World Premier International Research Center Initiative (WPI)
Executive Summary (For Extension Application Screening)

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

A. Progress Report of the WPI Center

I. Summary

As it enters its eighth year, the institute's momentum and scientific impact continue to increase rapidly. Many metrics support this claim: the number of scientific discoveries and breakthroughs that are reducing the identified roadblocks has increased dramatically as have the technology transfers to industry; the number of industrial partnerships has increased as have the number of international universities seeking partnerships with I^2CNER. The high-impact transformational reforms being instituted by the Kyushu University Administration that I^2CNER has driven, as well as I^2CNER's strategy for furthering technology-driven research, is positioning Kyushu University as a world-wide leader. The continual evolution of I^2CNER's research themes is forging new partnerships with other departments within Kyushu University, which are essential to ensure the vitality of the Institute and its ability to overcome the technological barriers preventing Japan from transitioning to a carbon neutral society. I^2CNER has become integrated into the very fabric of Kyushu University and the overall international energy research landscape. Despite the advances, many roadblocks are still to be overcome, but the Institute, through its new partnerships with mathematics, political and social sciences, and economics, is prepared to address these challenges. I^2CNER is already making vital contributions toward the development of a future carbon neutral society, and the institute's plans for the future are targeted to ensure Japan meets its energy needs while achieving its carbon reduction targets by 2050.

II. Items

1. Overall Image of Your Center

I^2CNER's mission remains to develop the foundations for development of energy systems that will address Japan's future energy needs while minimizing the nation's CO_2 emissions by 70-80% from the 1990 levels by 2050. To carry out its mission, I^2CNER's research is driven by well-defined milestones and targets that are identified in roadmaps of the underlying technologies. Our roadmaps are developed in by our Energy Analysis Division (EAD). The three principles in the roadmap are the creation of energy cost effective systems with increased efficiency, lower carbon intensity, and advanced CO_2 management. The research teams are by necessity composed of scientists and engineers from disparate disciplines including chemistry, physics, materials science, mechanics, geoscience, and biomimetics, and the research addresses phenomena that span many decades in spatial and temporal scales. The research teams are dynamic, with new disciplinary partnerships being formed and dissolved. By way of example, there is a fusion project between the natural sciences and applied math for energy engineering, e.g., two-phase flows in geomaterials and persistent homology, that emerged as a new frontier in I^2CNER's research endeavors that stem from our new interactions with the Institute of Mathematics for Industry (IMI) of Kyushu University (KU). I^2CNER research synergistically couples theory, computer modeling, and simulation with experimental methodologies to accelerate the realization of solutions to the challenges identified in the roadmaps. In other words, I^2CNER's research activities and goals are by nature interdisciplinary, mission-oriented, and are performed across research cluster (division) boundaries and international borders.

I^2CNER's mission is enhanced by its Satellite Center at the University of Illinois, which serves to advance an impressive number of collaborations across the USA, including top-tier US universities, prestigious national laboratories, and government agencies. In addition, the Illinois Satellite is enabling KU to execute its reform and revitalization program for the internationalization of its education and research missions. The Satellite Center provides the setting for young Japanese faculty, as well as graduate and undergraduate students, to be immersed in collaborative research in an international environment. To reinforce its research portfolio, I^2CNER has expanded its network of collaborations with leading internationally recognized research teams in institutions in Europe, Asia, and Australia.

2. Research Activities

I^2CNER's research activities are conducted within its technical divisions in partnership with the EAD, which ensures continuous assessment of techno-economic relevance and feasibility of the research. Within the divisions, research is organized into projects, with each project having well-defined milestones on a roadmap toward a final target. Toward this goal, within each project, research efforts by individual researchers target the corresponding milestones. Since inception, the Institute has realized 12 of the short-term and 4 of the mid-term milestones in our project roadmaps, realized a NEDO Target in the Hydrogen Storage division, and exceeded the gas selectivity target for our nanometer membrane for CO_2 separation in the CO_2 Capture and Utilization division. A selection of the Institute's breakthrough results/achievements are presented in terms of the milestones and targets of the respective project roadmaps.

Molecular Photoconversion Devices: Photocatalytic water splitting is limited by the slow kinetics of the hydrogen evolution reaction. To overcome this, by 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 valence band edge under solar illumination is the mechanism responsible for the degradation in a most exciting novel photovoltaic technology (hybrid perovskite devices) in the presence of moisture. By controlling water and oxygen ingress, the perovskite film exhibited reduced recombination carrier and suppressed formation of metallic lead, which led to improved device stability. The estimated device lifetime of 4,000 hrs is one of the longest ever reported with 18% power conversion.

Catalytic Materials Transformations: The discoveries on biomimetic catalysis by PI Ogo are an exemplar of continuous progress toward roadmap milestones. The group first reported in *Science* a functional [NiFe]-based model of [NiFe]hydrogenase enzymes, which can heterolytically activate hydrogen to form a hydride complex. That work was followed by a successful development of a new synthetic [NiFe]-based catalyst for O_2 reduction via an O_2 adduct. This is the first example worldwide of a side-on iron (IV) peroxo complex of an O_2-tolerant hydrogenase mimic. These accomplishments underlie future developments of small molecule fuel cells that do not involve precious metal catalysts, and at the same time set the framework for small molecule activation, an area of crucial importance to energy technologies.

Thermal Science and Engineering: The focus of Prof. Miljkovic's (Illinois) research on novel micro/nanostructures for coalescence induced droplet jumping and adsorbent nanomaterials has led to transformational efficiency enhancements in energy and water applications by fundamentally manipulating heat-fluid-surface interactions across multiple length and time scales. Specifically, the discovery of these novel nanomaterials and coatings has immense technological impact on renewable and non-renewable power generation, thermal management, and building energy technologies.

PI Saha's foundational studies on solid-vapor adsorption phenomena for the rational design of high-uptake adsorbent materials, as well as surface wettability due to hydrocarbon adsorption from the atmosphere, have led to the discovery of highly porous (> 3000 2/g) Metal-Organic Frameworks with ultra-high water and ethanol uptake. These accomplishments that meet the short-term milestones in the respective project roadmaps are re-writing the foundational knowledge base in the field of surface science by quantifying the environmental effects on sample wettability and adsorption.

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. The "polymer-wrapped carbon" approach developed by the group of PI Nakashima of 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 fuel cell electrodes with high performance and long lifetime.

The commercialization of electrochemical devices such as the solid-oxide electrolyzers is currently limited by the performance of the air electrode, as these typically experience rapid degradation under operation. Surface composition, surface reactions, and the degradation mechanism are longstanding puzzles that must be addressed for wide-scale technology adoption. Using the advanced surface analysis technique known as Low Energy Ion Scattering and atomistic simulations, the groups of PIs Kilner (Imperial College, London) and Ishihara discovered that pristine surfaces are inactive for oxygen adsorption, and that instead, such systems must rely on active site mediated mechanisms, known as vacancies, for adsorption to occur. Major contributors to this team were postdocs Druce and Tellez, who were both promoted to the rank of assistant professor, and tenured associate Professor Staykov.

CO_2 Capture and Utilization: Using a newly designed phase-separated-type CuPd nano-alloy catalyst, PI Yamauchi and Prof. Kenis (Illinois) succeeded in developing a highly efficient CO_2 electroreduction process to produce ethylene and ethanol (C_2 products) in electrochemical CO_2 reduction (up to 63% Faradaic efficiency, which is among the highest reported values for C_2 production in the literature). This is a 10-fold increase in performance relative to the levels reported prior to this work, and is achieved at the smallest reported overpotential (< 0.7 V).

Hydrogen Storage: In a collaborative effort, PIs Akiba and Horita discovered that defect formation is the activation mechanism for hydrogen absorption of TiFe intermetallics by High Pressure Torsion processing. It should be noted that TiFe was abandoned as a renewable energy storage medium due to the fact that it was notoriously difficult to activate at room temperature and low pressure. The discovery already led to commercialization of the activation approach by cold rolling or mechanical milling. Pursuing this research further, PI Akiba obtained higher effectiveness of the high-pressure torsion (HPT) processing to activate TiFe-based alloys through the addition of Mn. In a parallel project, 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.

