energy conversion membranes, ECS Transactions, 68 (1), 2565-2572.
669	Cook, S.N. and Tuller, H.L. (2015), The Direct Measurement of Ionic Piezoresistance, Materials Research Society Symposium Proceedings, 1730, 7-13.
670	Kabir, K.M.A., Alam, K.C.A., Sarker, M.M.A., Rouf, R.A. and Saha, B.B. (2015), Effect of Mass Recovery on the Performance of Solar Adsorption Cooling System, Energy Procedia, 79, 67-72.
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672	Sultan, M., Miyazaki, T., Saha, B.B., Koyama, S. and Maisotsenko, V.S. (2015), Steady-state Analysis on Thermally Driven Adsorption Air-conditioning System for Agricultural Greenhouses, Procedia Engineering, 118, 185-192.
673	Jribi, S., Miyazaki, T., Jerai, F., Saha, B.B., Koyama, S., Maeda, S. and Maruyama, T. (2015), CFD Simulations of Heat Exchanging Adsorber/Desorber Employing Activated Carbon-Ethanol Pair, 2015 JSRAE Annual Conference, C143-1-4.
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675	Shi, L., Dames, C., Lukes, J.R., Reddy, P., Duda, J., Cahill, D.G., Lee, J., Marconnet, A., Goodson, K.E., Bahk, J.-H., Shakouri, A., Prasher, R.S., Felts, J., King, W.P., Han, B. and Bischof, J.C. (2015), Evaluating broader impacts of nanoscale thermal transport research, <i>Nanoscale and Microscale Thermophysical Engineering</i> , 19 (2), 127-165.
676	Lee, S.-W., Wang, T., Selyanchyn, R., Korposh, S. and James, S.W. (2015), Optical fiber sensing of human skin emanations, <i>Proceedings of SPIE - The International Society for Optical Engineering</i> , 9655, 96551K.
677	Kitamura, K., Honda, H., Takaki, S. and Mitani, Y. (2015), Experimental study of two-phase fluid flow in the porous sandstone by P-wave velocity and electrical Impedance measurement, <i>Proceedings of the 12th SEGJ International Symposium</i> , 174-176.
678	Choi, J., Amir, E., Xu, T. and Valocchi, A.J. (2015), Learning relational Kalman filtering, <i>Proceedings of the National Conference on Artificial Intelligence</i> , 4, 2539-2546.
679	Asakawa, K., Hyakudome, T., Ishihara, Y. and Nakamura M. (2015), Development of an underwater glider for virtual mooring and its buoyancy engine, <i>2015 IEEE Underwater Technology</i> , UT 2015, 7108263.
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681	Kitamura, K., Nishizawa, O., Ito, T. and Finley, R.J. (2015), Heterogeneous two-phase flow in homogeneous porous sandstone, <i>3rd International Workshop on rock physics</i> .
682	Wang, J., Cai, X. and Valocchi, A. (2015), Spatial evolutionary algorithm for large-scale groundwater management, <i>Genetic and Evolutionary Computing</i> , 329, 131-142.
683	Matsuoka, K., Nakamura, M., Nishi, H., Mochizuki, S., Ueda, T. and Sawada K. (2015), Research of gliding performance of the plesiosaurus, <i>Proceedings of the International Offshore and Polar Engineering Conference, 2015-January</i> , 502-509.
684	Mo, K., Tung, H.-M., Chen, X., Yun, D., Miao, Y., Chen, W., Aimer, J., Novak, A. and Stubbins, J.F. (2015), In-situ synchrotron X-ray study of the elevated temperature deformation response of SS 316L pressurized creep tubes, <i>ASTM Special Technical Publication, STP 1576</i> , 244-255.
	B.4. Other English articles (Book chapters)
685	Adachi, C., Lee, S., Nakagawa, T., Shizu, K., Goushi, K., Yasuda, T. and Potscavage, W.J. (2015), Organic light-emitting diodes (OLEDs): Materials, photophysics, and device physics, <i>Organic Electronics Materials and Devices</i> , 43-73.
686	Yagi, K. (2015), Tribology: Friction, wear and lubrication, <i>Hydrated Materials: Applications in Biomedicine and the Environment</i> , 19-32.
	B.5. Articles written in other than English (Articles in Japanese)
687	Kikuchi, M., Kawaguchi, S. and Takahara, A. (2015), Molecular Conformation of Polysulfobetaine Brushes Immobilized on SiO ₂ Nanoparticles, <i>Journal of the Japan Society of Colour Material</i> , 88 (10), 341-347.
688	Yamamoto, S., Kubozono, T., Kojo, K. and Takahara, A. (2015), Development of Total Internal Reflection Raman Microscope with an Apparatus for Adhesion Test and Changes in Depolarization Ratio of Polymer Brush by Compressive Force, <i>Kobunshi Ronbunshu</i> , 72 (11), 673-680.
689	Moriga, T., Aoyama, N. and Tanaka, K. (2015), An Effect of R-value (NCO/OH Molar Ratio) on Sealing Properties of Polyurethane Gaskets, <i>Journal of the Society of Rubber Science and Technology, Japan</i> , 88 (7), 257-262.
690	Tsuwaki, M., Kasahara, T., Edura, T., Oshima, J., Kunisawa, E., Ishimatsu, R., Matsunami, S., Imato, T., Adachi, C., Shoji, S. and Mizuno, J. (2015), Fabrication of a Portable Electrochemiluminescence-induced Fluorescence Detection Chip with Microfluidic Excitation Source for Point-of-care Diagnostics, <i>IEEJ Transactions on Sensors and Micromachines</i> , 135 (6), 230-235.
691	Sato, T., Akamine, K., Takahara, A. and Otsuka, H. (2015), Macromolecular Design of Alkoxyamine-containing Radically Reactive Polymers Based on Dynamic Covalent Chemistry, <i>Kobunshi Ronbunshu</i> , 72 (6), 341.
692	Yamabe, J., Awane, T., Itoga, H., Matsunaga, H. and Matsuoka, S. (2015), Hydrogen diffusion behavior of various austenitic stainless steels, <i>JCOSSAR 2015</i> , 134-141.

693	Ogawa, Y., Matsunaga, H., Yoshikawa, M., Yamabe, J. and Matsuoka, S. (2015), Effect of high-pressure hydrogen gas environment on fatigue life characteristics of low alloy steel SCM435 and carbon steel SM490B, <i>JCOSSAR</i> 2015, 142-147.
694	Matsunaga, H. Kuwano, Y., Ogawa, Y., Itoga, H., Yamabe, J. and Matsuoka, S. (2015), Fatigue crack growth properties of high-strength austenitic stainless steel HP160, <i>JCOSSAR</i> 2015, 148-153.
695	Fukuda, K. (2015), Influences of hydrogen environment on the friction and wear of metallic materials, <i>Toraibarojisuto/Journal of Japanese Society of Tribologists</i> , 60 (10), 632-637.
696	Sawae, Y. (2015), Friction and wear of polymers in hydrogen environment, <i>Toraibarojisuto/Journal of Japanese Society of Tribologists</i> , 60 (10), 638-644.
697	Kawano, R., Kaneko, K., Hara, T., Yamada, K., Sato, Y., Higashida, K. and Kikuchi, M. (2015), Decorated dislocations with fine precipitates observed by FIB-SEM slice-sectioning tomography, <i>Tetsu-To-Hagane/Journal of the Iron and Steel Institute of Japan</i> , 101 (8), 422-425.
698	Yamaguchi, T. (2015), Dynamics of Adhesion and Debonding, <i>Koubunshi</i> , 64 (6), 350.
699	Narasaki, M., Ikuta, T., Nishiyama, T. and Takahashi, K. (2015), Thermal Transport in an Individual Multi-Walled Carbon Nanotube Defected by Focused Ion Beam Irradiation, <i>Japan Journal of Thermophysical Properties</i> , 29 (4), 179-184.
700	Yamada, Y., Kusaba, A., Ikuta, T., Nishiyama, T., Takahashi, K. and Takata, Y. (2015), Study of condensation on hydrophobic surface with nanoscale hydrophilic regions, <i>Transactions of the JSME</i> , 81 (823), 14-00495.
701	Ishikawa, H., Nakatani, J., Kikuchi, Y. and Hirao, M. (2015), Recycling system design that incorporates robustness and flexibility against variation risk, <i>Haikibutsu Shigen Junkan Gakkai Ronbunshi</i> , 26, 1-15.
	B.5. Articles written in other than English (Article in Chinese)
702	Jia, L., Tang, D.-W. and Zhang, X. (2015), Experimental study of ultrafast carrier dynamics in polycrystalline ZnTe nanofilm, <i>Wuli Xuebao/Acta Physica Sinica</i> , 64 (8), 087802.
	B.5. Articles written in other than English (Review articles in Japanese)
703	Kawaguchi, D. and Tanaka, K. (2015), An Importance of Polymer Chemistry to Adhesion Phenomena, <i>Journal of the Adhesion Society of Japan</i> , 51 (9), 434-440.
704	Semoto, T., Yamauchi, T. and Yoshizawa, K. (2015), Molecular Dynamics Study on Mechanisms of Interfacial Adhesion between Poly (<i>p</i> -phenylene sulfide) and Epoxy Resin, <i>Journal of the Adhesion Society of Japan: Adhesion</i> , 51 (3), 80-88.
705	Nakanotani, H. and Adachi, C. (2015), High performance organic light-emitting diodes based on thermally-activated delayed fluorescence materials, <i>Journal of the Vacuum Society of Japan</i> , 58 (3), 73-78.
	B.5. Articles written in other than English (Proceedings in Japanese)
706	Yoshida, A., Fujio, Y. and Xu, C.-N. (2015), Development of novel mechanoluminescent fibers, <i>Phosphor Research Society, The 359th Meeting Technical Digest</i> , 7-12.
707	Tanaka, K. and Kojio K. (2015), The 45th summer seminar - For realization of sustainable society by time- and space-domain controls of fibers, <i>Sen'i Gakkaishi</i> , 71 (6), 267.
708	Kawaguchi, D. and Tanaka, K. (2015), Surface and Interfacial Effects on Chain Dynamics in Thin Films, <i>Journal of the Adhesion Society of Japan</i> , 51 (5), 144-150.
	B.5. Articles written in other than English (Book chapters in Japanese)
709	Shundo, A. and Tanaka, K. (2015), Physical properties and mesoscopic heterogeneity of supramolecular hydrogels, <i>Frontier in Self-assembled Materials</i> .
710	Higaki, Y. and Takahara, A. (2015), Polymer Prush, <i>New Tribology Materials, Tribology Design Manual</i> , 403-406.
	B.5. Articles written in other than English (Magazine articles in Japanese)
711	Shundo, A. (2015), Interdisciplinary research fields, <i>Kobunshi</i> , 64 (11), 719.
712	Ishihara, T. (2015), New Oxide Ion Conductor, <i>Chemistry</i> , 70 (4), 70-71.

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

- List up to 10 main presentations during FY2015 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	Nicola H. Perry, Evaluating Thin Film Defect Equilibria and Kinetics by In Situ Optical Transmission: Application to Sr(Ti,Fe)O _{3-δ} Electrodes, 40th International Conference and Exposition on Advanced Ceramics and Composites (ICACC), Daytona Beach, USA, Jan. 27, 2016 (Invited).
2	Shigenori Fujikawa, Molecular separation by a free-standing and nanometer-thick membrane, The International Chemical Congress of Pacific Basin Societies 2015 (Pacifichem2015), Honolulu, USA, Dec. 17, 2015 (Invited).
3	Miho Yamauchi, Catalyst Development For the Realization of Carbon-Neutral Energy Cycles, The International Chemical Congress of Pacific Basin Societies 2015 (Pacifichem2015), Honolulu, USA, Dec. 16, 2015 (Invited).
4	Masanobu Kubota, Fretting Fatigue in Hydrogen and the Effect of Impurity Addition to Hydrogen on Fretting Fatigue Properties, 3rd World Congress on Petrochemistry and Chemical Engineering, Atlanta, USA, Dec. 2, 2015 (Plenary).
5	Yasuyuki Takata, Thermophysical Property Measurement of High Pressure Hydrogen up to 100MPa, 3rd International Workshop on Heat Transfer Advances for Energy Conservation and Pollution Control, Taipei, Taiwan, Oct. 17, 2015 (Plenary).
6	Etsuo Akiba, Hydrogen and Fuel Cell Developments in Japan, World Hydrogen Technologies Convention (WHTC 2015), Sydney, Australia, Oct. 13, 2015 (Plenary).
7	Kenshi Itaoka, Focus groups and interviews with stakeholders of the Tomakomai CCS project before the decision on the project site, International Energy Agency (IEA) Greenhouse Gas R&D Programme, The 5 th Social Research Network Meeting, Cambridge, UK, Jul. 6, 2015 (Invited).
8	Xing Zhang, Laser Flash Raman Spectroscopy Method for Thermophysical Characterization of Nanomaterials, Nineteenth Symposium on Thermophysical Properties, Boulder, USA, Jun. 25, 2015, (Keynote).
9	John A. Kilner, Surface and Near-Surface Characterisation of Electroceramic Materials for Solid Oxide Electrode Surfaces: from bulk ceramics to real devices, 14th International Conference European Ceramic Society, Toledo, Spain, Jun. 24, 2015 (Keynote).
10	Takeshi Tsuji, Continuous monitoring of injected CO ₂ using ambient noise and controlled seismic source, International Energy Agency (IEA) Greenhouse Gas R&D 10th Monitoring Network Meeting, Berkeley, USA, Jun. 10, 2015 (Invited).

C. Major Awards

- List up to 10 main awards received during FY2015 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	Yasunori Kikuchi The SCEJ Award for Outstanding Young Researcher, The Society of Chemical Engineers, Japan, 2016

2	Zenji Horita Medal of Honor with Purple Ribbon, Government of Japan, 2015
3	Shigenori Fujikawa The Nanotechnology Prize, Institute of Systems, Information Technologies and Nanotechnologies (ISIT), 2015
4	Shigeru Koyama IIR Science and Technology Medal, International Institute of Refrigeration, 2015
5	Harry L. Tuller President, International Society of Solid State Ionics, 2015
6	Toyoki Kunitake The Kyoto Prize, Inamori Foundation, 2015
7	Takeshi Tsuji Ozawa Yoshiaki Award, The Geological Society of Japan, 2015
8	Shintaro Ida The Chemical Conversion of Light Energy Prize 2015, Presto on Chemical Conversion of Light Energy, Japan Science and Technology Agency
9	John A. Kilner The John E. Dorn Memorial Lecture, Department of Materials Science and Engineering, Northwestern University, 2015
10	<u>Kaveh Edalati</u> , Akito Yamamoto, <u>Zenji Horita</u> , and <u>Tatsumi Ishihara</u> Most Cited Papers of Scripta Materialia, 2010-2015, "Paper: K. Edalati, A. Yamamoto, Z. Horita, T. Ishihara, "High-pressure torsion of pure magnesium: Evolution of mechanical properties, microstructures and hydrogen storage capacity with equivalent strain", Scripta Materialia, Vol. 64, No. 9, pp. 880-883, 2011", Elsevier

FY 2015 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".

<Results at the end of FY2015>									
Principal Investigators Total:26									
Name (Age)	Affiliation (Position title, department, organization)	Academic degree, specialty	Working hours (Total working hours: 100%)				Starting date of project participation	Status of project participation (Describe in concrete terms)	Contributions by PIs from overseas research institutions
			Work on center project		Others				
			Research activities	Other activities	Research activities	Other activities			
Center director <u>Petros Sofronis</u> (58)	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	<ul style="list-style-type: none"> • Directs and Administers the Institute • Travels to Kyushu University to participate in events and engage with researchers (50% time) • Promotes I²CNER's interests worldwide to various universities, government agencies, laboratories, and industry on a daily basis • Intensive trans-Pacific electronic communication, including e-mail, videoconferencing, etc. 	<ul style="list-style-type: none"> • Manages and directs I²CNER's operations
Tatsumi Ishihara (54)	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	<ul style="list-style-type: none"> • Located at I²CNER • Participates in research/events as Associate Director, Lead PI of Molecular Photoconversion Devices Division 	
Chihaya Adachi (52)	Prof., Department of Applied Chemistry, Kyushu University	Dr. of Eng., Materials science and device physics	60%	20%	10%	10%	2010, Dec.1 st	<ul style="list-style-type: none"> • Located at I²CNER • Participates in research/events 	

Atsushi Takahara (60)	Prof., Institute for Materials Chemistry and Engineering, Kyushu University	Dr. of Eng., Surface and Interface Characterization	60%	20%	10%	10%	2010, Dec.1 st	<ul style="list-style-type: none"> • Located at I²CNER • Participates in research/events
Seiji Ogo (52)	Prof., International Institute for Carbon-Neutral Energy Research, Kyushu University	Dr. of Science, Green Chemistry	90%	10%	0%	0%	2010, Dec.1 st	<ul style="list-style-type: none"> • Located at I²CNER • Participates in research/events as Lead PI of Catalytic Materials Transformations Division
Zenji Horita (62)	Prof., International Institute for Carbon-Neutral Energy Research, Kyushu University	Ph.D., Dr. of Eng., Materials Science	90%	10%	0%	0%	2010, Dec.1 st	<ul style="list-style-type: none"> • Located at I²CNER • Participates in research/event
Naotoshi Nakashima (64)	Prof., International Institute for Carbon-Neutral Energy Research, Kyushu University	Ph.D., Nanocarbon science, Supramolecular science	85%	15%	0%	0%	2010, Dec.1 st	<ul style="list-style-type: none"> • Located at I²CNER • Participates in research/events
Kazunari Sasaki (51)	Prof., International Institute for Carbon-Neutral Energy Research, Kyushu University	Dr. of Science and technology, Fuel cell materials, Inorganic materials	90%	10%	0%	0%	2010, Dec.1 st	<ul style="list-style-type: none"> • Located at I²CNER • Participates in research/events
Etsuo Akiba (64)	Prof., International Institute for Carbon-Neutral Energy Research, Kyushu University	Dr. of Science, Materials science	70%	30%	0%	0%	2010, Dec.1 st	<ul style="list-style-type: none"> • Located at I²CNER • Participates in research/events as Lead PI of Hydrogen Storage Division
<u>Harry L. Tuller</u> (70)	Prof., Department of Materials Science and Engineering, Massachusetts Institute of Technology	Eng. Sc. D., Functional electroceramic materials	35%	5%	45%	15%	2010, Dec.1 st	<ul style="list-style-type: none"> • Primarily located at partner institution • Participates in research • Visited I²CNER for three weeks to participate in events and work on collaborative research projects • Discussion via Internet

<u>John A. Kilner</u> (69)	Prof., Department of Materials, Imperial College, London	Ph.D., Materials for solid oxide fuel cells and electrolysers	50%	5%	45%	0%	2010, Dec.1 st	<ul style="list-style-type: none"> Primarily located at partner institution Participates in research Visited I²CNER for five weeks to participate in events and work on collaborative projects Regular discussion via Internet
Joichi Sugimura (58)	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	<ul style="list-style-type: none"> Located at I²CNER Participates in research/events
Yasuyuki Takata (59)	Prof., International Institute for Carbon-Neutral Energy Research, Kyushu University	Dr. of Eng., Thermal Engineering	70%	30%	0%	0%	2010, Dec.1 st	<ul style="list-style-type: none"> Located at I²CNER Participates in research/events as Associate Director, Lead PI of Thermal Sciences and Engineering Division
<u>Xing Zhang</u> (54)	Prof., Department of Engineering Mechanics, Tsinghua University, China	Ph.D., Thermal Science	10%	10%	45%	35%	2010, Dec.1 st	<ul style="list-style-type: none"> Primarily located at partner institution Participates in research/events Visited I²CNER for six weeks to participate in events and work on collaborative projects Discussion via Internet
<u>Brian P. Somerday</u> (47)	Dr., Sandia National Laboratories (until the end of February 2016) Dr., South West Research Institute, USA (from March 2016)	Ph.D., Materials Science and Engineering	20%	15%	35%	30%	2010, Dec.1 st	<ul style="list-style-type: none"> Primarily located at partner institution Participates in research as Lead PI of Hydrogen Materials Compatibility Division Visited I²CNER for two weeks to participate in events and work on collaborative projects Participates in meetings/events via videoconference system

Setsuo Takaki (63)	Prof., International Institute for Carbon-Neutral Energy Research, Kyushu University	Dr. of Engineering	90%	10%	0%	0%	2011, April.1 st	<ul style="list-style-type: none"> • Located at I²CNER • Participates in research/events
<u>Reiner Kirchheim</u> (72)	Prof., The Institut für Metallphysik, University of Göttingen, Germany	Ph.D., Hydrogen in Metals, Thermodynamics of alloys, Interstitial solution and diffusion in glasses	20%	20%	40%	20%	2011, April.1 st	<ul style="list-style-type: none"> • Primarily located at partner institution • Participates in research • Visited I²CNER for one week to participate in events and work on collaborative projects • Discussion via Internet
Miho Yamauchi (42)	Associate Prof., International Institute for Carbon-Neutral Energy Research, Kyushu University	Dr. of Science, Chemistry	100%	0%	0%	0%	2012, Jan. 1 st	<ul style="list-style-type: none"> • Located at I²CNER • Participates in research/events
Ken Sakai (54)	Prof., Department of Chemistry Faculty of Sciences, Kyushu University	Ph.D., Inorganic Chemistry	80%	10%	0%	10%	2012, Jan.16 th	<ul style="list-style-type: none"> • Located at I²CNER • Participates in research/events
<u>Ian Robertson</u> (58)	Prof., Dean of Engineering, University of Wisconsin-Madison, Chief Science Advisor to the Director	Ph.D., Metallurgy	20%	5%	25%	50%	2012, April.1 st	<ul style="list-style-type: none"> • Primarily located at partner institution • Participates in research/events as Chief Science Advisor to the Director • Discussion via Internet

<u>Andrew A. Gewirth</u> (56)	Prof., Chemistry, University of Illinois	Ph.D., Chemistry	20%	5%	60%	15%	2012, April.1 st	<ul style="list-style-type: none"> • Primarily located at partner institution • Participates in research • Serves as a member of the Illinois Satellite Advisory Committee and IPRC • Visited I²CNER for one week to participate in events and work on collaborative projects • Discussion via Internet 	Accepting students from I ² CNER
<u>Kenneth T. Christensen</u> (42)	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	<ul style="list-style-type: none"> • Primarily located at partner institution • Participates in Research • Serves as a member of the Illinois Satellite Advisory Committee and IPRC • Visited I²CNER for two weeks to participate in events and work on collaborative projects • Discussion via Internet 	
Shigenori Fujikawa (45)	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	<ul style="list-style-type: none"> • Located at I²CNER • Participates in research/events as Lead PI of CO₂ Capture and Utilization Division 	
Takeshi Tsuji (36)	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	<ul style="list-style-type: none"> • Located at I²CNER • Participates in research/events as Lead PI of CO₂ Storage Division 	

Hiroshige Matsumoto (49)	Prof., International Institute for Carbon-Neutral Energy Research, Kyushu University	Dr. of Engineering	90%	10%	0%	0%	2010, Dec.1 st	<ul style="list-style-type: none"> • Located at I²CNER • Participates in research/events as Lead PI of Electrochemical Energy Conversion Division
Bidyut B. Saha (50)	Prof., International Institute for Carbon-Neutral Energy Research, Kyushu University	Dr. of Engineering	80%	15%	0%	5%	2010, Dec.1 st	<ul style="list-style-type: none"> • Located at I²CNER • Participates in research/events

Researchers unable to participate in project in FY 2015

Name	Affiliation (Position title, department, organization)	Starting date of project participation	Reasons	Measures taken
N/A				

Biographical Sketch of a New Principal Investigator

Name (Age)	Hiroshige Matsumoto (49)
<i>NOTE: Place an asterisk (*) by the name of investigators considered to be ranked among the world's top researchers.</i>	
Current affiliation (Position title, department, organization)	Professor, International Institute for Carbon-Neutral Energy Research (I ² CNER), Kyushu University
Academic degree, specialty	Dr. of Engineering, Solid Electrochemistry
<p>Research and education history</p> <p>(Education)</p> <p>1996 Ph.D. Engineering, The University of Tokyo</p> <p>1993 M.S. Engineering, The University of Tokyo</p> <p>1991 B.S. Engineering, The University of Tokyo</p> <p>(Research)</p> <p>2015-present Lead Principal Investigator of the Electrochemical Energy Conversion research Division (from July 2015) International Institute for Carbon-Neutral Energy Research (I²CNER), Kyushu University</p> <p>2013-present Professor, Hydrogen Production Research Division International Institute for Carbon-Neutral Energy Research (I²CNER), Kyushu University</p> <p>2009-2013 Professor, Environmental Research Division INAMORI Frontier Research Center, Kyushu University</p> <p>2004-2008 Associate Professor Dept. Applied Chemistry, Faculty of Engineering, Kyushu University</p> <p>2003-2004 Research Associate Institute of Multidisciplinary Research for Advanced Materials, Tohoku University</p> <p>1996-2002 Research Associate Center for Integrated Research in Science, Nagoya University</p>	
<p>Achievements and highlights of past research activities</p> <p>Proton-conducting solid oxides are a material to conduct researches for both basic science and practical applications. As an example of basic research, Matsumoto has been demonstrated a reversible conductivity change with respect to the precipitation/dissolution of platinum nanoparticles as one of the rare example of nanoionics effect, which will be a new material design principle. For practical application, steam electrolysis is a main research topic for the production of renewable hydrogen. BaZr_{0.44}Ce_{0.36}Y_{0.2}O_{3-δ} has been found as a highly conductive and highly stable in high steam condition, and demonstrated high performance steam electrolysis working with energy efficiency higher than 90%.</p> <p>"Surface proton conducting metal oxide nanoparticles" is a new type of ion conducting solid material: Matsumoto has proposed to use the surface of metal oxide instead of interior of the grains that has been the conventional place for the conventional ion conductors, and demonstrated high proton conductivity at room temperature in sulfated titanium oxide nanoparticles; ion conduction of ceramic material has never taken place at such a low temperature before. The material is now being applied to water electrolysis with a special structure suitable for these proton-conducting nanoparticles, that is, "water absorbing porous electrolyte cell."</p>	
Achievements	

(1) International influence

- a) *Guest speaker, chair, director, or honorary member of a major international academic society in the subject field,*
1. Board member, The Solid State Ionics Society of Japan
 2. Board member International conference on Solid State Proton conductor
 3. International Advisory board of Prospect of Proton Conductor Cells
- b) *Holder of a prestigious lectureship,*
1. Hiroshige Matsumoto, KWATI LEONARD, Young-Sung Lee, Yuji Okuyama, "Influence of Dopant Levels on the Proton-Conducting Properties of ZCY and BZCY system", Materials Science and Technology 2015 (MS&T15) (Key lecture), Columbus, Ohio, United States of America ,October 4-October 8, 2015.
 2. Hiroshige Matsumoto, "Hydrogen production via steam electrolysis using proton-conducting rare-earth metal oxides (in Japanese)", 32nd Symposium on Rare earths, Kagoshima, Japan 21-May, 2015.
- c) *Member of a scholarly academy in a major country,*
1. Electrochemical Society of Japan
 2. The Chemical Society of Japan
 3. The Ceramic Society of Japan
 4. Catalysis Society of Japan
- d) *Recipient of an international award(s) ,*
- e) *Editor of an influential journal, etc.*
1. Associate Editor, Chemistry Letters (The Chemical Society of Japan)(2012-2014)
 2. Guest Editor, Solid State Ionics (Elsevier, Special issue of 19th Int. Conf. on Solid State Ionics, 2013, Kyoto, Japan)
 3. Editor, Electrochemistry (2008, 2009)

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

1. JSPS Grant in Aid for Scientific Research - Challenging Exploratory Research, "Water electrolysis working under small gravity using water-absorbing porous electrolyte and hydrophobic electrodes", 3,000,000 JPY, FY2014-2015.
 2. JST CREST, "Synthesis of methane through the reduction of carbon dioxide using hydrogen generated from the renewable energy" (as a co-investigator), 66,000,000 JPY, FY2014-2019.
 3. JST, SIP, "New steam electrolysis", 74,376,900 JPY*, 2014-2018, JST/ALCA awarded in 2013 has been reformed to this project.
 4. JST, ALCA, "New steam electrolysis", 74,376,900 JPY*, 2013-2015, awarded in July 2013.
 5. JST, A-STEP, "Development of gas diffusion layer using electrospinning method", 1,700,000 JPY*, 2012-2013, awarded in November 2012.
 6. "Development of gas diffusion layer using electrospinning method", JST, A-STEP, 1,700,000 JPY (2012-2013)
 7. JST, ALCA (Feasible study), "Fuel cell using hydrogen-containing organic fuel", 5,000,000 JPY FY2011-2012.
 8. JST, A-STEP, "Development of microtubular electrochemical cell fabric", 1,700,000 JPY, FY2011-2012.
- * Indirect budget included.