CO_2 Storage: The coupled pore-scale flow dynamics of CO_2 and brine in geologic media represents a critical component of accurately predicting large-scale migration of injected CO_2. PI Christensen's (Notre Dame University) work in this area is the first quantitative study of liquid CO_2-water flow in a porous micromodel at reservoir-relevant conditions. His studies clarified the importance of inertial forces during CO_2 bursts through the rock and also the occurrence of flow within trapped water ganglia that could promote enhanced dissolution of CO_2 into the resident brine. The implication of these results is that pore-scale models of liquid CO_2 migration must be modified to account for such dynamic flow processes, which can greatly alter macroscale migration of CO_2 in geologic reservoirs. The group of PI Tsuji developed a novel monitoring method to quantify CO_2 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 CO_2 saturation with monitoring-derived seismic velocity. This monitoring system is currently deployed in an ongoing CO_2 sequestration project at a coal-fired power plant in Saskatchewan, Canada.

Hydrogen Materials Compatibility: Using state-of-the-art microstructural characterization and computational modeling, the groups of PIs Robertson (University of Wisconsin-Madison) and Sofronis (Illinois/Kyushu) discovered the link between hydrogen-enhanced plasticity and material failure. They found that the evolution of the material microstructure by hydrogen mediated plasticity in synergism with hydrogen-enhanced decohesion brings about material failure. The significance of this development is in predicting the lifetime of metal components in a high-pressure hydrogen gas environment. Quantitative insights into the hydrogen effects on intergranular cracking were further investigated by PI Kirchheim (Göttingen University) through a thermodynamic treatment of new surface creation accompanying fracture. Closed form 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.

Energy Analysis: In addition to developing the division project roadmaps, the EAD has carried out a number of technoeconomic studies on important energy challenges for Japan and the impact of the I^2CNER solution pathways on CO_2 emissions reduction. Collaborating with WPI Visiting Professor Hirose from Toyota Motor Corporation and using geographic information system analysis, Prof. Itaoka, leader of the EAD, 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. The analysis concluded that the most effective approach is to locate the hydrogen stations in a way that minimizes average distance between potential customers and the nearest hydrogen stations. The analysis also demonstrated that more hydrogen stations need to be located in internal city locations, especially in every prefectural capital. Lastly, the important metropolitan areas that are not covered by the existing/planned stations and which need to be covered by new stations were identified.

In a collaborative study with PI Yamauchi, Prof. Itaoka explored the possibility of importing low carbon fuel based on renewable energy from abroad, where renewable energy sources are more abundant or carbon capture and storage is more feasible, consistent with the conditions of the locations' natural environments. The study is based on a life-cycle assessment of the carbon neutral cycle (CN) of PI Yamauchi, in which oxalic acid is converted into glycolic acid using electricity, and 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-CO_2/kWh in 2014) and those emissions can be further reduced by increasing the efficiency of the production of glycolic acid by a polymer electrolyte alcohol electrosynthesis cell.

3. Feeding research outcomes back into society

The relevance of the I^2CNER research efforts and objectives to enabling the green innovation initiative of the government of Japan is demonstrated by the large number (81) of collaborative projects in which its researchers are involved with industry (e.g. Toyota, Nissan, Honda, Kyocera, Mitsubishi, Hitachi, JX Nippon Oil and Energy, Air Liquide, and JFE Steel Corporation). A total of 33 projects resulted in technology transfer. Moreover, 7 additional ongoing projects in collaboration with industry are primed for technology transfer. Since inception, I^2CNER filed for 178 patents and was granted 46 patents.

The following are representative examples for each division: i) PI Ishihara's transfer of dual carbon battery technology for energy recovery from automobiles to Ricoh Co. Ltd., ii) PI 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 using solar energy, iii) PI 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 pump, iv) Prof. Akiba is working with IWATANI Co. Ltd to develop high performance hydrogen absorbing alloys suitable for stationary hydrogen storage; v) PI Yamauchi's synthetic method for the preparation of atomically well mixed Fe-Ni nanoalloys has been transferred to Daido Steel, vi) PI Fujikawa's functional nanomembrane technology for gas separation has been transferred to Nanomembrane Technology Inc. for upscale development, vii) PI Tsuji's innovative continuous CO_2 monitoring system in collaboration with the Japan Oil, Gas and Metals National Corporation (JOGMEC) has been transferred and deployed in the ongoing CO_2 sequestration project in Saskatchewan, Canada, viii) PI Sugimura's studies of diamond-like carbon (DLC) coatings in collaboration with Kitz corporation on the wear of candidate coatings in the presence of hydrogen contributed to the development of 100 MPa hydrogen flow valve, which is now in practical use in hydrogen refueling stations; ix) Prof. Itaoka's study on the hydrogen refueling stations and supply infrastructure for Japan have been submitted to the Ministry of Economy, Trade and Industry of Japan in the form of 73-page report in February 2017.

To pursue technology transfer in a more strategic framework, I^{2}CNER established the Industrial Advisory Board and the Industrial Research Division (IRD) in Spring 2017. The purpose of the Board is to advise I^{2}CNER on opportunities for interactions with industry and technology transfer, and the purpose of the IRD is to advance technology transfer with companies which are funding projects that have a clear association with I^{2}CNER's research, and which agree to have one of their employees immersed in I^{2}CNER laboratories as WPI Visiting Professor. The first such project is "mobile energy storage for low-carbon society," sponsored by Mazda Motor Corporation.

4. Interdisciplinary Research Activities

I^{2}CNER provides unique opportunities for bottom-up research, giving researchers opportunities to create and establish new research directions. Young researchers in particular have formed an important part of I^{2}CNER. From internal reporting, they have initiated 30 international collaborations and 12 collaborations within Japan. Young professors supported by I^{2}CNER were particularly prolific in their collaborations. Of note are Associate Professor Staykov, who was involved in collaborations in 4 different divisions of I^{2}CNER, Assistant Professor Perry, who initiated 5 international collaborations, and Assistant Professor Orejon, who initiated 9 international collaborations. As a result of the work performed from these collaborations and others, young researchers in I^{2}CNER have secured 12 sources of internal and/or external funding. To promote the establishment of new and creative research directions, young faculty have been awarded competitive internal seed funding. In one example, internal funding awarded to Assistant Professor Perry and Assistant Professor Ertekin (Illinois) focusing on combined computational and experimental studies of oxygen exchange on electrode surfaces laid the ground work for the NSF/JSPS sponsored PIRE (Partnerships in International Research and Education) project "Integrated Computational Materials Engineering for Active Materials and Interfaces in Chemical Fuel Production." The PIRE program is a high-visibility joint program of the US National Science Foundation and JSPS that seeks to foster international collaborations and support the development of global citizenry.

In FY 2015 and FY 2016, with assistance from the KU Executive Vice President in Charge of Research and Industrial Collaboration, Professor Wakayama, I^{2}CNER started a new initiative on Applied Math for Energy. The competitive funding 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 I^{2}CNER's Applied Math Initiative. The Institute received several proposals in response to the call, and after rigorous screening by the Internal Programs Review Committee, 5 applications were selected in FY 2015 and 2 in FY 2016 as "seed projects," the idea being to foster close, ongoing collaboration between I^{2}CNER and other KU units, in particular, the IMI. I^{2}CNER's annual symposia are used as platforms to explore fusion of disciplines and come up with action plans for nurturing new cross-cutting interdisciplinary research directions and guiding new faculty hires. By way of example, major outcomes of the 2016 and 2017 symposia is that they helped in the establishment respectively of computational science and applied math as integral components of I^{2}CNER's research portfolio. In addition, the symposium on applied math has had ripple effects beyond I^{2}CNER, with mathematicians now interacting with engineers at I^{2}CNER, Kyushu University, and the University of Illinois, as demonstrated by joint proposal submissions to international funding agencies.

The disparate nature of the disciplines involved in the I^{2}CNER research fields facilitates interdisciplinary work through collaborations across division boundaries. The work by PIs Kilner and Ishihara that led to the understanding of the oxygen transport kinetics in solid oxide fuel cells and involved a large number of postdocs and young faculty lies at the intersection of surface science, materials science, electrochemistry, and theoretical and molecular chemistry. Similarly, the collaboration of PI Somerday (Southwest Research Institute) with Associate Professor Staykov that involved mechanical metallurgy and density functional theory calculations led to the understanding of how oxygen adsorbed on metal surfaces can inhibit hydrogen uptake, thus mitigating hydrogen accelerated fatigue, which is a severe degradation mechanism, as another collaboration between PIs Somerday, Kirchheim, and Sofronis has demonstrated.