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

1. Iwahara, H., Shimura, T., Matsumoto, H., "Protonic Conduction in Oxides at Elevated Temperatures and Their Possible Applications", (2000) *Electrochemistry*, 68 (3), pp. 154-161. (91 citations)
2. Matsumoto, H., Kawasaki, Y., Ito, N., Enoki, M., Ishihara, T., Relation between electrical conductivity and chemical stability of BaCeO₃-based proton conductors with different trivalent dopants", (2007)

Electrochemical and Solid-State Letters, 10 (4), pp. B77-B80. (83 citations)

3. Matsumoto, H., Shimura, T., Iwahara, H., Higuchi, T., Yashiro, K., Kaimai, A., Kawada, T., Mizusaki, J., "Hydrogen separation using proton-conducting perovskites", (2006) Journal of Alloys and Compounds, 408-412, pp. 456-462. (63 citations)
4. Ma, G., Matsumoto, H., Iwahara, H., "Ionic conduction and nonstoichiometry in non-doped $Ba_xCeO_{3-\alpha}$ ", (1999) Solid State Ionics, 122 (1-4), pp. 237-247. (63 citations)
5. Matsumoto, H., Hamajima, S., Yajima, T., Iwahara, H., "Electrochemical Hydrogen Pump Using $SrCeO_3$ -Based Proton Conductor: Effect of Water Vapor at the Cathode on the Pumping Capacity", (2001) Journal of the Electrochemical Society, 148 (10), pp. D121-D124. (55 citations)
6. Matsumoto, H., Shimura, T., Higuchi, T., Tanaka, H., Katahira, K., Otake, T., Kudo, T., Yashiro, K., Kaimai, A., Kawada, T., Mizusaki, J., "Protonic-electronic mixed conduction and hydrogen permeation in $BaCe_{0.9-x}Y_{0.1}Ru_xO_{3-\alpha}$ " (2005) Journal of the Electrochemical Society, 152 (3), pp. A488-A492. (41 citations)
7. Katahira, K., Matsumoto, H., Iwahara, H., Koide, K., Iwamoto, T., "Solid electrolyte hydrogen sensor with an electrochemically-supplied hydrogen standard", (2001) Sensors and Actuators, B: Chemical, 73 (2-3), pp. 130-134. (40 citations)
8. Matsumoto, H., Nomura, I., Okada, S., Ishihara, T., "Intermediate-temperature solid oxide fuel cells using perovskite-type oxide based on barium cerate", (2008) Solid State Ionics, 179 (27-32), pp. 1486-1489. (37 citations)
9. Ito, N., Matsumoto, H., Kawasaki, Y., Okada, S., Ishihara, T., "Introduction of In or Ga as second dopant to $BaZr_{0.9}Y_{0.1}O_{3-\delta}$ to achieve better sinterability", (2008) Solid State Ionics, 179 (9-10), pp. 324-329. (37 citations)
10. Matsumoto, H., Hamajima, S., Iwahara, H., "Electrochemical hydrogen pump using a high-temperature- proton conductor: Improvement of pumping capacity", (2001) Solid State Ionics, 145 (1-4), pp. 25-29. (36 citations)
11. Matsumoto, H., Okubo, M., Hamajima, S., Katahira, K., Iwahara, H., "Extraction and production of hydrogen using high-temperature proton conductor", (2002) Solid State Ionics, 152-153, pp. 715-720. (35 citations)
12. Matsumoto, H., Iida, Y., Iwahara, H., "Current efficiency of electrochemical hydrogen pumping using a high-temperature proton conductor $SrCe_{0.95}Yb_{0.05}O_{3-\alpha}$ ", (2000) Solid State Ionics, 127 (3), pp. 345-349. (35 citations)
13. Shimura, T., Esaka, K., Matsumoto, H., Iwahara, H., "Protonic conduction in Rh-doped $AZrO_3$ (A=Ba, Sr and Ca)", (2002) Solid State Ionics, 149 (3-4), pp. 237-246. (34 citations)
14. Kobayashi, T., Abe, K., Ukyo, Y., Matsumoto, H., "Study on current efficiency of steam electrolysis using a partial protonic conductor $SrZr_{0.9}Yb_{0.1}O_{3-\alpha}$ " (2001) Solid State Ionics, 138 (3-4), pp. 243-251. (32 citations)
15. Sakai, T., Matsushita, S., Matsumoto, H., Okada, S., Hashimoto, S., Ishihara, T., "Intermediate temperature steam electrolysis using strontium zirconate-based protonic conductors", (2009) International Journal of Hydrogen Energy, 34 (1), pp. 56-63. (30 citations)

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

Biographical Sketch of a New Principal Investigator

Name (Age)	Bidyut Baran Saha (51)
Affiliation (Position title, department, organization)	Professor, International Institute for Carbon-Neutral Energy Research (I ² CNER), Kyushu University
Academic degree, specialty	Dr. of Engineering, Mechanical Systems Engineering
<p>Research and education history</p> <p>(Research)</p> <p>2016-present Principal Investigator of the Thermal Science and Engineering Division, Professor (2016-present), International Institute for Carbon-Neutral Energy Research (I²CNER), Kyushu University</p> <p>2016-present Professor, Department of Mechanical Engineering, Faculty of Engineering, Kyushu University</p> <p>2013-2015 Professor, Program for Leading Graduate Schools, Green Asia Education Center, Kyushu University</p> <p>2010-2013 Professor, Department of Mechanical Engineering, Faculty of Engineering, Kyushu University</p> <p>2010-2013 Professor, International Education Center, Kyushu University</p> <p>2009-2010 Senior Research Fellow, Mechanical Engineering Department, National University of Singapore</p> <p>2009-2010 Visiting Professor, Research and Education Center of Carbon Resources, Kyushu University</p> <p>2006-2008 Associate Professor, Interdisciplinary Graduate School of Engineering Sciences, Kyushu University</p> <p>2001-2006 Associate Professor, Institute for Materials Chemistry and Engineering, Kyushu University</p> <p>2000-2001 Associate Professor, Department of Mechanical Systems Engineering Sciences, Tokyo University of Agriculture and Technology</p> <p>1997-2000 Assistant Professor, Department of Mechanical Systems Engineering Sciences, Tokyo University of Agriculture and Technology</p> <p>1993-1994 Research Scholar, Department of Mechanical Systems Engineering, Tokyo University of Agriculture and Technology</p> <p>1991-1992 Bose Fellow, Bose Center for Advanced Study in Natural Sciences, University of Dhaka, Bangladesh</p> <p>(Education)</p> <p>1997 Ph.D. in Engineering, Mechanical Systems Engineering, Tokyo University of Agriculture and Technology, Japan</p>	

1990	M.Sc. in Applied Mathematics, Faculty of Science, Dhaka University, Bangladesh
1987	B.Sc. (Hon's) in Mathematics, Faculty of Science, Dhaka University, Bangladesh
<p>Achievements and highlights of past research activities <i>(Describe qualifications as a top-caliber researcher if he/she is considered to be ranked among the world's top researchers.)</i></p> <p>(1) Minimum heat source temperature for single and multi-stage adsorption chillers. A thermodynamic formulation has been developed to calculate the minimum temperature of the driving heat source for an advanced solid sorption cooling device. It is also validated with experimental data. This formalism has been developed from the rigor of Boltzmann distribution function and the condensation approximation of adsorptive molecules. An interesting and useful finding has been established from this formalism that it is possible to construct a solid sorption refrigeration device that operates in a cycle transferring heat from a low temperature source to a heat sink with a driving heat source at a temperature close to but above ambient. (Sources: International Journal of Refrigeration, Vol. 29, Issue 7, pp. 1175-1181, 2006; Applied Physics Letters, Vol. 91, 111902, 2007.)</p> <p>(2) Thermodynamic framework for calculating the specific heat capacity and isosteric heat of adsorption of a single component adsorbent + adsorbate system A thermodynamic framework for calculating the specific heat capacity and isosteric heat of adsorption of a single component adsorbent + adsorbate system has been derived and developed using the classical thermodynamics, and these are essential for the design of adsorption processes. The derived formulations of the specific heat capacity and isosteric heat of adsorption are compared with experimentally measured values of various adsorbent + adsorbate systems. The study results contributed significantly in filling up the information gap with respect to the state of adsorbed phase to dispel the confusion as to what is the actual state of the adsorbed phase. (Sources: Applied Physics Letters, Vol. 90, 171902, 2007; Applied Physics Letters, Vol. 90, 171902, 2007.)</p> <p>(3) Development of temperature-entropy (T-s) diagram of CaCl₂-in-silica gel + water system The thermodynamic property surfaces for a single-component adsorbent + adsorbate system are derived and developed from the view point of classical thermodynamics, thermodynamic requirements of chemical equilibrium, Gibbs law and Maxwell relations. They enable us to compute the entropy and enthalpy of the adsorbed phase, the isosteric heat of adsorption, specific heat and the adsorbed phase volume quite precisely. These simple equations are amenable with ease for calculating the energetic performances of any adsorption system. This is yet another contribution towards narrowing the information gap in the nature of the adsorbed phase. We have also evolved and elucidated the temperature-entropy diagrams of (i) CaCl₂-in-silica gel + water system for cooling applications, and (ii) activated carbon (Maxsorb III) + methane system for gas storage. (Sources: International Journal of Heat and Mass Transfer, Vol. 52, No. 1-2, pp. 516-524, 2009; Langmuir, Vol. 25, No. 4, pp. 2204–2211, 2009.)</p>	
<p>Achievements</p> <p>(1) International influence</p> <p><i>a) Guest speaker, chair, director, or honorary member of a major international academic society in the subject field</i></p> <ul style="list-style-type: none"> • General Chairman, International Conference on Innovative Materials for Processes in Energy Systems, IMPRES2016, Sicily, Italy, October 2016. • Invited Lecture, International Forum for Green Asia, Fukuoka, Japan, November 2015. • Keynote Speaker, IX Minsk International Seminar "Heat Pipes, Heat Pumps, Refrigerators, Power Sources", Minsk, Belarus, September 2015 • Keynote Speaker, Polygeneration 2015, Chennai, India, February 2015. • Invited Lecture, the First SERIUS Series Symposium, Bangalore, India, April 2014. • Organizer: Global Strategy for Green Asia – MJIIT Joint Workshop, Malaysia-Japan International Institute of Technology, Kuala Lumpur, February 2014 • Keynote Speaker, the 22nd National and 11th International ISHMT-ASME Heat and Mass Transfer Conference, IIT Kharagpur, India, December 2013. 	