5. International Research Environment

The environment at I^{2}CNER provides a rich platform to pursue transformative research in non-traditional and highly multi-disciplinary environments, bringing together researchers from domestic and international settings to address issues critical to Japan's transition to a carbon neutral society. A total of 196 internationally recognized researchers have visited the Institute and a total of 214 distinguished visitors have been hosted by I^{2}CNER. The environment fosters communication between local and international members through regular research exchanges, seminars, and symposia. The I^{2}CNER environment fosters excellence in its young researchers. Based on internal reporting, since the Institute was established, 40 I^{2}CNER graduate students, post-docs, and young faculty have visited universities and institutions abroad as part of research collaborations, and I^{2}CNER itself has hosted over 35 graduate students, post-docs, and visiting professors from abroad. I^{2}CNER prepares its post-docs and young faculty for impactful research careers: it has sent nearly 56 researchers to professorship positions at various levels (excluding Kyushu University), and 14 are making impact at private companies and/or research institutes. As part of its commitment to fostering globally-aware researchers starting from the undergraduate level, I^{2}CNER annually sends approximately 5 undergraduate students from KU to carry out research in the laboratories at the University of Illinois, while also hosting 5 undergraduate students from Illinois who participate in summer research programs in I^{2}CNER laboratories.

The I^{2}CNER Administrative Office is in close communication with the existing KU International Student and Researchers Support Center, and offers full-time support to overseas researchers in the invitation procedures, including visa application processing and accommodations on campus. To help overseas researchers adapt smoothly into the new culture and research environment, the

Administrative Office i) offers additional training and workshop opportunities, ii) introduced an English version of various application forms, guidelines, and university regulations, and iii) introduced an English version of the Web Safety Training Module, which all new I^{2}CNER members are required to complete prior to conducting experiments in the laboratory. Additionally, the Administrative Office provides extensive living assistance with medical checkups, off-campus accommodations, travel arrangements for family members, and introduction to the Japanese social insurance system.

6. Organizational Reforms

These can be summarized as follows: i) the University of Illinois was designated as a collaborating institution on leading-edge research related to the carbon-neutral energy research, ii) Director Sofronis was given full authority for all I^{2}CNER operations by President Kubo and EVP Wakayama, iii) the cross-appointment employment system was institutionalized and applied throughout KU, iv) the Intra-university faculty transfer system was established, v) I^{2}CNER faculty involvement with teaching is increasing, vi) KU introduced I^{2}CNER's merit-based salary system across all units, vii) I^{2}CNER's flexibility with travel expenses of renowned visitors from overseas was adopted across KU, viii) KU provided support in the form of administrative personnel, building infrastructure, tenured faculty positions, ix) administrative staff have a good command of English, x) KU undergraduate students were sent to the University of Illinois for research experiences, xi) I^{2}CNER was adopted as a model concept of the internationalization of research and education, KU established the Kyushu University Platform of Inter/Transdisciplinary Energy Research (Q-PIT), xii) EVP Wakayama led the efforts to integrate I^{2}CNER with KU and expand collaborations with other units, e.g. IMI, and xiii) faculty council regulations were changed dramatically.

7. Others

Evidence of I^{2}CNER's international stature and relevance can be seen in its 1408 journal publications, of which, 89 were published in journals with an impact factor greater than 10. On a related note, since its inception, 230 of the Institute's publications have been cited between 10 and 19 times, 72 have been cited 20-29 times, 38 have been cited 30-39 times, 22 have been cited 40-49 times, and 44 have been cited 50 or more times.

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Progress Report of the WPI Center
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Host Institution	Kyushu University	Host Institution Head	Chiharu Kubo
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*Write your report within 30 pages. (The attached forms are in addition to this page count.) Keep the length of your report within the specified number of pages.

Common Instructions:

*Please prepare this report based on the current (31 March 2017) situation of your WPI center.

*Use yen (¥) when writing monetary amounts in the report. If an exchange rate is used to calculate the yen amount, give the rate.

1. Overall Image of Your Center (write within 2 pages including this page)

Describe the Center's current identity and overall image. For centers that have had a change in their directors, describe that transition and the effects of the change.

・On the sheets in Appendix 1-1~7, list the Principle Investigators, and enter the number of center personnel, a chart of the center's management system, a campus map showing the center's locations on the campus, and project funding.

I[2]CNER's vision is to enable energy technologies that hold promise for alleviating Japan's lack of primary energy resources and energy security concerns, which are caused by Japan's current heavy reliance on imported fossil fuels. In executing this vision, I[2]CNER aims to create a carbon-neutral society (CNS) through basic research underlying technology which, when deployed, leads to a large reduction of greenhouse gas (GHG) emissions (70-80% by 2050 from 1990 levels). This reduction goal is in line with the G8 commitment announced in 2009. We aim to expedite our efforts by considering economic efficiency and safety issues when developing new technology. As a whole, we consider 3E+S (Environment, Energy security, Economy, and Safety) as basic view points for the vision.

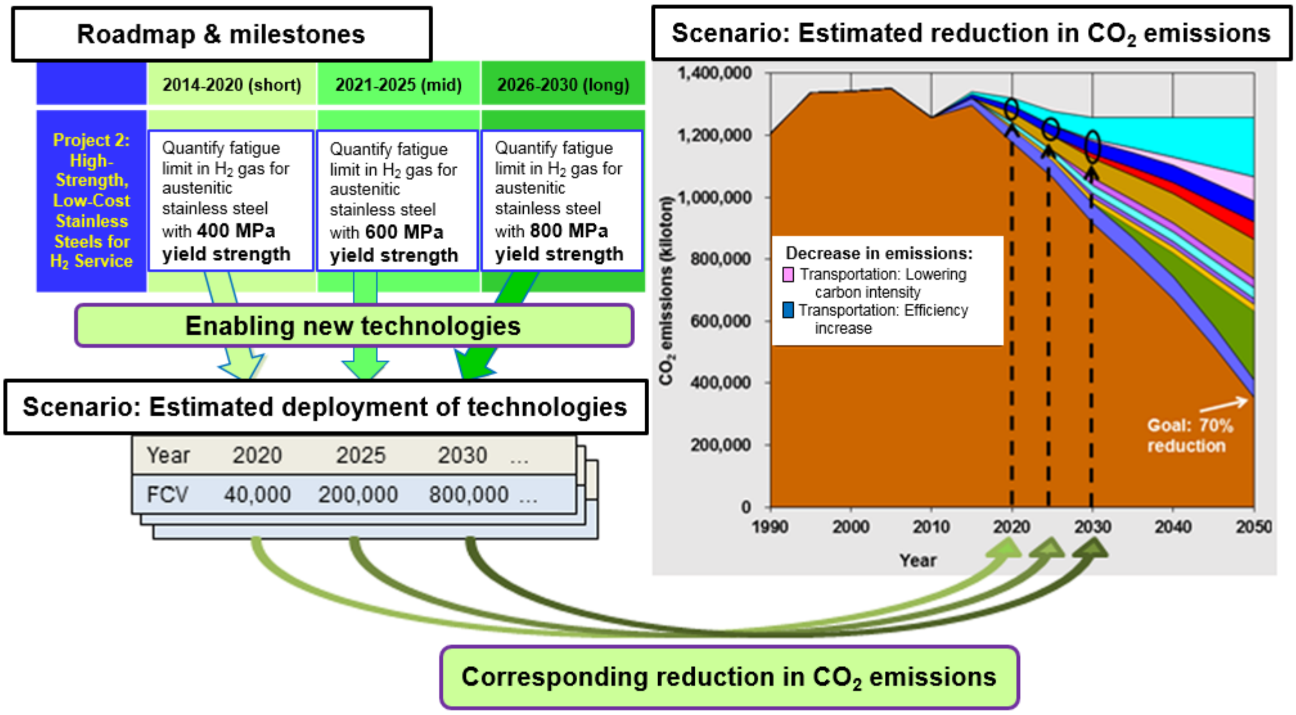


Figure 1. Flowchart showing the research roadmap and milestones for Project 2 in the Hydrogen Compatible Materials division for the development of a hydrogen-resistant high strength steel for hydrogen refueling stations and fuel cell vehicles (FCV), the enabling relationship of these milestones to the projected deployment of FCV technology, and then the calculated effect of this deployment on reducing CO_2 emissions.