- Keynote Speaker, the 6th International Meeting on Advanced Thermofluids (IMAT2013), Singapore, November 2013.
- Keynote Speaker, 11th China-Japan-Korea Symposium on Carbon Materials to Save the Earth – Materials and Devices for New Energies and Environmental Protection (CSE2013), Nagasaki, November 2013.
- General Chairman, International Conference on Innovative Materials for Processes in Energy Systems, IMPRES2013, Fukuoka, Japan, October 2016.
- Keynote Speaker, International Conference on Green Energy and Technology (ICGET), Kitakyushu, Japan, August 2013.
- Plenary Lecture, 10th China-Japan-Korea Symposium on Carbon Materials to Save the Earth – Materials and Devices for New Energies and Environmental Protection (CSE2012), Guangzhou, China, November 2012.
- Plenary Lecture, 2nd KIER-Kyushu U. Joint Symposium on Green System and Materials, Jeju, Korea, September 2012.
- Keynote Speaker, VIII Minsk International Seminar Heat Pipes, Heat Pumps, Refrigerators, Power Sources, Minsk, Belarus, September 12-15, 2011.
- Keynote Speaker, 4th Workshop on Solar Desalination Water Treatment and Utilization, Jeju, South Korea, June 2011.
- General Chairman, International Conference on Innovative Materials for Processes in Energy Systems, IMPRES2010, Singapore, December 2010.
- General Co-chair: International Conference on Environmental Aspects of Bangladesh (ICEAB10), Kitakyushu, Japan, September 4, 2010.
- Keynote Speaker, 2nd European Conference on Polygeneration, Tarragona, Spain, March 31, 2011.
- Invited Speaker, Solar Energy Conclave, New Delhi, January 2010.
- Invited Lecture, 16th Mathematics Conference, BUET, Dhaka, December 2009.
- Keynote Speaker, Heat Powered Cycle Conference 2009, Berlin, September 2009.
- General Secretary, The 8th Asian Thermophysical Properties Conference, Fukuoka, Japan, August 2007.
- Invited Lecture, International Seminar on the Future of Heat Cascading and Energy Systems, Tokyo, December 2006.
- Plenary Lecture, 8th Cross Straits Symposium on Materials, Energy and Environmental Sciences, Busan, Korea, November 2006.
- Keynote Speaker, Cryogenics and Refrigeration – Proceedings of ICCR'2008, Shanghai, China, April 2008.
- Keynote Speaker, International Seminar on Clean Energy, Durgapur, India, October 2007.
- General Secretary, International Seminar on Thermally Powered Sorption Systems, Fukuoka, Japan, December 2003.
- Keynote Speaker, International Conference on Building Systems and Facilities Management, Singapore, October 2003.
- Plenary Lecture, 2nd Japan-Korea Joint Symposium on Energy and Environment, Fukuoka, Japan, October 2002.
- Keynote Speaker, KSMTE Spring Conference 2002, Masan, South Korea, April 2002.
- Keynote Speaker, BSME-ASME International Conference on Thermal Engineering, Dhaka, Bangladesh, January 2002.

b) Holder of a prestigious lectureship

- Journal Management, Kyushu University, 2013, 2014, 2015.
- Thermally Powered Cooling Systems, University Teknologi Petronas, Malaysia, 2015.
- Solar Powered Adsorption Cooling, University Kebangsaan Malaysia, Malaysia 2011.

c) Member of a scholarly academy in a major country

- Executive Member, Heat Pump and Thermal Storage Technology Center of Japan (HPTCJ), Low Temperature Heat Utilization Research Group.
- Member, American Society of Mechanical Engineers (ASME).
- Member, the Japan Society of Mechanical Engineers (JSME).
- Member, Japanese Society of Refrigeration and Air Conditioning Engineers (JSRAE).
- Member, Japan Society of Thermophysical Properties.
- Life Member, Indian Society for Heat and Mass Transfer.
- Life Member, Bangladesh Mathematical Society.
- Life Member, Japanese Universities Alumni Association in Bangladesh (JUAAB).

d) Recipient of an international award(s)

- ITEX Silver Medal for the invention “Innovative Solar adsorption Chiller”, at (23rd International Invention, Innovation and Technology Exhibition, Malaysia), Kuala Lumpur, May 2012.
- Best Presentation Paper Award, the 5th Asian Conference on Refrigeration and Air Conditioning (ACRA2010), Tokyo, Japan (Award issued on 1 March 2012).
- IES Prestigious Engineering Achievement Award 2009 for the Development of Adsorption Desalination cum Cooling Technology, 31 August 2009
- Outstanding Paper Award, The 9th Cross Straits Symposium on Materials, Energy and Environmental Engineering, Pohang, South Korea, 2007.
- Outstanding Paper Award, The 6th Cross Straits Symposium on Materials, Energy and Environmental Engineering, Pohang, South Korea, 2004.
- Selected as One of the Best Ten Papers, International Ab-Sorption Heat Pump Conference, Montreal, Canada, 1996.
- Best Paper Award, Japanese Society of Refrigeration and Air Conditioning Engineers (JSRAE), 1995.

e) Editor of an influential journal, etc.

- Editor-in-Chief, EVERGREEN Joint Journal of Novel Carbon Resource Sciences & Green Asia Strategy, http://www.tj.kyushu-u.ac.jp/leading/en/c_publication/evergreen.php
- Managing Guest Editor, Applied Thermal Engineering, Special Issue: <http://ees.elsevier.com/ate/>
- Editorial Advisory Board, Applied Thermal Engineering, <http://ees.elsevier.com/ate/>
- Honorary Editorial Advisor, Ganit Journal of the Bangladesh Mathematical Society, <http://bdmathsociety.org/>
- Editorial Board Member, Advances in Mechanical Engineering, Hindawi Publishing Corporation, <http://www.hindawi.com/journals/ame/>
- Editorial Board Member (Up to 2008), Engineering Sciences Reports, Kyushu University, Japan, ISSN: 1346-7883, <http://www.tj.kyushu-u.ac.jp/info/online/index.php>
- Editorial Advisory Board Member, Open Mechanical Engineering Journal (OMEJ), ISSN: 1874-155X, <http://www.bentham.org/open/tomej/>
- Editorial Advisory Board Member, Open Thermodynamics Journal (OTHerJ), Bentham Science Publishers, USA. ISSN: 1874-396X, <http://www.bentham.org/open/totherj/index.htm>
- Guest Editor, Heat Transfer Engineering Journal (<http://www.ingentaconnect.com/content/tandf/uhte>), ISSN: 0145-7632, Special Issue “Application of Sorption Technologies for Energy Efficiency”.
- Editorial Board Member, Fundamental Journal of Thermal Science and Engineering, (http://www.frdint.com/fundamental_journal_thermal_science_engineering_edit.html) ISSN: 2249-975X

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

- Chakraborty (Nanyang Technological University, Singapore, PI), K.C. Leong (NTU, Collaborator) and **B.B. Saha** (Collaborator), “Development of metal organic frameworks for heat transmission applications, Ministry of Education, Singapore, Project No. MOE2014-T2-2-061, duration: 1 June 2015 to 31 May 2018, amount: S\$ 768, 939.
- T. Maruyama (Group Leader, Calsonic Kansei Corp.), T. Miyazaki (Group Leader), **B.B. Saha** (Investigator), J. Miyawaki (Investigator), S. Koyama (Investigator), Research and development of highly-efficient waste heat driven cooling heat pump for vehicles, Thermal Management Materials and Technology Research Association, METI Project, duration: 2014-2017, amount: JPY 218 million.
- Y. Takata (Coordinator), H. Daiguji (Group Leader), S. Koyama (Group leader), **B.B. Saha** (Investigator), et al., “Interfacial metafluidics”, *Core Research for Evolutional Science and Technology (CREST) Project*, duration: 2011-2016, amount: JP Yen 350 million.
- **B.B. Saha** (Coordinator), H. Mori, Y. Hamamoto, K. Kariya and A. Eto, “Performance evaluation of adsorption chillers powered by fuel cell waste heat”, Project No. C05, International Center for Hydrogen Research, duration: 2010-2013, amount: JP Yen 1 million per year.
- **B.B. Saha** (Coordinator) and K. Kariya (Investigator), “Study on water adsorption onto zeolite coated heat exchanger towards the improvement of adsorption chiller”, *Ministry of Education, Science, Sports and Culture, Japan, “Science and Technology Project”*, Project No. 23560235, duration: 2011-2013, amount: JP Yen 4.9 million.

- K.C. Ng (PI), **B.B. Saha** (Co-PI) and T.H. Wee (Investigator), "Solar-Powered Adsorption Desalination (AD): A Pilot Test Program to Achieve 1.5 kWh/m³", National University of Singapore (NUS) for the ARF grant, WBS R265-000-222-112 and King Abdullah University of Science & Technology (KAUST) grant WBS R265-000-286-597, duration: April 2008 – March 2011, amount US\$ 4.7 million.

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

1. Modeling the performance of two-bed, silica gel-water adsorption chillers, *International Journal of Refrigeration*, 22 (3), 194-204, 1999, (number of citations: 206).
2. Solar/waste heat driven two-stage adsorption chiller: the prototype, *Renewable Energy*, 23 (1), 93-101, 2001, (number of citations: 192).
3. Computer simulation of a silica gel-water adsorption refrigeration cycle--the influence of operating conditions on cooling output and COP, *ASHRAE Transactions*, 101 (2), 348-357, 1995, (number of citations: 189).
4. Experimental investigation of a silica gel-water adsorption refrigeration cycle--The influence of operating conditions on cooling output and COP, *ASHRAE Transactions*, 101 (2), 358-366, 1995, (number of citations: 187).
5. Waste heat driven dual-mode, multi-stage, multi-bed regenerative adsorption system, *International Journal of Refrigeration*, 26 (7), 749-757, 2003, (number of citations: 160).
6. Computational analysis of an advanced adsorption-refrigeration cycle, *Energy*, 20 (10), 983-994, 1995, (number of citations: 144).
7. Experimental investigation of the silica gel-water adsorption isotherm characteristics, *Applied Thermal Engineering*, 21 (16), 1631-1642, 2001, (number of citations: 140).
8. Performance evaluation of a low-temperature waste heat driven multi-bed adsorption chiller, *International Journal of Multiphase Flow*, 29 (8), 1249-1263, 2003, (number of citations: 123).
9. A new generation cooling device employing CaCl₂-in-silica gel-water system, *International Journal of Heat and Mass Transfer*, 52 (1), 516-524, 2009, (number of citations: 115).
10. Heat exchanger design effect on the system performance of silica gel adsorption refrigeration systems, *International Journal of Heat and Mass Transfer*, 43 (24), 4419-4431, 2000, (number of citations: 92).
11. Silica gel water advanced adsorption refrigeration cycle, *Energy*, 22 (4), 437-447, 1997, (number of citations: 83).
12. Study on an activated carbon fiber-ethanol adsorption chiller: Part I-system description and modeling, *International Journal of Refrigeration*, 30 (1), 86-95, 2007, (number of citations: 81).
13. Multi-bed regenerative adsorption chiller—improving the utilization of waste heat and reducing the chilled water outlet temperature fluctuation, *International Journal of Refrigeration*, 24 (2), 124-136, 2001, (number of citations: 81).
14. Experimental investigation of activated carbon fibers/ethanol pairs for adsorption cooling system application, *Applied Thermal Engineering*, 26 (8), 859-865, 2006 (number of citations: 78).
15. Operational strategy of adsorption desalination systems, *International Journal of Heat and Mass Transfer*, 52 (7), 1811-1816, 2009, (number of citations: 70).
16. An overview of developments in adsorption refrigeration systems towards a sustainable way of cooling, *Applied Energy*, 104, 554-567, 2013, (number of citations: 69).
17. Experimental investigation of an advanced adsorption refrigeration cycle, *ASHRAE Transactions*, 103 (2), 50-58, 1997, (number of citations: 68).
18. Experimental study on performance improvement of a four-bed adsorption chiller by using heat and mass recovery, *International Journal of Heat and Mass Transfer*, 49 (19), 3343-3348, 2006, (number of citations: 64).
19. Study on an activated carbon fiber-ethanol adsorption chiller: Part II-performance evaluation, *International Journal of Refrigeration*, 30 (1), 96-102, 2007, (number of citations: 62).
20. Experimental investigation on activated carbon-ethanol pair for solar powered adsorption cooling applications, *International Journal of Refrigeration*, 31 (8), 1407-1413, 2008, (number of citations: 61).
21. On the thermodynamic modeling of the isosteric heat of adsorption and comparison with experiments, *Applied Physics Letters*, 89 (17), 171901, 2006 (number of citations: 56).
22. Theoretical insight of physical adsorption for a single-component adsorbent+ adsorbate system: I. Thermodynamic property surfaces, *Langmuir*, 25 (4), 2204-2211, 2009, (number of citations: 55).
23. A study on the kinetics of ethanol-activated carbon fiber: theory and experiments, *International Journal of Heat and Mass Transfer*, 49 (17), 3104-3110, 2006, (number of citations: 54).
24. A new cycle time allocation for enhancing the performance of two-bed adsorption chillers, *International*

- Journal of Refrigeration, 32 (5), 846-853, 2009 (number of citations: 51).
25. Study on a waste heat-driven adsorption cooling cum desalination cycle, *International Journal of Refrigeration* 35 (3), 685-693, 2012, (number of citations: 48).
 26. Thermodynamic modeling of a solid state thermoelectric cooling device: Temperature–entropy analysis, *International Journal of Heat and Mass Transfer*, 49 (19), 3547-3554, 2006, (number of citations: 48).
 27. Evaluation of adsorption parameters and heats of adsorption through desorption measurements, *Journal of Chemical & Engineering Data*, 52 (6), 2419-2424, 2007, (number of citations: 46).
 28. Study on solar/waste heat driven multi-bed adsorption chiller with mass recovery, *Renewable Energy*, 32 (3), 365-381, 2007, (number of citations: 46).
 29. Study on adsorption refrigeration cycle utilizing activated carbon fibers. Part 1. Adsorption characteristics, *International Journal of Refrigeration*, 29 (2), 305-314, 2006, (number of citations: 46).
 30. Study on adsorption of methanol onto carbon based adsorbents, *International Journal of Refrigeration*, 32 (7), 1579-1586, 2009, (number of citations: 44).
 31. Isotherms and thermodynamics for the adsorption of n-butane on pitch based activated carbon, *International Journal of Heat and Mass Transfer*, 51 (7), 1582-1589, 2008 (number. of citations: 44).
 32. Study on an advanced adsorption desalination cycle with evaporator–condenser heat recovery circuit, *International Journal of Heat and Mass Transfer*, 54 (1), 43-51, 2011, (number of citations: 42).
 33. Two-stage non-regenerative silica gel-water adsorption refrigeration cycle, *ASME Advanced Energy Systems Division*, 40, 65-69, 2000, (number of citations: 42).
 34. Performance evaluation of combined adsorption refrigeration cycles, *International Journal of Refrigeration*, 34 (1), 129-137, 2011 (number of citations: 40).
 35. Thermodynamic formalism of minimum heat source temperature for driving advanced adsorption cooling device, *Applied Physics Letters*, 91 (11), 111902, 2007 (number of citations: 40).
 36. Study on a dual-mode, multi-stage, multi-bed regenerative adsorption chiller, *Renewable Energy*, 31 (13), 2076-2090, 2006 (number of citations: 40).
 37. Improved isotherm data for adsorption of methane on activated carbons, *Journal of Chemical & Engineering Data*, 55 (8), 2840-2847, 2010, (number of citations: 39).
 38. How heat and mass recovery strategies impact the performance of adsorption desalination plant: theory and experiments, *Heat Transfer Engineering* 28 (2), 147-153, 2007, (number of citations: 39).
 39. Performance evaluation of multi-stage, multi-bed adsorption chiller employing re-heat scheme, *Renewable Energy*, 33 (1), 88-98, 2008, (number of citations: 38).
 40. Carbon dioxide adsorption isotherms on activated carbons, *Journal of Chemical & Engineering Data*, 56 (5), 1974-1981, 2011, (number of citations: 36).
 41. Solar-assisted dual-effect adsorption cycle for the production of cooling effect and potable water, *International Journal of Low-Carbon Technologies*, 4 (2), 61-67, 2009 (number. of citations: 36).
 42. Adsorption desalination quenches global thirst, *Heat Transfer Engineering*, 29 (10), 845-848, 2008, (number of citations: 36).
 43. An overview on adsorption pairs for cooling, *Renewable and Sustainable Energy Reviews*, 19, 565-572, 2013, (number of citations: 35).
 44. Specific heat capacity of a single component adsorbent-adsorbate system, *Applied Physics Letters*, 90 (17), 2007, (number of citations: 35).
 45. Parametric study of a two-stage adsorption chiller using re-heat—The effect of overall thermal conductance and adsorbent mass on system performance, *International Journal of Thermal Sciences*, 45 (5), 511-519, 2006, (number of citations: 35).
 46. Entropy generation analysis of two-bed, silica gel-water, non-regenerative adsorption chillers, *Journal of Physics D: Applied Physics*, 31 (12), 1471, 1998 (number of citations: 35).
 47. Numerical simulation and performance investigation of an advanced adsorption desalination cycle, *Desalination*, 308, 209-218, 2013, (number of citations: 33).
 48. Waste heat driven multi-bed adsorption chiller: heat exchangers overall thermal conductance on chiller performance, *Heat Transfer Engineering* 27 (5), 80-87, 2006, (number of citations: 33).
 49. Study on adsorption refrigeration cycle utilizing activated carbon fibers. Part 2. Cycle performance evaluation, *International Journal of Refrigeration*, 29 (2), 315-327, 2006, (number of citations: 33).
 50. Parametric study of a silica gel-water adsorption refrigeration cycle--The influence of thermal capacitance and heat exchanger UA-values on cooling capacity, power density, and COP, *ASHRAE Transactions*, Vol. 103 (1), 139-148, 1997, (number of citations: 33).