In drawing our vision, we consider two major principles, efficiency increase (EI) in energy conversion and energy use, and lowering the carbon intensity (LCI) of fuel and electricity to adopt and develop future technologies. EI can be applied to existing systems, but is also achieved by replacing existing systems with new technology. LCI in electricity and fuel supply-use pathways is achieved using either renewables, nuclear, or carbon capture and storage (CCS). There can be many possible scenarios (combinations of technology options) that would allow us to achieve the targeted GHG emissions reduction. By prioritizing different LCI and EI technologies, renewables, and CCS, we developed 5 scenarios. The extent of development and deployment timing of these technologies creates the variability among the scenarios. Each of the 5 I²CNER scenarios results in 70% emissions reduction by 2050: A (development of important EI technologies and balanced deployment of renewables and CCS), B (very large penetration of renewables for LCI and development of important EI technologies), C (large deployment of CCS for power and industries, especially for coal, and development of important EI technologies), D (balanced application of LCI technologies, including limited nuclear power due to public concern about safety), and E (balanced application of LCI technologies, including lifetime extension of large nuclear plants). I²CNER's research efforts are intimately tied to these five scenarios because the short-, mid-, and long-term milestones of each of our division roadmaps were established in consideration for the removal of the roadblocks in the development and deployment timing of the various promising technology options in the scenarios. As an example, for a typical research project in one of I²CNER's research divisions, Figure 1 shows how the relationship between the milestones of the project roadmap enables the implementation of the corresponding technologies that are necessary to achieve the corresponding GHG emission reduction under scenario A.

The updating of the I²CNER roadmap and research portfolio for the removal of roadblocks toward CNS is carried out by the continuous interaction among the technical divisions and the Energy Analysis Division and is informed by the Institute's scientific exchanges with a stellar list of distinguished scientists from 24 partnering institutions across the globe that includes the Southwest Research Institute, Texas; University of Wisconsin-Madison; MIT; the National Fuel Cell Research Center at the University of California, Irvine; and the State of California Air Resources Board (CARB) in the U.S.; Imperial College, London, and the University of Oxford in the UK; and the University of Göttingen in Germany.

A unique and important component of I²CNER is the Satellite Institute at the University of Illinois at Urbana Champaign (UIUC), which facilitates complementary research activities and pioneers student and researcher exchanges with the US. A Memorandum of Understanding (MoU) for all levels of interaction between Kyushu and Illinois, and a specific agreement for undergraduate student exchange are in place.

Our researchers have joint publications with researchers from 621 institutions around the world, and 214 internationally recognized researchers visited I²CNER for scientific interaction and exchange. The Institute's researchers are globally engaged and have been responsible for organizing, co-organizing, or serving on the scientific committees of 159 international conferences, 191 international conference sessions/symposia or workshops, and 48 I²CNER international workshops.

The environment at I²CNER provides a rich platform for young researchers to pursue transformative research in a non-traditional and highly multi-disciplinary and international setting. Of the 85 young researchers, 19 went on to take faculty positions at universities in Japan (excluding Kyushu University) and the world and 7 moved to industry and national laboratory positions. Fusion of disciplines is fostered by several initiatives, including annual support for competitive research initiatives by young researchers that are rigorously assessed by the Internal Programs Review Committee. A vital interdisciplinary program seeded in the last two years is the fusion of applied math with energy engineering, based on the Institute's burgeoning relationship with Kyushu University's (KU) Institute of Mathematics for Industry (IMI) and various departments at the UIUC.

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 (81) of collaborative projects in which its researchers are involved with industry (e.g. Toyota, Nissan, Honda, Kyocera, Mitsubishi, Hitachi, JX Nippon Oil and Energy, Air Liquide, and JFE Steel Corporation). A total of 33 projects resulted in technology transfer events. An additional 7 ongoing projects in collaboration with industry may result in further technology transfer. Since inception, I²CNER filed for 178 patents and was granted 46 patents.

I²CNER is spearheading KU's globalization efforts within the University Reform Revitalization Program, and I²CNER faculty are instructors in the international programs of KU. I²CNER's operational principles in research served as an example for the establishment of the KU Platform for Trans/Interdisciplinary Energy Research (Q-PIT) on October 1, 2016, an umbrella organization to integrate campus efforts in research and education on energy across its various units, including social sciences, economics, law, and political sciences.

In summary, I²CNER is as a highly successful research and education test bed. It is a national and global experiment an experiment that *tackles key scientific challenges along the path to providing Japan with carbon-neutral and sustainable energy supplies, despite limited energy resources,* through internationalization of scientific research and education in Japan, the U.S., and the world at large.

2. Research Activities (within 15 pages)

2-1. Research results to date

Describe issues of a global level that the Center has challenged, and give the results. Select 20 representative results achieved during the period from 2010 through March 2017. Number them [1] to [20] and provide a description of each. Place an asterisk (*) in front of those results that could only have been achieved by a WPI center.

- In Appendix 2-1, list the papers underscoring each research achievement (up to 40 papers) and provide a description of each of their significance.

I^{2}CNER's research activities are carried out within its technical divisions in collaboration/interaction with the Energy Analysis Division (EAD) to continuously assess techno-economic relevance and feasibility. Within the divisions, research is organized in projects, with each project having well defined milestones on a roadmap toward a final target (see Figure 1). According to I^{2}CNER's scenarios, the I^{2}CNER mission will be realized when all project targets across all divisions are achieved. Toward this goal, within each project, research efforts by individual researchers are targeting the corresponding milestones. Since inception, we realized 12 of the short-term and 4 of the mid-term milestones in our project roadmaps, and realized a NEDO Target in the Hydrogen Storage division. In the following some of our best accomplishments will be presented related to the advancement of the institute toward its roadmap targets. As a summary,

1) **Extended stability in hybrid perovskite photovoltaics (PI Adachi)**

One of the division's targets is to develop high efficiency and high stability solar cells and light-emitting diodes. The Adachi group has been studying stability issues in one of the most promising photovoltaic technologies: hybrid organic/inorganic perovskite (PSC) materials. Results using a thermally stimulated current (TSC) method, X-ray photoelectron spectroscopy, and time-of-flight (TOF) secondary ion mass spectrometry on fresh and degraded PSCs revealed that one source of degradation is the formation of metallic lead by the decomposition of the perovskite compound in the presence of water and oxygen under solar irradiation [1,2]. We reduced oxygen and water ingress into the perovskite solar cells by fabricating the perovskite films in a high purity nitrogen atmosphere, resulting in a 2.5 factor improvement in lifetime [1]. The introduction of benzoquinone (BQ) into the precursor solution used for fabrication of the perovskite films further increased [2]. The presence of BQ reduces perovskite crystal formation, resulting in uniform, flat perovskite films with larger grains. The improved film formation reduced carrier recombination, suppressed the formation of metallic lead, and improved device stability. The estimated device lifetime of 4,000 hrs (Figure 2.1) is one of the longest ever reported. Further optimization increased the power conversion efficiency to ~18%, along with stability. The Division's goal is to reach power conversion efficiencies >20% with lifetimes >10,000 hrs. *These results exceed the benchmark of 12% for Project 1 in the Molecular Photoconversion Devices division's roadmap and are approaching the short-term milestone.*

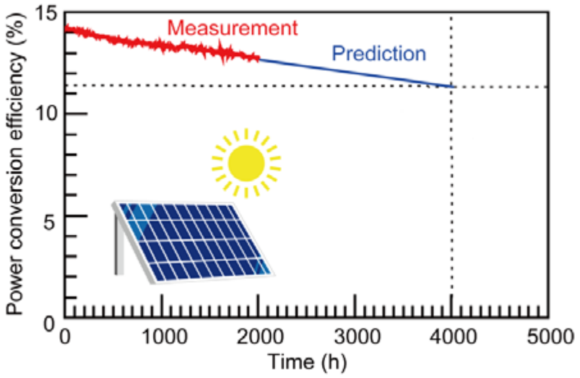


Figure 2.1. Stability of perovskite solar cell showing the lifetime prediction of 4000 h when efficiency is reduced to 80% of the initial performance.