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

Inventor of Intellectual Property (Patent)

1. K.C. Ng, A. Myat, H. Yanagi, K. Thu, **B.B. Saha** and I. Leong, "A dehumidifier and a method of dehumidification", **Patent No. 183110**, Date of Grant: 19 January 2015.
2. B.B. Saha, A. Chakraborty, T.Y. Al-Ghasham, K.C. Ng, K. Thu and H. Yanagi, "Apparatus and method for improved desalination", **Patent No. 170810**, Date of Grant: 16 October 2014.
3. Deepak Pahwa, **Bidyut Baran Saha**, Anil Kumar Choudhary, Rajan Sachdev and Kuldeep Singh Malik, "Hybrid heat exchangers and method of manufacture thereof", WIPO/PCT: WO 2015/104719 A2, Publication Date: 16 July 2015.
4. K.C. Ng, W.S. Loh, K.A. Rahman and **B.B. Saha**, "Method and system for storing natural gas", PCT Application No.: **PCT/SG2011/000217**, Publication Date: 22 December 2011, WO2011/159259. Indonesia Patent Application No. W00201300116.
5. K.C. Ng, A. Myat, H. Yanagi, K. Thu, **B.B. Saha** and I. Leong, "A dehumidification and a method of dehumidification", PCT Application No.: **PCT/SG2011/000028**, Publication Date: 28 July 2011, WO2011/090438.
6. **B.B. Saha**, K.C. Ng, A. Chakraborty and K. Thu, "Desalination system and method", PCT: WO 2011/010205 A1.
7. K.C. Ng, K. Thu, H. Yanagi, **B.B. Saha**, A. Chakraborty, T. Al-Ghasham, Apparatus and method for improved desalination, PCT Patent Application No: PCT/SG2009/000223, **WO 2009/157875**, December 2009 and PCT Application No. 2011022878, Grant date: 16 October 2014.
8. S. Koyama, **B.B. Saha**, A. Chakraborty, K. Srinivasan and K. Kuwahara, "Hybrid refrigeration system", Publication No. WO/2009/145278, Date December 3, 2009, International Application No. PCT/JP2009/059817.
9. K.C. Ng, X.L. Wang, L.Z. Gao, A. Chakraborty, **B.B. Saha**, S. Koyama, "Pressurized-cycle based electro-adsorption chiller (PEAC)" **WO 2006/135346 A1**, Application No. **PCT/SG2006/000163**, International Publication Date: 21 December 2006.
10. **B.B. Saha**, S. Koyama, K.C. Ng, X.L. Wang, L.Z. Gao, A. Chakraborty, A. Akisawa and T. Kashiwagi, "Adsorption refrigerator", **WO 135026 A1**, Application No. **PCT/JP2006/312070**, Publication Date: 21 December 2006.
11. K.C. Ng, X.L. Wang, L.Z. Gao, A. Chakraborty, **B.B. Saha**, S. Koyama, A. Akisawa and T. Kashiwagi, "Apparatus and method for desalination", Patent No.: US 8535486 B2, Publication Date: 17 September 2013.
12. K.C. Ng, X.L. Wang, L.Z. Gao, A. Chakraborty, **B.B. Saha**, S. Koyama, A. Akisawa and T. Kashiwagi, "Apparatus and method for desalination", **WO 2006/121414**, Application No. PCT/SG2006/000157, Publication Date: 16 November 2006. Patent No.: US 8,535,486 B2, Grant Date: 17 September 2014.
13. H.T. Chua, K.C. Ng, A. Malek, T. Kashiwagi, A. Akisawa, and **B.B. Saha**, "A regenerative adsorption process and multi-reactor regenerative adsorption chiller", **WO 2000/033932**, Application No. **PCT/SG99/000136**, Publication Date: 15 June 2000.

Records of FY2015 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 [00 month, 00 year].

	Goal set in the "Post-interim evaluation revised center project"	Results at end of FY 2015	Final goal (Date: March 2020)
Researchers	172 <78, 45%> [29, 17%]	166 <80, 48%> [18, 11%]	177 <81, 46%> [33, 19%]
Principal investigators	25 <9, 36%> [1, 4%]	26 <10, 38%> [1, 4%]	25 <9, 36%> [3, 12%]
Other researchers	147 <69, 47 %> [28, 19%]	140 <70, 50%> [17, 12%]	152 <72, 47%> [31, 20%]
Research support staff	70	53	70
Administrative staff	21	21 (17, 81%)	21 (17, 81%)
Total	263	240	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 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.

<FY2015 (April, 2015~ March, 2016)>

Researcher	Position at I ² CNER	Affiliated with I ² CNER for:	Former Affiliation	Affiliation after I ² CNER
Nguyen Thi Thanh Nga	Postdoctoral Researcher	1 year	Kyushu University (PhD student)	(Currently at I ² CNER)
Kaveh Edalati	Assistant Professor, Postdoctoral Researcher	1 year, 2 years	Kyushu University	(Currently at I ² CNER)
Stephen Lyth	Associate Professor, Assistant Professor	1 year, 3 years and 9 months	Tokyo Institute of Technology	(Currently at I ² CNER)
Yuki Terayama	Postdoctoral Researcher	11 months	Asahi Intecc	(Currently at I ² CNER)
Helena Tellez Lozano	Assistant Professor	5 months	Imperial Collage London, UK	(Currently at I ² CNER)

Niste Vlad Bogdan	Postdoctoral Researcher	4 months	University of Southampton (PhD student)	(Currently at I ² CNER)
Smid Brestilav	Postdoctoral Researcher	4 months	JSPS Postdoctoral Research Fellow (NIMS)	(Currently at I ² CNER)
Bidyut Baran Saha	Professor (PI)	3 months	Kyushu University, Japan	(Currently at I ² CNER)
Aleksandar Staykov	Associate Professor (3), Associate Professor (2), Assistant Professor (1),	3 months (3), 1 year and 1 month (2), 3 years and 7 months (1),	Kyushu University, Japan	(Currently at I ² CNER)
John Druce	Assistant Professor, Postdoctoral Researcher	3 months, 3 years and 11 months	Imperial Collage London, UK	(Currently at I ² CNER)
Singh Shiwani	Postdoctoral Researcher	2 months	Jawaharlal Nehru Centre for Advanced Scientific Research, India	(Currently at I ² CNER)
Nuguroho Agung Pambudi	Postdoctoral Researcher	1 month	Sebelas Maret University, Indonesia	(Currently at I ² CNER)
Huaijun Lin	Postdoctoral Researcher	1 month	Kyushu University, Japan	(Currently at I ² CNER)
Masamichi Nishihara *	Assistant Professor	5 years	Kyushu University, Japan	Kyushu University, Japan
Kiminori Shitashima *	Associate Professor	4 years 10 months	Central Research Institute of Electric Power Industry, Japan	Tokyo University of Marine Science and Technology, Japan
Limin Guo	Postdoctoral Researcher	3 years 4 months	Tohoku University, Japan	Huazhong University of Science and Technology, China
Fei Jiang	Postdoctoral Researcher	3 years	Kyushu University, Japan	Yamaguchi University, Japan
Mohamed Reda Berber	Postdoctoral Researcher	3 years	Kyushu University, Japan	Tanta University, Egypt
Hoda Sadat Emami Meibody	Postdoctoral Researcher	2 years 8 months	CNRS, France	TBD
Ma Wei	Postdoctoral Researcher	2 years and 6 months	Kyushu University, Japan	Wenzhou Institute of Biomaterials and Engineering, China
Alexander Rene Parent	Postdoctoral Researcher	2 years 4 months	Yale University, USA	North Dakota State University, USA
Kevin Lee White	Postdoctoral Researcher	1 year 1 month	Kyushu University, Japan	Akron Ascent Innovations, USA

* Appointment not renewed after March 31, 2016

Yutaka Yamada	Postdoctoral Researcher	1 year	Kyushu University (PhD student)	Okayama University, Japan
Askounis Alexandros	Postdoctoral Researcher	4 months	The University of Edinburgh (PhD student)	JSPS postdoctoral research fellow Kyushu University

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 at Urbana-Champaign (UIUC)	Andrew Gewirth	

< Partner institutions>

Institution name	Principal Investigator(s), if any	Notes
Air Resources Board of the State of California (CARB)		
Bandung Institute of Technology		
University of Edinburgh		Prof. Khellil Sefiane appointed as KU Professor in July 2015, currently holds the title of WPI Professor
Dalian Institute of Chemical Physics		
Department of Energy, Energy Efficiency and Renewable Energy		
Helmholtz Institute Forschungszentrum Juelich		New (Interactions commenced in FY2015)
Imperial College London	John Kilner	
Massachusetts Institute of Technology	Harry Tuller	
Max-Planck Institute		
Mohawk Innovative Technology		
Norwegian University of Science and Technology (NTNU)/SINTEF		
Sandia National Laboratories	Brian Somerday (thru February 2016)	
Southwest Research Institute	Brian Somerday (from March 2016)	New (Interactions commenced in FY2015)
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 Irvine/NFCRC		
University of Göttingen	Reiner Kirchheim	
University of New South Wales		New (Agreement negotiations in progress)
University of Norte Dame	Kenneth Christensen	
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 FY2015:

Total: 2,286,895,514 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)
Miho Yamauchi	CREST	JST	24,765,000
Miho Yamauchi	CREST	JST	4,550,000 (FY2016 287,300,000)
Joichi Sugimura	R&D Project (Useful Technology of Hydrogen)	NEDO	393,537,000
Chihaya Adachi	Exploratory Research for Advanced Technology (ERATO)	JST	228,996,000
Seiji Ogo	KAKENHI (Specially Promoted Research)	JSPS	117,300,000
Kazunari Sasaki	Demonstration Research on a Hydrogen-based Society through Collaboration among Industry, University, Government and Local Community	MEXT	108,542,000

COMPETITIVE FUND

RECIPIENT	NAME OF GRANT	FUNDED BY	PERIOD	TOTAL (JPY)
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 O ₂ sensor application				
Guo Limin	KAKENHI (Young Researcher B)	JSPS	FY 2014-15	4,030,000
Dye-sensitized mesoporous Ta ₃ N ₅ photocatalysts for water splitting under visible light with longer wavelengths up to ~600 nm				
Mohamed R. Berber	KAKENHI (Young Researcher B)	JSPS	FY 2014-15	2,340,000
A step towards the real world application of polymer electrolyte fuel cells: improvement of durability				
Yuki Honda	KAKENHI (Young Researcher B)	JSPS	FY 2014-15	3,900,000
Mechanism Analysis and Improvement of Fluorescence Changes of the Green Fluorescent Protein-based Citrate Indicators				
Ki-Seok Yoon	KAKENHI (Scientific Research C)	JSPS	FY2015-17	4,940,000
Unraveling the electron transfer mechanism of New [NiFe]hydrogenase surpassing platinum catalyst:				
Stephen Lyth	KAKENHI (Young Researcher B)	JSPS	FY2015-16	4,420,000
Doped Graphene Foam as a Model Oxygen Reduction Reaction Electrocatalyst System				
Nicola Perry	KAKENHI (Young Researcher B)	JSPS	FY2015-16	4,030,000
Optimization of grain boundary architecture and chemistry for efficient, durable SOFC/SOEC electrodes				
Hiroshige Matsumoto	SIP	JST	FY2014-18	48,750,000
Novel steam electrolysis				
Ikuo Taniguchi	ALCA	JST	FY2014-15	4,550,000
Preparation of nanogel immobilized membranes and the CO ₂ separation properties				
Yuki Terayama	Matching Planner Program	JST	FY2015-16	1,695,200
Development of Reversible Cell for Fuel Cell and Water Electrolysis with Water-Absorbing Porous Electrolyte				

COMMISSIONED RESEARCH

<u>RECIPIENT</u>	<u>FUNDED BY</u>	<u>PERIOD</u>	<u>TOTAL (JPY)</u>
Masanobu Kubota	Air Liquid Laboratories	FY2014-15	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	Mizuho Information & Research Institute	FY2015	6,624,728

Research on public understanding of CCS

Kenshi Itaoka	Toyota	FY2015	15,507,362
Research for domestic hydrogen station deployment model			
Kiminori Shitashima	University of Tokyo	FY2015	13,659,374
Ocean resource use promotion technical development program, Development of large-area survey system for discovery for ocean mineral resources			
Kiminori Shitashima	Kochi University	FY2015	2,200,000
Development of multi-channel integration control system for hydrothermal vent observation technology			
Takeshi Tsuji	JSPS (Bilateral Joint Research Projects: Egypt)	FY2015-16	3,094,880
Serpentine rocks: a potential georeactor for CO ₂ sequestration			
Tatsumi Ishihara	JSPS (International Joint Research Program: PIRE Program)	FY2015-20	49,500,000
Integrated Computational Materials Engineering for Active Materials and Interfaces in Chemical Fuel Production			

JOINT RESEARCH

<u>RECIPIENT</u>	<u>FUNDED BY</u>	<u>PERIOD</u>	<u>TOTAL (JPY)</u>
Petros Sofronis	JFE Steel	FY2014-15	2,040,000
Effect of Hydrogen on Fatigue S-N Curves			
Masanobu Kubota	Nippon Steel & Sumitomo Metal corporation	FY2014-15	1,944,000
Fundamental Studies on Fretting Fatigue and Crack Growth Behavior of Small Crack			
Hiroshige Matsumoto	Kyocera	FY2014-15	2,850,000
Research on low-temperature sintering of ceramic materials			
Miho Yamauchi	Toyota Central R&D Labs	FY2014-15	2,000,000
Synthesis of homogeneous solid-solution Fe-Ni nanoalloys for sensor applications			
Hiroshige Matsumoto	Honda	FY2014-15	3,420,000
Development of novel hydrogen production method			
Masanobu Kubota	Air Liquid Laboratories	FY2014-15	20,400,000
Effect of Impurities Contained in Hydrogen Gas on Inhibition of Hydrogen Embrittlement in Steels			
Hiroshige Matsumoto	Panasonic	FY2014-15	5,760,000
Joint research on epitaxially-prepared high-proton-conducting thin film metal oxides			
Ikuo Taniguchi	Tosoh	FY2015	1,000,000
Natural gas purification by membrane separation with novel amines			
Tatsumi Ishihara	Zeon	FY2015	1,300,000
Development of nanosheet electrodes for high efficiency dye-sensitized solar cells (DSSCs)			
Tatsumi Ishihara	Zeon	FY2015	1,300,000

Development of novel organic dyes for high efficiency dye-sensitized solar cells (DSSCs)

Takeshi Tsuji	JOGMEG	FY2015	440,000
Development of seismic monitoring system for injected CO ₂ distribution using a continuous and controlled source			
Masanobu Kubota	Nippon Steel & Sumitomo Metal Corporation	FY2015-16	1,944,000
Development of method for fatigue performance evaluation based on fretting fatigue properties and small crack propagation properties			
Takeshi Tsuji	Shikoku Research Institute	FY2015	600,000
Fault characterization using geophysical approaches			
Masamichi Nishihara	Nissan Chemical Industries	FY2015-16	1,000,000
Development of novel ionomers for polymer electrolyte membrane fuel cells			
Hiroshige Matsumoto	Kyocera	FY2015-16	25,000,000
Research on low-temperature sintering of ceramic materials			

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 FY2015 and give up to three examples of the most representative ones using the table below.

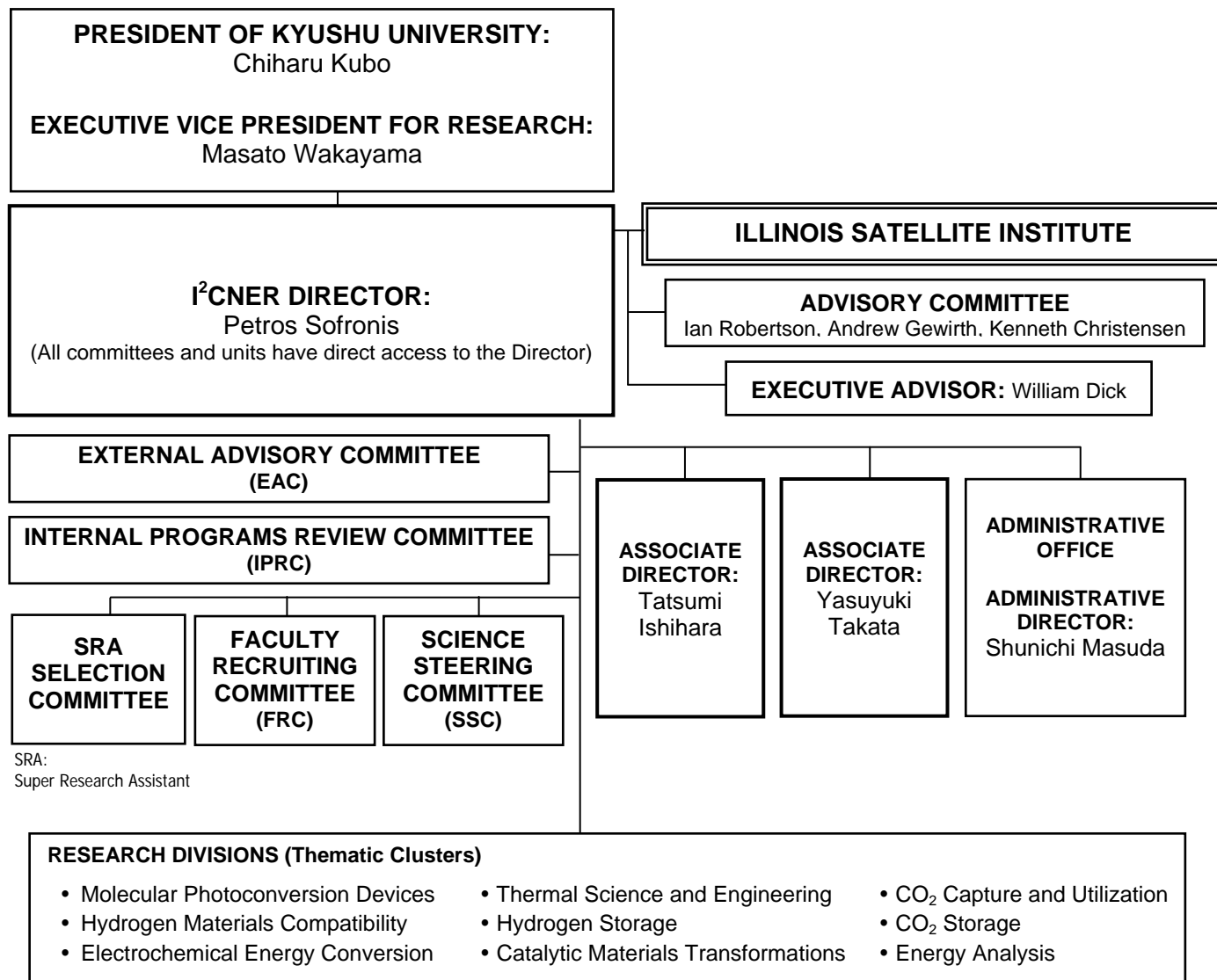
FY 2015	
Major examples (meeting title and place held)	Number of participants
I ² CNER Annual Symposium 2016, I ² CNER Hall, Ito Campus, Kyushu University February 1-2, 2016	From domestic institutions: 127 From overseas institutions: 125
I ² CNER International Workshop 2016, Ito Campus, Kyushu University February 4, 2016	From domestic institutions: 304 From overseas institutions: 76
The First Pacific Rim Thermal Engineering Conference, Hawaii Conference Chair, PI Takata March 13-17, 2016	Total 500 - 600

4. Center's management system

- Please diagram management system in an easily understood manner.

I²CNER ORGANIZATIONAL STRUCTURE

(As of April 1, 2016)



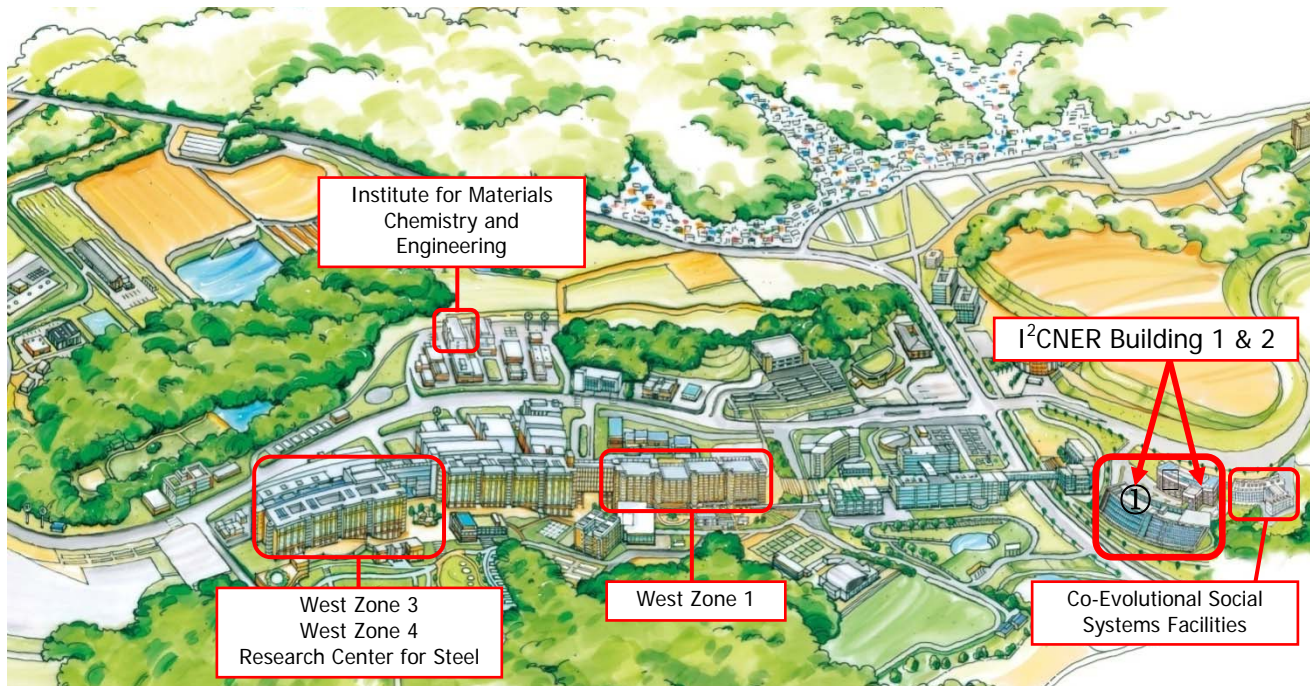
- If any changes have been made in the management system from that in the "Post-interim evaluation revised center project," please describe them. Please describe any changes made in the administrative director, head of host institution, and officer(s) in charge at the host institution (e.g., executive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

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.

With the support of EVP Wakayama, I²CNER reorganized its divisions in response to a critical evaluation by the Internal Programs Review Committee (IPRC) in FY2013. Specifically, two of its divisions (Hydrogen Production and Fuel Cells) were dissolved and two new divisions with more specific, focused targets (Molecular Photoconversion Devices, led by Prof. Ishihara, and Electrochemical Energy Conversion, led by Prof. Matsumoto) were created.

Campus Map

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



6. FY2015 Project Expenditures (the exchange rate used: 1USD=100JPY)

i) Overall project funding

Cost Items	Details	Costs (10,000 dollars)
Personnel	Center director and Administrative director	22
	Principal investigators (no. of persons):17	223
	Other researchers (no. of persons):77	359
	Research support staffs (no. of persons):25	56
	Administrative staffs (no. of persons):23	101
	Total	761
Project activities	Gratuities and honoraria paid to invited principal investigators (no. of persons):51	4
	Cost of dispatching scientists (no. of persons):0	0
	Research startup cost (no. of persons):27	37
	Cost of satellite organizations (no. of satellite organizations):1	198
	Cost of international symposiums (no. of symposiums):1	2
	Rental fees for facilities	257
	Cost of consumables	27
	Cost of utilities	34
	Other costs	59
		Total
Travel	Domestic travel costs	14
	Overseas travel costs	55
	Travel and accommodations cost for invited scientists (no. of domestic scientists):53 (no. of overseas scientists):49	16
	Travel cost for scientists on secondment (no. of domestic scientists):1 (no. of overseas scientists):3	2
		Total
Equipment	Depreciation of buildings	82
	Depreciation of equipment	1,537
	Total	1,619
Other research projects	Projects supported by other government subsidies, etc.	144
	Commissioned research projects, etc.	1,234
	Grants-in-Aid for Scientific Research, etc.	277
		Total
	Total	4,740

	Ten thousand dollars
WPI grant	1,270
Costs of establishing and maintaining facilities	27
Establishing new facilities (Number of facilities:0m ²)	Costs paid: 0
Repairing facilities (Building 2) (Number of facilities:5,000m ²)	Costs paid: 24
Others	3
Cost of equipment procured	582
Name of equipment: Nanoindenter	Number of units:1 Costs paid: 73
Name of equipment: Surface Energy Analyzer	Number of units:1 Costs paid: 20
Others	489

ii) Costs of Satellites and Partner institutions

Cost Items	Details	Costs (10,000 dollars)
Personnel	Principal investigators (no. of persons):2	/
	Other researchers (no. of persons):6	
	Research support staffs (no. of persons):16	
	Administrative staffs (no. of persons)	
	Total	124
Project activities		55
Travel		18
Equipment		0
Other research projects		0
	Total	197

Status of Collaboration with Overseas Satellites

1. Coauthored Papers

- List the refereed papers published in FY2015 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. 2016 and not described in Appendix 1.