*2) **Visualization of the active site of a photocatalyst (PI Ishihara)**

Photocatalytic water splitting is limited by the slow kinetics of the hydrogen evolution reaction. To overcome this, co-catalysts are often incorporated into photocatalytic systems. However, their working mechanism is not well understood, and this lack of understanding hinders the design and optimization of large-scaled hydrogen production systems. We have reported the first demonstration and visualization of single atom co-catalysts embedded as dopants in two-dimensional titania nanosheets [3]. Isolated rhodium atom dopants are incorporated into the titania nanosheets, acting as active sites and co-catalyzing water oxidation and reduction. At optimal doping concentrations, the hydrogen production rate is a factor of ten better than that of the undoped sheets. Atomistic first-principles simulations reveal the mechanisms by which the isolated Rh dopants induce changes to the water molecule adsorption and dissociation energy landscape on the nanosheets. We extended this work to map the full reaction mechanism of oxygen evolution on these nanosheets. We then assessed the full spectrum of transition metals as candidate dopants for experimentally synthesized nanosheets. Our work combines atomistic computational modeling with experimental 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. These efforts hold promise for the design of active sites of photocatalyst to improve activity, and *address the short-term milestone for project 2-2 of the Molecular Photoconversion Devices division.*

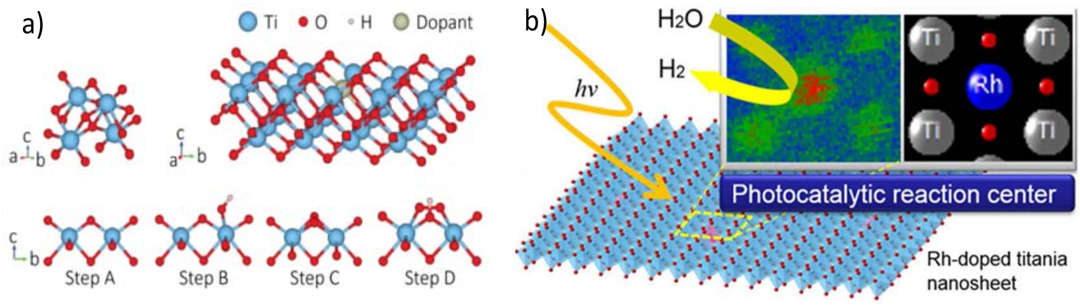


Figure 2.2. Two-dimensional titania nanosheets doped with isolated Rh species have been shown to exhibit accelerated rates of hydrogen production compared to the undoped systems [3].

*3) **Activation of TiFe by HPT for hydrogen storage (PIs Akiba and Horita)**
TiFe is an excellent candidate for stationary hydrogen storage applications due to its low price, high storage capacity per unit volume, low hydrogenation temperature, and reversible hydriding/dehydriding. Although TiFe was proposed as a hydrogen storage material four decades ago, its application was abandoned because of its difficult activation (Fig. 2.3a), requiring conditions of high pressure and high temperature, and rapid deactivation in air. However, our team discovered a novel manner of circumventing this roadblock. In 2011-2012, we found that mechanical processing of TiFe via high-pressure torsion (HPT) results in fast room-temperature hydrogen storage without any activation process (Fig. 2.3b) [4]. The HPT-processed material remained active even after exposure

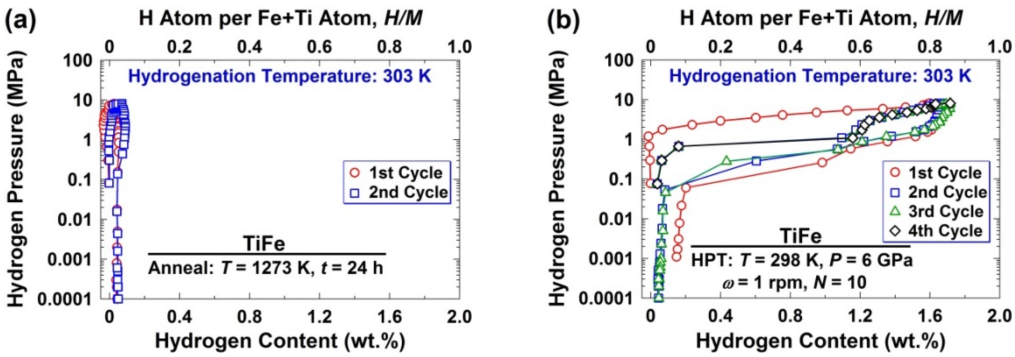


Figure 2.3. Activation of TiFe for hydrogen storage at room temperature by introduction of lattice defects via HPT process. a) Hydrogen content of traditionally processed material, b) Hydrogen content after HPT processing.

to air for over one year. Detailed examinations in 2013-2014 confirmed that the activation of TIFe is mainly due to the generation of lattice defects and grain boundaries, which act as quick pathways for hydrogen transport. This discovery was not limited to TiFe, as we observed similar phenomenon in other materials such as TiFe-Mn, Mg_2Ni and TiV (2015-2016) [5,6]. *This finding achieved the short-term milestone for Project 3 of the Hydrogen Storage Division*. The HPT processed sample is small and not appropriate for commercial applications. To achieve the *mid-term milestone of the Project 3 and scale-up the size of active TiFe material*, we optimized two commercial processes: cold rolling (2014) and mechanical milling (2015). We found that TiFe processed by these two commercial methods absorb hydrogen without any activation process.

*4) **A functional [NiFe] hydrogenase mimic that catalyzes electron and hydride transfer from H_2 (PI Ogo)**
The search for biomimetic hydrogen activation was crowned with our report of a functional [NiFe]-based catalyst (Figure 2.4) [7], the first synthetic analog for H_2 activation in the world. The new catalyst consists of Ni and Fe centers linked by a pair of thiolates, as seen in the natural enzyme. Structural investigations were performed by a range of techniques, including x-ray diffraction and neutron scattering, resulting in detailed crystal structures that can be analyzed to understand the mechanism of catalysis. The hydrido substrate bridges the Fe and Ni, being predominantly associated with the Fe center. The hydridic character of the substrate is manifested by the liberation of H_2 upon reactions with strong acids. By activating hydrogen, this new system is capable of catalytically reducing substrates by both electron transfer and hydride transfer pathways. *The accomplishment meets the short-term milestone for Project 1 in the Catalytic Materials Transformations Division's roadmap.*

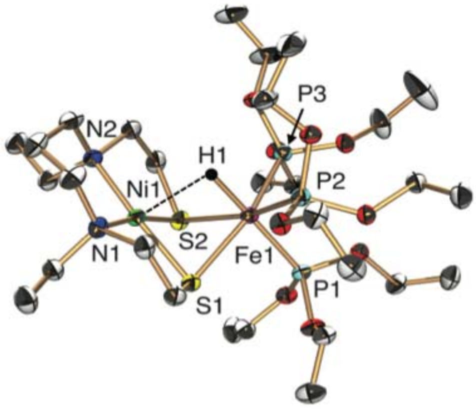


Figure 2.4. Bio-inspired catalyst for hydrogen activation.

*5) **A high-valent iron(IV) peroxo core derived from O_2 (PI Ogo)**
A second major advance, also coming from the Ogo team, focuses on bio-inspired molecular catalysts for oxygen reduction. Dioxygen-tolerant [NiFe] hydrogenases catalyze not only the conversion of H_2 into protons and electrons but also the reduction of O_2 to H_2O. Chemists have long sought to mimic such bifunctional catalysts to facilitate analysis and catalyst optimization. Compared to the enzyme, the synthetic catalysts are far more compact (about 1% the weight), and thus more practical for device applications. The Ogo group reports a new [NiFe]-based catalyst for O_2 reduction. Structural investigations revealed that the catalyst operates via the first example of a side-on iron(IV) peroxide intermediate. Because of its connection to hemoglobin, iron-O_2 chemistry is an ancient art, so this advance is very important. The breakthrough was uncovered by systematic redesign of the H_2 catalyst, which revealed that the organic ligand attached to Fe completely controls the catalyst's selectivity for H_2 vs O_2 [8]. Ogo's program has now provided catalysts for both the oxygen [9] and hydrogen sides of a prototype biomolecular fuel cell. The research group's next step is to further modify the hydrogen and oxygen splitting catalysts so they can be applied in a working fuel cell. Realization of such a fuel cell will be a crucial step the path to making fuel cells affordable enough for daily life. *This fulfills the short-term milestone for Project 1 of the Catalytic Materials Transformation* division.

*6) **CO_2-free electric power circulation via direct charge and discharge using the glycolic acid/oxalic acid redox couple (PI Yamauchi)**
This discovery by PI Yamauchi involves a CO_2-free way to distribute electric power by exploiting an incredibly simple, bio-derived redox couple. The components of the couple are glycolic acid (GC) and oxalic acid (OX), both of which occur widely in nature. Direct electric power storage in GC ensures high stability and transportability 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

electro-reduction is the suppression of hydrogen evolution even in acidic aqueous media (Faraday efficiency of 70–95%, pH 2.1). CO_2-free power generation was also achieved via electro-oxidation of GC with an alkaline fuel cell [10]. Key advantages of this emerging technology are the high energy density of the components and the robustness of titania nanospheres that mediate the electron-transfer. The establishment of an efficient electric power distribution method is required to realize a sustainable society powered by renewable-energy-based electricity, such as solar photovoltaic, wind turbine, and wave electricity. *This achievement is directly relevant to the Catalytic Materials Transformation division's long-term target for Project 2.*

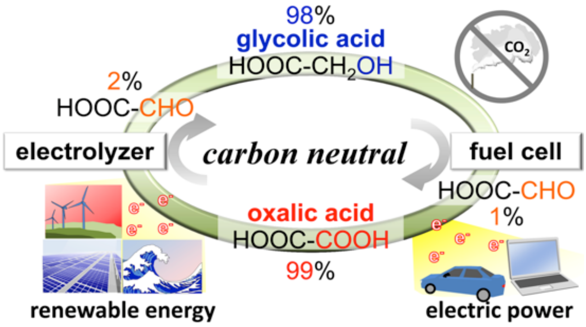


Figure 2.5. Schematic of a carbon-neutral energy circulation by highly selective electrocatalyses using the glycolic acid/oxalic acid redox couple.

*7) **Fundamental understanding of coalescence-induced droplet jumping (PI Takata)**

Water vapor condensation on superhydrophobic surfaces has received much attention in recent years due to the ability of such surfaces to shed microscale water droplets via coalescence-induced droplet jumping, resulting in heat transfer, anti-icing, anti-bacterial, and self-cleaning performance enhancement [11,12]. We demonstrated for the first time the coalescence-induced removal of water nanodroplets ($R \approx 500$ nm)[11]. Furthermore, we obtained an understanding of jumping directionality by developing a novel and discipline-cross-cutting single-camera technique capable of providing three-dimensional (3D) information through the use of focal plane manipulation, termed "focal plane shift imaging" (FPSI) [13]. The outcomes of this work demonstrate the ability to passively shed nanometric water droplets, which has the potential to further increase the efficiency of systems that can harness jumping droplets for a wide range of energy and water applications. Furthermore, the outcomes provide a powerful imaging platform for the study of dynamic droplet processes that result in out-of-plane motion such as sliding, coalescence, or impact. The knowledge gained from this work is being applied to the development of more compact condensers for HVAC&R and power generation industries, anti-icing surfaces, and highly efficient electronics thermal management devices. *This accomplishment meets the short-term milestone of Project TP-3 (Thermal Transport at the Nanoscale) and HMT-1 (Phase Change Heat Transfer) of the Thermal Science and Engineering division's roadmap.*

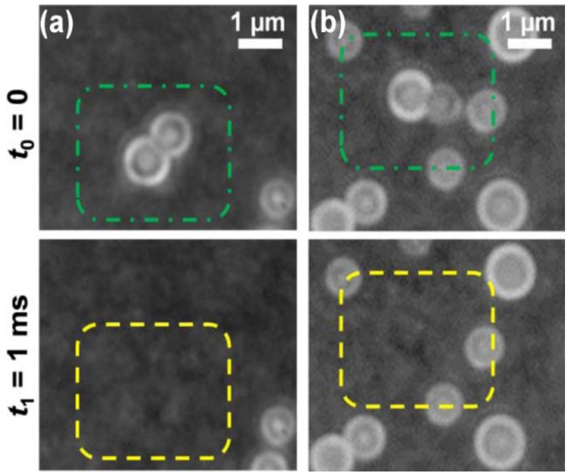


Figure 2.6. Time-lapse images captured via top-view optical microscopy of steady-state water condensation on a superhydrophobic carbon nanotube surface. Condensing nanoscale droplets underwent spontaneous jumping after coalescence.

*8) **Development of novel functionalized adsorbents for HVAC applications (PI Saha)**

In this study, the adsorption characteristics of ethanol onto two promising adsorbents were investigated for developing high performance adsorption chillers [14,15]. The two new adsorbents were KOH4-PR and KOH6-PR. Laser Diffraction Particle Size Analysis revealed that both samples had narrow particle size distributions, with normalized particle amount reaching 50% at particle diameters of 26 and 23 μm for KOH4-PR and KOH6-PR, respectively, Figure 2.7. Adsorption isotherm measurements showed the uptake capacity of KOH4-PR/ethanol to be as high as 1.43 kg·kg^{-1} while

Figure 2.7. Photos showing preparation of KOH6-PR absorbent, and SEM micrograph showing particle size distribution.

one kg of KOH6-PR was able to adsorb ~2 kg of ethanol, the highest demonstrated to date [16]. The predicted performance of KOH6-PR/ethanol pairs is 1.54 times that of Maxsorb-III. The developed KOH6-PR/ethanol pair enables the further penetration of adsorption chiller technology into the vapor compression dominated HVAC&R market. *These results are targeting the mid-term milestone of Project HMT-2 (Adsorption) and meet the short-term milestones of Projects HMT-2 and TES-1 (Waste Heat Driven Adsorption).*

*9) **Air electrodes in high temperature electrochemical devices: An atomistic study of composition and mechanisms (PI Kilner)**

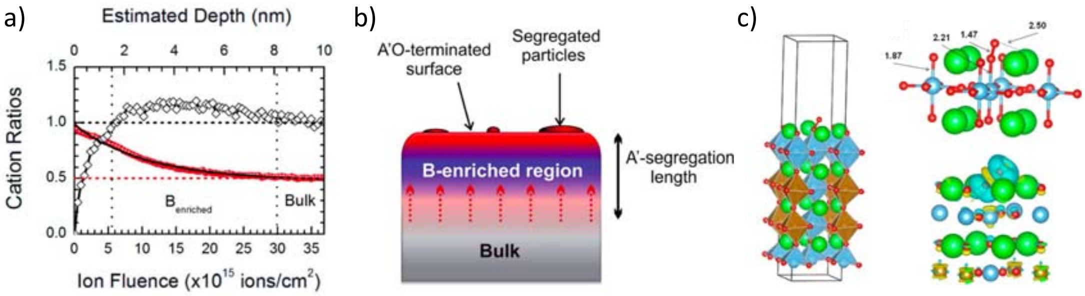


Figure 2.8. a) Measured compositional profile shows segregation of cations to the surface, b) Schematic of measured composition profile. The segregation is closely linked to performance degradation, c) Atomistic modelling has unveiled a vacancy-assisted mechanism for surface exchange.

The commercialization of electrochemical devices is currently limited by the performance of the air electrode, as these typically experience rapid degradation under operation. Surface composition, surface reactions, and the degradation mechanism are longstanding puzzles that must be addressed for wide-scale technology adoption. Using advanced surface analysis techniques, we have identified two previously unknown characteristics, Figure 2.8a,b, that are universal to a large class of $A_{1-x}A'_xBO_3$ perovskite oxide air electrodes and closely linked to their degradation [17]. First, under operation the surface quickly reorganizes to a termination consisting entirely of A, A′, and O ions, covering the catalytically active B cations. Second, there is a rapid segregation of substituted cations to produce a majority A′O rich near-surface region. Using this knowledge of the surface composition, we computationally modelled the adsorption and incorporation of molecular oxygen onto electrode surfaces [18]. Our analysis shows that pristine surfaces are inactive for oxygen adsorption, and that systems must rely on active site mediated mechanisms, known as vacancies, for adsorption to occur [19]. These new insights highlight the critical need for rational design of surfaces to enhance performance; a finding that was previously not recognised. This interdisciplinary effort lies at the intersection of surface science, materials science, electrochemistry and theoretical and molecular chemistry. *Additionally, these results meet the short- and a mid-term milestones for solid oxide cells in Project 1 of the Electrochemistry Energy Conversion division's roadmap.*

*10) **Novel electrocatalyst based on polymer-wrapping of carbon nanotubes (PI Nakashima)**