Overseas Satellite: University of Illinois, Urbana-Champaign (Total: 14 papers)

No.	Author names and details
(-)	Tsuji, T., Jiang, F. and <i>Christensen, K.</i> (2016), Characterization of immiscible fluid displacement processes with various capillary numbers and viscosity ratios in 3D natural sandstone, <i>Advances in Water Resources</i> , 95, 3-15.
(-)	Kim, B., Hillman, F., Ariyoshi, M., Fujikawa, S. and <i>Kenis, P.J.A.</i> (2016), Effects of composition of the micro porous layer and the substrate on performance in the electrochemical reduction of CO ₂ to CO, <i>Journal of Power Sources</i> , 312, 192-198.
(-)	Wang, S., Martin, M.L., Robertson, I.M. and <i>Sofronis, P.</i> (2016), Effect of hydrogen environment on the separation of Fe grain boundaries, <i>Acta Materialia</i> , 107, 279-288.
(103)	<i>Dadfarnia, M.</i> , Nagao, A., Wang, S., Martin, M.L., Somerday, B. P. and <i>Sofronis, P.</i> (2015), Recent advances on hydrogen embrittlement of structural materials, <i>International Journal of Fracture</i> , 196 (1), 223-243.
(126)	Robertson, I.M., <i>Sofronis, P.</i> , Nagao, A., Martin, M.L., Wang, S., Gross, D.W. and <i>Nygren, K.E.</i> (2015) Hydrogen Embrittlement Understood, <i>Metallurgical and Materials Transactions A</i> , 46, 2323-2341
(127)	<i>Dadfarnia, M.</i> , <i>Martin, M.L.</i> , Nagao, A., Sofronis, P. and Robertson, I.M. (2015), Modeling hydrogen transport by dislocations, <i>Journal of the Mechanics and Physics of Solids</i> , 78, 511-525.
(252)	<i>Ma, S.</i> , Sadakiyo, M., Luo, R., Heima, M., Yamauchi, M. and <i>Kenis, P.J.A.</i> (2015), One-step electrosynthesis of ethylene and ethanol from CO ₂ in an alkaline electrolyzer, <i>Journal of Power Sources</i> , 301, 219-228.
(472)	Kim, S.H., Mohseni, P.K., Song, Y., Ishihara, T. and <i>Li, X.</i> (2015), Inverse metal-assisted chemical etching of InP produces smooth high aspect ratio nanostructures, <i>Nano Letters</i> , 15 (1), 641-648.
(-)	Ida, S., Kim, N., <i>Ertekin, E.</i> , Takenaka, S. and Ishihara, T. (2015), Photocatalytic reaction centers in two-dimensional titanium oxide crystals, <i>Journal of the American Chemical Society</i> , 137, 239-244.
(-)	Tellez, 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, <i>Progress in Photovoltaics: Research and Applications</i> , 23 (10), 1219-27.
(-)	Kim, N.H., Turner, E.M., Ida, S. and <i>Ertekin, E.</i> , Oxygen evolution reaction on doped and undoped lepidocrocite TiO ₂ nanosheets: design rules for the identification of optimal dopant species from first principles, manuscript currently under revision for publication (Invited Article, <i>Journal of Materials Research</i>).

(-)	Song, Y., Mohseni, P.K., Kim, S.H., Shin, J.C., Ishihara, T, Adesida, I., and <i>Li, X.</i> (2016), Ultra-high Aspect Ratio InP Junctionless FinFETs by a Novel Wet Etching Method, IEEE Device Research Letters, 37 (8), 7485851, 970-973.
(-)	Nagao, A., <i>Dadfarnia, M.</i> , Sofronis, P. and Robertson, I.M., (2016) Hydrogen embrittlement mechanisms, Encyclopedia of Iron, Steel, and Their Alloys, CRC Press.
(-)	Chavan, S., Cha, H., Orejon, D., Nawaz, K., Singla, N., Yeung, Y.-F., Park, D., Kang, D. H., Chang, Y., Takata, Y. and <i>Miljkovic, N.</i> , Heat Transfer through a Condensate Droplet on Hydrophobic and Nanostructured Superhydrophobic Surfaces, ACS Nano, In Review

2. Status of Researcher Exchanges

- Using the below tables, indicate the number and length of researcher exchanges in FY2015. 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>

	Under 1 week	From 1 week to 1 month	From 1 month to 3 months	3 months or longer	Total
FY2015	11 8	0 0	0 2	0 0	11 10

<From satellite>

	Under 1 week	From 1 week to 1 month	From 1 month to 3 months	3 months or longer	Total
FY2015	5 8	0 3	0 0	0 0	5 11

FY 2015 Visit Records of World Top-caliber Researchers from Abroad

Researchers Total: 37

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)
Sang-Young Lee	Assoc. Prof., Ulsan National Institute of Science and Technology (UNIST), Korea	Ph.D., Chemical Engineering	<ul style="list-style-type: none"> • Top 50 basic research awards (NRF, 2014) • Kangwon Top 10 Patent Awards (2012) • NET Awards (2007) 	2015/5/15	I ² CNER Seminar Series Presentation
Zhiqun Lin	Prof., Georgia Institute of Technology, USA	Ph.D., Polymer Science & Engineering	<ul style="list-style-type: none"> • ISU Award for Early Achievement in Research (2010) • Young Engineering Faculty Research Award, College of Engineering at ISU (2009) • NSF CAREER Award (2009) 	2015/6/5	I ² CNER Seminar Series Presentation
Valeriy S. Maisotsenko	Prof Emeritus, Chief Scientist and Founder, Coolerado Corp and Idalex Technologies Inc., USA	D.Sc., Heating Engineering, Refrigeration Engineering, Heat Transfer Thermodynamics , Air-conditioning	<ul style="list-style-type: none"> • The 2007 Sustainable Business Silver Medal of Honor award (2007) • The History Channel and Invent Now Award (2007) • Governor's Excellence in Renewable Energy Award (2008) 	2015/6/24	I ² CNER Seminar Series Presentation
Esko Kauppinen	Prof., Department of Applied Physics, Aalto University, Finland	Ph.D., Gas Phase Synthesis of Nanomaterials, including Carbon Nanotubes and Fullerenes and Polymer-drug Composite Nanoparticles	<ul style="list-style-type: none"> • Finnish Association for Aerosol Research (FAAR) Award(1992) • Air Pollution Control Research Award of 2001 	2015/7/10	I ² CNER Seminar Series Presentation

Xing Zhang	Prof., Department of Engineering Mechanics, Tsinghua University, China	Ph.D., Thermal Science	<ul style="list-style-type: none"> • Significant Contribution Awards from the 10th 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) 	2015/7/19-2015/8/16 2016/1/24-2016/2/18	Joint Research Joint Research, Participation in I ² CNER Annual Symposium, Hydrogen Forum and International Workshop as Principal Investigator
Andrew Gewirth	Prof., Chemistry, University of Illinois, USA	Ph.D., Chemistry	<ul style="list-style-type: none"> • 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) 	2015/7/27-2015/8/1	Joint Research, Participation in Site Visit
Kenneth Christensen	Prof., College of Engineering, University of Notre Dame, USA	Ph.D., Theoretical and Applied Mechanics specializing in experimental fluid mechanics	<ul style="list-style-type: none"> • Dean's Award for Excellence in Research from the College of Engineering, UIUC (2012) • François Frenkiel Award for Fluid Mechanics from APS-DFD (2011) • NSF CAREER Award (2007) • AFOSR Young Investigator Award (2006) 	2015/7/27-2015/8/1 2016/1/30-2016/2/5	Participation in Site Visit and Division Meetings as Principal Investigator Joint Research, Participation in I ² CNER Annual Symposium and International Workshop as Principal Investigator

Brian Somerday	Dr., Sandia National Laboratories, USA (until the end of February 2016) Dr., South West Research Institute, USA (from March 2016)	Ph.D., Materials Science and Engineering	<ul style="list-style-type: none"> • DOE Hydrogen and Fuel Cell Program Achievement Award (2014) • Best Poster Award, ASME 12th Fuel Cell Science, Engineering, and Technology Conference (2014) 	2015/7/29-2015/8/4 2016/1/30-2016/2/8	Joint Research, Participation in Division Meeting(Retreat) Joint Research, Participation in I ² CNER Annual Symposium, International Workshop and Division Meeting(Retreat) as Principal Investigator
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Harry Tuller	Prof. Department of Materials Science and Engineering, Massachusetts Institute of Technology, USA	Eng. Sc. D., Functional Electroceramic Materials	<ul style="list-style-type: none"> • 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) 	2015/8/7- 2015/8/18 2016/1/30- 2016/2/5	Joint Research Joint Research, Participation in I ² CNER Annual Symposium, Hydrogen Forum and International Workshop as Principal Investigator
Unggul Priyanto	Chairman, Agency for Assessment and Application of Technology (BPPT), Indonesia	Dr., Engineering for Optimization of Coal Liquefaction Process	• N/A	2015/10/6	I ² CNER Seminar Series Presentation

Eniya Listiani Dewi	Deputy Chairperson of Technology for Agroindustrial and Biotechnology, BPPT, Indonesia	Dr., Electron Transfer Phenomenon on the Nanocatalysts, Hydrocarbon Polymer Materials, PEM-Fuel Cells and Zinc-Air Fuel Cell Batteries Engineering	<ul style="list-style-type: none"> • Mizuno Award (2003) • Koukenkai Award (2003) • Asia Excellent Award • Best Scientist Award 	2015/10/6	I ² CNER Seminar Series Presentation
Olivier Guillon	Prof., Director, Institute of Energy and Climate Research, Forschungszentrum Juelich GmbH, Germany	Ph.D., Field Assisted Sintering Technology, Phase Transformation of Nanoparticles, Solid Oxide Fuel/Electrolytic Cells	<ul style="list-style-type: none"> • DGM-Masing Prize (2010) • FEMS Materials Science and Technology Prize (2011) • R.L. Coble Award for Young Scholar (2011) 	2015/10/9	I ² CNER Seminar Series Presentation
John Kilner	Prof., Department of Materials, Imperial College, London, UK	Ph.D., Materials for Solid Oxide Fuel Cells and Electrolyzers	<ul style="list-style-type: none"> • Platinum Medal, Institute of Materials Minerals and Mining (2012) • Somiya Award, International Union of Materials Research Societies (2012) • Fellow, City and Guilds Institute of London (2007) • Royal Society Armourers and Brasiers' Company Prize, Royal Society (2005) • Verulam Medal, Institute of Materials, Minerals and Mining (2005) • Schoenbein Medal, European Solid Oxide Forum (2004) • Excellence in Teaching, Imperial College (1997) 	2015/10/25-2015/11/16 2015/1/27-2015/2/13	Joint Research Joint Research, Participation in I ² CNER Annual Symposium, Hydrogen Forum, International Workshop and Division Retreat as Principal Investigator

Bruno Ameduri	Research Director, The National Center for Scientific Research, France	Ph.D., Synthesis of Fluorinated Monomers, Telomeres, and (co)Polymers	<ul style="list-style-type: none"> • Special "Prime d'Excellence Scientifique" (2011) • Award for Outstanding Contribution and Innovation in Fluoropolymer Science (2012) 	2015/11/5	I ² CNER Seminar Series Presentation
Harold Drake	Prof., Department of Ecological Microbiology, University of Bayreuth, Germany	Ph.D., Microbiology	<ul style="list-style-type: none"> • C. M. Downs Award, University of Kansas (1976) • NIH Research Career Development Award (1978) 	2015/11/13	I ² CNER Seminar Series Presentation
Françoise Winnik	Prof., Department of Chemistry, University of Montreal, Canada	Ph.D., Organic Chemistry and Photochemistry	<ul style="list-style-type: none"> • Clara Benson award of the Canadian Institute of Canada (2006) 	2015/11/24	I ² CNER Seminar Series Presentation
Leslie Mabon	Lecturer in Sociology, Robert Gordon University, Scotland	Ph.D., Human Geography	<ul style="list-style-type: none"> • UK CCS Research Centre-International Collaboration Grant (with Research Centre for Innovative Technology for the Earth, Kyoto Japan) (£17,000) (2015/16) • GB Sasakawa Foundation-Scotland-Japan Workshops on Environmental Governance (£5,000) (2015/16) 	2015/12/16	I ² CNER Seminar Series Presentation
Marc Robert	Prof., University Paris Diderot, France	Ph.D., Molecular Electrochemistry	<ul style="list-style-type: none"> • The French Chemical Society prize (2006) 	2016/1/15	I ² CNER Seminar Series Presentation
Gwidon Stachowiak	Prof., School of Civil and Mechanical Engineering, Curtin University, Australia	Ph.D., Development of Methods for the Characterization of Multiscale 3D Surface Topographies	<ul style="list-style-type: none"> • Tribology Gold Medal (2014) 	2016/1/29	I ² CNER Seminar Series Presentation

Michael Celia	Prof., Civil and Environmental Engineering, Princeton University, USA	Ph.D., Civil Engineering	<ul style="list-style-type: none"> • AGU Hydrologic Sciences Award (2005) • Hydrology Days Award (2012) 	2016/1/29	I ² CNER Seminar Series Presentation
Christodoulos Chatzichristodoulou	Senior Scientist, Department of Energy Conversion and Storage, Technical University of Denmark, Denmark	Ph.D., Electrodes and Electrolytes for CO ₂ Reduction	<ul style="list-style-type: none"> • Manufacturing of Green Fuels from Renewable Energy (Invited speaker) (2015) • High Temperature Alkaline Electrolysis (Lecturer) (2014) 	2016/1/30- 2016/2/5	Participation in I ² CNER Annual Symposium, Hydrogen Forum and International Workshop