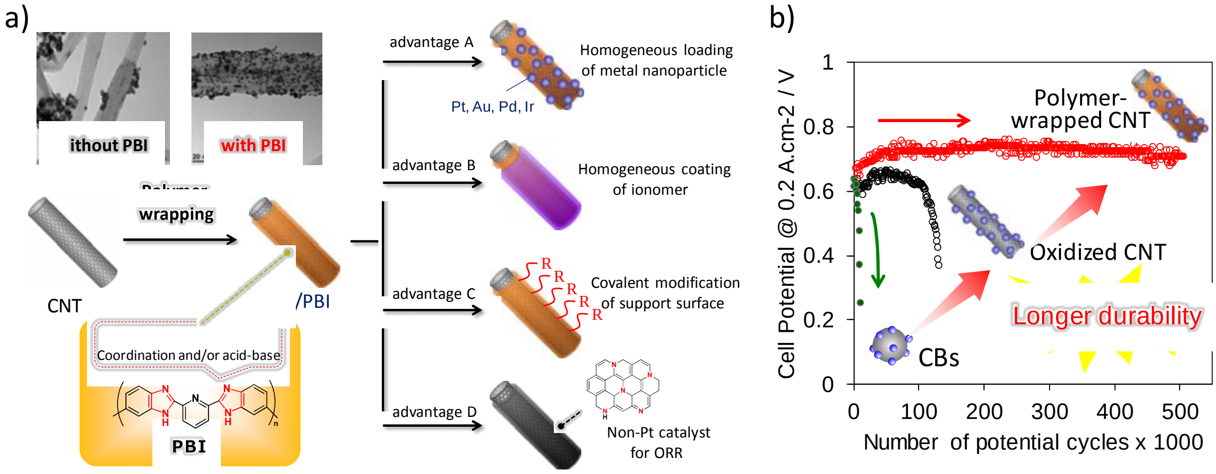


Figure 2.9. New approach to highly durable electrocatalysts based on polymer wrapping. a) Summary of the approach, b) Durability results showing no visible degradation in polymer wrapped systems up to 500,000 cycles.

To overcome the critical limiting feature of low durability of electrocatalysts, we have developed the use of polymer-wrapped carbon supports [20]. This unique approach has now been applied to produce a comprehensive set of metal nanoparticles including Pt, Au, Pd, Au-Pd core-shell and Ir, or homogeneous coatings of the proton-conductive layers, on the surface of carbon supports [21] (Figure 2.9a). Notably, they have demonstrated extremely high durability, with lifetimes of the polymer electrolyte fuel cell (PEFC) for single cell tests exceeding 500,000 cycles at 80˚C under humidified conditions (Figure 2.9b) [22] and > 400,000 cycles at 120 °C under non-humidified condition [21]. This polymer-wrapping technology opens new routes for developing next generation PEFCs with both exceptional durability enhancement and cost reduction. *These results exceed the stability target for PEFCs in Project 1 of the Electrochemical Energy Conversion division's roadmap, are contributing to the short-term milestone, and are promising toward the final target for 'non-Pt PEFC'.*

*11) **Intermediate temperature steam electrolysis (PI Matsumoto)**

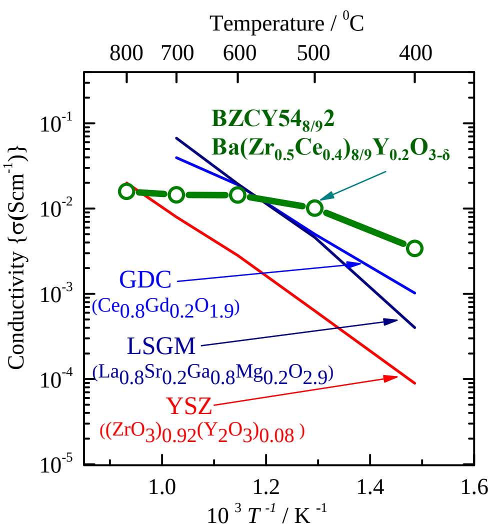


Figure 2.10. Ionic conductivity of (BZCY54$_{8/9}$2) compared with existing oxide-ion-conducting electrolyte materials.

The effective utilization of renewable energy demands methods to cleanly convert electricity into hydrogen or fuels. We focused our efforts on steam electrolysis for hydrogen production, currently the most energy-efficient process at intermediate temperatures in comparison to other water-electrolyzing techniques at intermediate temperature (600°C) [23,24]. We developed a conducting electrolyte exhibiting high performance at 600°C; conventional steam electrolyzers typically operate at 700 - 800°C. This low operation temperature was achieved through material composition optimization for high ionic conductivity and thermodynamic stability. Thus, our $Ba(Zr_{0.5}Ce_{0.4})_{8/9}Y_{0.2}O_{3-\delta}$ (BZCY54$_{8/9}$2) composition is the highest performing to date and has a comparable conductivity at 600°C to the most highly used electrolytes (GDC and LSGM), and can outperform them at the lower temperatures of 400-500 °C, Figure 2.10 [24]. In addition, our material has been confirmed to be stable in high concentration steam environments. We have also established a standard protocol for highly efficient intermediate temperature steam electrolysis. This approach, including electrolyte and electrode materials [25], cell processing, and fabrication, has been shared with Nippon Shoukubai Co. Ltd through collaborative research initiated in 2013. As a result, the commercialization of steam electrolyzers is ongoing, and large scale electrolyte/electrode assemblies have been produced. *The conductivity of this new material meets the short-term milestone in the Electrochemical Energy Conversion division's roadmap for Project 2.*

*12) **Inertial effects in liquid CO_2-water flow behavior for CO_2 storage (PI Christensen)**
The coupled pore-scale flow dynamics of CO_2 and brine in geologic media represents a critical component of accurately predicting large-scale migration of injected CO_2. This research focused on the first-ever experimental quantification of these pore-scale flow processes at reservoir-relevant conditions in 2D micromodels. The results obtained in both homogeneous and heterogeneous micromodels (inspired by real rock) provide a detailed picture of the flow physics during the migration of the CO_2 front, the evolution of individual menisci and the growth of the dendritic structures, so called fingers [26,27,28]. Velocity burst events, termed Haines jumps, were captured, during which the local Reynolds number was estimated to be up to O(100) in the CO_2 phase, indicating the significance of inertial effects. Pore drainage events were shown to be cooperative, and the zone of influence of such an event may extend beyond tens of pores, confirming, in a quantitative manner, that Haines jumps are non-local phenomena. The findings provide valuable insights into flow processes at the pore scale, which are of great benefit for the other research efforts going on within the division (e.g., model construction and upscaling). *This effort directly addresses the short-term milestone of Project 2 of the CO_2 Storage Division.*

*13) **Develop continuous and accurate monitoring system for injected CO_2 (PI Tsuji)**
We developed a seismic-monitoring-based method for monitoring CO_2 migration based on estimating the temporal variation of seismic velocity using ambient noise. Doing so allows a time-lapse survey to be conducted and to extract subsurface information using only passive seismometer data. The low cost of this approach makes it particularly attractive for long-term monitoring of CCS projects, both for migration monitoring and for leak detection. P-wave velocity variation can be interpreted as pore pressure increasing due to fluid injection [29], and allows us to estimate pore pressure variation within an aquifer formation. Based on this advance, we developed a novel monitoring method for injected CO_2 using a continuous and controlled seismic source (Figure 2.11). Our monitoring system is cost-effective, with high temporal resolution and high accuracy, compared to conventional monitoring approaches. Field experiments show that hourly-variation of surface-wave velocity can be monitored with better than 1 % accuracy [30], which is required to detect changes in seismic velocities associated with CO_2 leakage through the fault zone. Recently we have applied this technique in an ongoing CCS project in Canada [31]. The developed monitoring system has the potential to identify spatial distribution of CO_2 leakage in shallow formation. *This effort directly addresses the short-term milestone of Project 3 in the roadmap of the CO_2 Storage Division.*

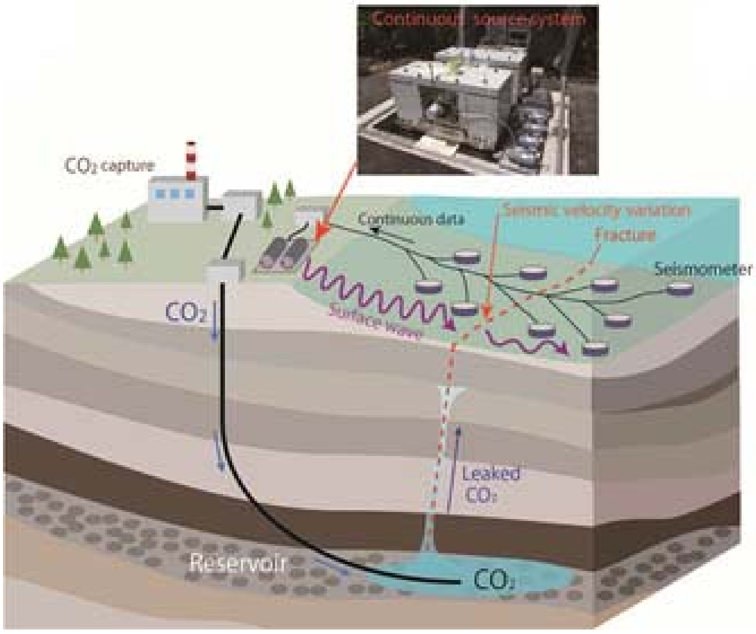


Figure 2.11. Continuous seismic monitoring of injected CO_2 and detection of leaked CO_2 with the monitoring device shown.