Anil Virkar	Distinguished Professor, Materials Science and Engineering, University of Utah, USA	Ph.D., Materials Science	<ul style="list-style-type: none"> • John Jeppson Award, American Ceramic Society (2013) • James I Mueller Award, American Ceramic Society (2013) • Dow Distinguished Lecturer: "Transport-Induced Instability in Electrochemical Devices: Fuel Cells, Batteries, Electrolyzers", Northwestern University (2012) • Elected Fellow of ASM International (2010) • Distinguished Lecture, National Cheng Kung University, Taiwan (2009) • Keynote Speaker (Lecture and Plaque), University of Pennsylvania (2009) • Distinguished Speaker (Lecture and Plaque), Pacific Northwest National Laboratory (2009) 	2016/1/30-2016/2/5	Participation in I ² CNER Annual Symposium, Hydrogen Forum and International Workshop
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Reiner Kirchheim	Prof., The Institut für Materialphysik, University of Göttingen, Germany	Ph.D., Hydrogen in Metals, Thermodynamics of Alloys, Interstitial Solution and Diffusion in Glasses	<ul style="list-style-type: none"> • 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-Denkmalze (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) 	2016/1/29- 2016/2/6	Participation in I ² CNER Annual Symposium, Hydrogen Forum and International Workshop as Principal Investigator
Ian Robertson	Prof., Dean of Engineering, Chief Science Advisor to the Director, University of Wisconsin-Madison, USA	Ph.D., Metallurgy	<ul style="list-style-type: none"> • 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) 	2016/1/30- 2016/2/3	Participation in I ² CNER Annual Symposium, as Principal Investigator

Elif Ertekin	Asst. Prof., Department of Mechanical Science & Engineering, University of Illinois, USA	Ph.D., Materials Science & Engineering	<ul style="list-style-type: none"> • 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 University (1999) 	2016/1/30- 2016/2/5	Joint Research, Participation in I ² CNER Annual Symposium, International Workshop and Division Meeting(Retreat)
Jörg Neugebauer	Director., Max-Planck-Ins- titut für Eisenforschung GmbH, Düsseldorf, Germany	Ph.D., Physics	<ul style="list-style-type: none"> • European Research Council (ERC) Advanced Grant (2012) • Member of the Academy of Sciences and Art in North Rhine-Westphalia (2010) • Honorary Professor at the Ruhr-University Bochum (2007) • DFG Habilitationsstipendium (1996) • DAAD Forschungsstipendium (1993) • Humboldt prize (1990) 	2016/1/30- 2016/2/2	Participation in I ² CNER Annual Symposium, Hydrogen Forum and International Workshop

Edward Seidel	Director, The National Center for Supercomputing Applications, Founder Prof., Department of Physics, Prof., Department of Astronomy, University of Illinois, USA	Ph.D., Relativistic Astrophysics	<ul style="list-style-type: none"> • Sidney Fernbach Award (2006) • Gordon Bell Prize (2001) • Heinz-Billing-Award (1998) 	2016/1/30- 2016/2/3	Participation in I ² CNER Annual Symposium
Luca De Gioia	Prof., Department of Biotechnology and Bioscience, University of Milan Bicocca, Italy	Ph.D. 化学	<ul style="list-style-type: none"> • Presented more than 100 posters and oral communications in national and international congresses • Co-author of more than 180 publications about protein chemistry and bioinorganic chemistry on peer-reviewed international journals (h-index = 38, November 2015) 	2016/1/30- 2016/2/5	Participation in I ² CNER Annual Symposium, Hydrogen Forum and International Workshop

John Keith	R.K. Mellon Faculty Fellow, Department of Chemical and Petroleum Engineering, University of Pittsburgh, USA	Ph.D., Chemistry	<ul style="list-style-type: none"> • Pittsburgh Business Times Who's Who in Energy (2014-2015) • R.K. Mellon Faculty Fellow in Energy (2013) • Insidehighered.com: Mover and Shaker (2013) • Alexander von Humboldt Postdoctoral Fellowship (2008-2010) • Phi Beta Kappa (2001) • American Chemical Society: Connecticut Valley Regional Award (2001) • Bradley Prize for outstanding undergraduate thesis in chemistry (2001) • American Chemical Society Analytical Chemistry Award (2000) 	2016/1/30-2016/2/5	Participation in I ² CNER Annual Symposium, Hydrogen Forum and International Workshop
Géraldine Theiler	Scientist, BAM (Federal Institute for Materials Research and Testing), Germany	Ph.D., Engineering	<ul style="list-style-type: none"> • Gave presentations in World Hydrogen Energy Conference (2006), World Tribology Congress (2013) and International Tribology Conference (2015) 	2016/1/30-2016/2/5	Participation in I ² CNER Annual Symposium, Hydrogen Forum and International Workshop

Bilge Yildiz	Assoc. Prof., Nuclear Science and Engineering, Materials Science and Engineering, Massachusetts Institute of Technology, USA	Ph.D., Nuclear Science and Engineering	<ul style="list-style-type: none"> • Charles W. Tobias Young Investigator Award (2012) • Somiya Award for International Collaboration (2012) • NSF CAREER Award (2011 – 2016) • ANS Faculty PAI Outstanding Teaching Award (2008) • Pacesetter Award, Argonne National Laboratory (2006) 	2016/1/31- 2016/2/7	Participation in I ² CNER Annual Symposium, Hydrogen Forum and International Workshop
Christopher San Marchi	Distinguished Member of Technical Staff, Sandia National Laboratories, USA	Ph.D., Materials Science	<ul style="list-style-type: none"> • The DOE Hydrogen and Fuel Cell Program achievement award (2014) • The DOE Annual Merit Review Award, Hydrogen Delivery and Safety, Codes and Standards (2014) 	2016/1/31- 2016/2/5	Participation in I ² CNER Annual Symposium, Hydrogen Forum and International Workshop

Xiaojia Wang	Asst. Prof., Department of Mechanical Engineering, University of Minnesota, USA	Ph.D., Mechanical Engineering	<ul style="list-style-type: none"> • Innovation Award for the poster presentation at IMECE (2009) • Xi'an Jiaotong University graduate First Prize Scholarship (2005) • "China Petroleum & Chemical" Fellowship (Nationwide) (2005) • Freshman First Prize Scholarship for graduate students (2004) • Excellent Graduate of Xi'an Jiaotong University (2004) • "Nan Fang Lu Ji" Fellowship (Nationwide) (2003) • Xi'an Jiaotong University First Prize Scholarship (2003) 	2016/1/31- 2016/2/5	Participation in I ² CNER Annual Symposium, Hydrogen Forum and International Workshop
Kondo-François Aguey-Zinsou	Assoc. Prof., School of Chemical Engineering, University of New South Wales, Australia	Ph.D., Heterogeneous Catalysis	<ul style="list-style-type: none"> • UNSW Research Excellence Award 2012 	2016/1/31- 2016/2/5	Participation in I ² CNER Annual Symposium, Hydrogen Forum and International Workshop
Ali Elkamel	Prof., Chemical Engineering, University of Waterloo, Canada	Ph.D., Chemical Engineering	<ul style="list-style-type: none"> • Outstanding Reviewer Status, Applied Energy (2015) • Best Reviewer Award for the International Journal of Process Systems Engineering (IJPSE) (2014) 	2016/2/19	I ² CNER Seminar Series Presentation
Keumnam Cho	Prof., Sungkyunkwan University, Korea	Ph.D., Mechanical Engineering	<ul style="list-style-type: none"> • Asian Academic Award (2007) 	2016/2/26	I ² CNER Seminar Series Presentation

Gerard Marriott	Prof., University of California, Berkeley, USA	Ph.D., Biochemistry	<ul style="list-style-type: none">Fluorescence Investigator Award	2016/3/18	I ² CNER Seminar Series Presentation
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State of Outreach Activities

- Using the table below, show the achievements of the Center's outreach activities in FY2015(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 FY2015 resulting from press releases and reporting.

Activities	FY2015(number of activities, times held)
PR brochure, pamphlet	5
Lectures, seminars for general public	12
Teaching, experiments, and training for elementary and secondary school students	22
Science cafe	2
Open houses	1
Participating, exhibiting in events	7
Press releases	14

Special Achievements

- 11th Japan-France Workshop on Nanomaterials-2nd WPI-Workshop on Materials Science
- Director Sofronis, Prof. Fujikawa, and Prof. Yamauchi gave lectures at the workshop, which was organized by 4 WPI Institutes, May 2015

Super Science High Schools (SSH) student workshop

- Prof. Helena Téllez gave a lecture to students, Aug. 2015

Homecoming Day

- I²CNER welcomed more than 40 alumni who attended the Homecoming Day of Kyushu University, Oct. 2015

6th World Hydrogen Technologies Convention

- I²CNER ran a booth and Profs. Akiba, Matsumoto, and Itaoka gave lectures, Oct. 2015

Books for general readers

- "Small Molecule Energy" by Prof. Seiji Ogo, Feb. 2016

FY 2015 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	Apr. 7, 2015	Nihon Keizai Shimbun	Interview about usage of hydrogen Akiba E. (Hydrogen Storage)
2	Apr. 20, 2015	Nihon Keizai Shimbun	Vision and challenge of hydrogen society Sasaki K. (Electrochemical Energy Conversion)
3	Apr., 2015	Nikkei Sangyo Shimbun, Nikkan Kogyo Shimbun, etc.	Development of hydrogen permeation system of 100 MPa hydrogen gas pressure-The highest gas pressure in the world Nagao A. (Hydrogen Materials Compatibility)
4	Jun. 9, 2015	Nikkei Sangyo Shimbun	An innovator in Japan. Advanced technology. Development of organic EL novel material. Adachi C. (Molecular Photoconversion Devices)
5	Jun. 23, 2015	Nishinippon Shimbun	Kyoto Prize Kunitake T. (CO ₂ Capture and Utilization)
6	Jun. 26, 2015	VOICE	At the forefront of the battle against global warming Xue Z. (CO ₂ Storage)
7	Jul. 2, 2015	Mainichi Shimbun	Mechanism of cell membrane Kunitake T. (CO ₂ Capture and Utilization)
8	Jul. 29, 2015	Nihon Keizai Shimbun	Increasing the efficiency of electric power generation of fuel cells Sasaki K. (Electrochemical Energy Conversion)
9	Oct. 1, 2015	Nihon Keizai Shimbun	Hybrid-FC powered by SOLIDIA received GOOD DESIGN AWARD Sasaki K. (Electrochemical Energy Conversion)
10	Oct. 1, 2015	Sankei Shimbun, Nihon Keizai Shimbun, Science Portal, excite news, zakzak, Sankei News	Found new geological formation controlling earthquake off the Kii peninsula Tsuji T. (CO ₂ Storage)
11	Oct. 12, 2015	Nikkan Dempa Shimbun	Workshop on Industrialization of Organic Light Electroluminescent Products Adachi C. (Molecular Photoconversion Devices)
12	Oct. 20, 2015	Nikkei Sangyo Shimbun	Organic Electroluminescence, Cheap But Brilliant Light Adachi C. (Molecular Photoconversion Devices)

13	Nov. 2, 2015	Nikkei Sangyo Shimbun	Novel energy Sasaki K. (Electrochemical Energy Conversion)
14	Nov. 2, 2015	Nishinippon Shimbun, Asahi Shimbun, Yomiuri Shimbun, Nihon Keizai Shimbun	Medal with Purple Ribbon Horita Z. (Hydrogen Storage)
15	Nov. 4, 2015	Nikkei Sangyo Shimbun, Asahi Shimbun	Enzyme for both sides of fuel cells Ogo S. (Catalytic Materials Transformations)
16	Nov. 9, 2015	Nihon Keizai Shimbun	Breakthrough in continuous monitoring of CO ₂ leaks from storage sites Tsuji T., Ikeda T. (CO ₂ Storage)
17	Nov. 10, 2015	Tekko Shimbun	Research Center for Steel, Kyushu University Takaki S. (Hydrogen Materials Compatibility)
18	Nov. 26, 2015	Nikkan Kogyo Shimbun	Durability enhancement of polymer electrolyte fuel cell Nakashima N. (Electrochemical Energy Conversion Devices)
19	Nov. 26, 2015	Yomiuri Shimbun	Improvement of productive technologies Takaki S. (Hydrogen Materials Compatibility)
20	Dec. 11, 2015	Bangladesh Sangbad Sangstha	Japanese Team meets DU VC Saha B.B. (Thermal Science and Engineering)
21	Dec. 15, 2015	Nihon Keizai Shimbun	High purity separation of semiconducting carbon nanotubes Nakashima N. (Electrochemical Energy Conversion Devices)
22	Dec. 22, 2015	Nihon Keizai Shimbun	Tailwind for Startup Companies Adachi C. (Molecular Photoconversion Devices)
23	Feb. 16, 2016	Nikkan Kogyo Shimbun	Kyushu University has developed the glue that can be used on wet surfaces and high humid environment Takahara A., Higaki Y. (Molecular Photoconversion Devices)
24	Feb. 25, 2016	Nishinippon Shimbun, Asahi Shimbun, Nihon Keizai Shimbun, Sankei Shimbun	Towards the Development of Materials for Smartphone Displays by a Kyushu University Startup Company of Organic Electroluminescent Products Adachi C. (Molecular Photoconversion Devices)
25	Mar. 10, 2016	Secchakuzai Shimbun	Glue can be used on wet surface -Application of the principle of barnacles- Takahara A., Higaki Y. (Molecular Photoconversion Devices)