*14) **A novel approach for CO_2 capture through nanometer membranes (PI Fujikawa)**
Gas selectivity and flux of a membrane are main factors in gas separation. Membrane thickness directly connects to its gas flux performance and, thus, many efforts have been devoted to the preparation of thin and free-standing membranes without gas leaks to improve membrane gas flux. We successfully prepared 20-100 nanometer-thick and free-standing membrane from polymers

possessing CO_2 affinity sites, resulting in gas permeation selectivities of 14.4 (CO_2/N_2) and 14.1 (CO_2/H_2). To the best of our knowledge, this is the first example of gas separation by a free-standing nanomembrane with the thickness of a few tens of nanometers. *This achievement is a proof-of-concept of our approach, and meets the two short-term milestones in the CO_2 Capture and Utilization division's roadmap for Project 1.* Based on these achievements, we developed inorganic nanomembranes with CO_2 selectivity. Based on insights from theoretical approaches, we incorporated aromatic caboxylic acids into nanomembranes of titanium dioxide (TiO_2) (~100 nm). The selectivity of the TiO_2 composite with phthalic acid (PA@TiO_2) layer alone was $\alpha(CO_2/N_2)$~140 under small pressure differences [32]. *This exceeds our ultimate target value of the gas selectivity ($\alpha(CO_2/N_2)$~40)*, and means the technology is potentially suitable for separating CO_2 from air.

*15) **Bimetallic Cu-Pd catalyst with different mixing patterns for the electroreduction of CO_2 (PI Yamauchi)**

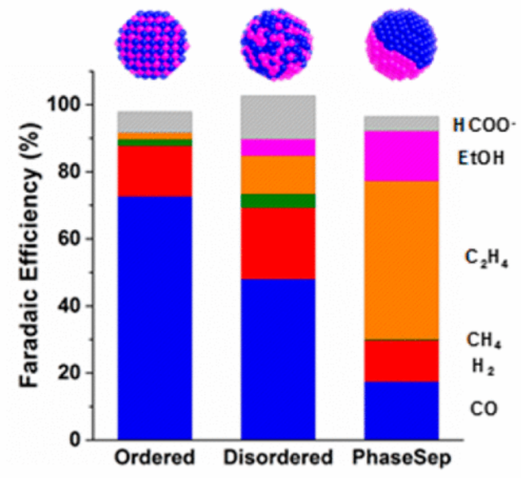


Figure 2.12. Faradaic efficiency (selectivity) for the electroreduction of CO_2 to different C_1-C_2 products as a function of the atomic arrangements for a bimetallic CuPd catalyst.

Copper is known to be the "only" transition metal catalyst capable of reducing CO_2 to significant amounts of C_2 hydrocarbons (ethylene and ethanol). However, the selectivity toward such products is low (typically <30%). In this work, we studied a variety of bimetallic CuPd catalysts with different morphologies (ordered, disordered, phase-separated) and compositions (Cu:Pd = 1:1, 1:3, 3:1) with the aim of understanding the key factors that determine the selectivity of CO_2 electroreduction toward different C_1-C_2 products [33]. The ordered CuPd catalyst was found to exhibit the highest selectivity toward C_1 products (>80%) when compared to the disordered and phase-separated CuPd catalysts (Figure 2.12). Additionally, the phase-separated CuPd and Cu_3Pd were found to achieve higher selectivity for C_2 products (>60%) than $CuPd_3$ and ordered CuPd. The results indicate that a high density of Cu atoms is required for the formation of C_2 products and the reaction proceeds via a C_1 dimerization mechanism. Additionally, they indicate that geometric effects rather than electronic effects play a more important role in determining the selectivity of bimetallic CuPd catalysts. The understanding that the selectivity of CO_2 electroreduction on Cu based bimetallics can be tuned by altering the geometric arrangement can potentially be used to design other bimetallic catalysts. This insight is needed to advance non-precious metal catalysis for converting CO_2 to useful products. *This achievement meets the short-term milestone of Project 2 of the CO_2 Capture and Utilization division's roadmap.*

*16) **Next-generation high-strength, low-cost alloy for hydrogen service (PI Takaki)**

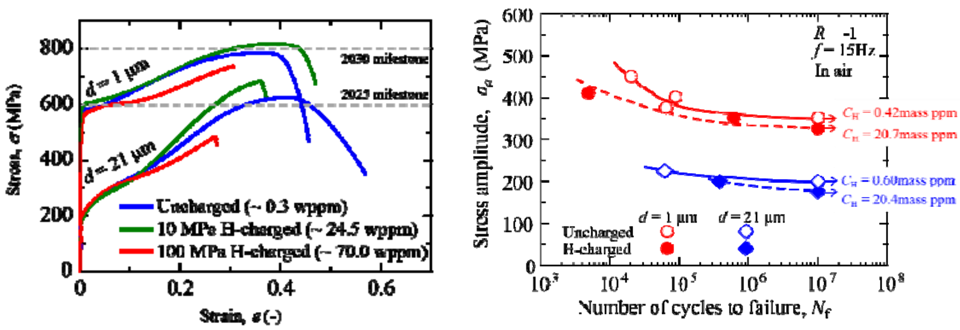


Figure 2.13. Data for Fe-16Cr-10Ni with ultra-fine grain size (d = 1 μm) and conventional grain size (d = 21 μm). (Left) Tensile stress vs. strain data after exposure to hydrogen gas up to 100 MPa, (Right) Stress amplitude vs. cycles to failure relationships with hydrogen concentration indicated for each data set.

Our group has pioneered the process of ultra-grain refinement in austenitic stainless steels. By applying this process to the low-cost experimental alloy Fe-16Cr-10Ni, yield strength was increased

three-fold (to 600 MPa) relative to the conventional grain sized material (Fig. 2.13 left). As for hydrogen compatibility, two metrics were met: tensile ductility and fatigue life. As shown in Fig. 2.13 (left), the strain to failure of ultra-fine grain (UFG) Fe-16Cr-10Ni remains above 30% after exposure to 100 MPa hydrogen [34,35]. Regarding fatigue life, the fatigue limit (stress amplitude at 10^7 cycles) for UFG Fe-16Cr-10Ni is not degraded by hydrogen (~20 wppm), as shown in Fig 2.13 (right). To date, there is no other austenitic stainless steel with such strength that is also hydrogen-resistant.
This achievement fulfills the mid-term milestone in Project 2 and represents significant progress toward the ultimate target of the Hydrogen Materials Compatibility division. One technological implication of this achievement is that low-cost, high-strength UFG stainless steels could replace the benchmark (i.e. SUS316) stainless steel in hydrogen fuel systems. While these results have not been transferred to industry, the commercial-scale production of UFG stainless steels was recently demonstrated by a couple of steel making companies*.
(* revised in the final version)

*17) **Mechanism of fretting fatigue in hydrogen (PI Somerday)**
Understanding fretting fatigue, the coupled problem of cyclic stress and frictional contact, is technologically imperative, since it can lead to component failure. This work demonstrated that hydrogen-induced degradation is more severe for fretting fatigue compared to conventional fatigue (i.e. cyclic stress only). In the plot of cyclic stress amplitude vs. number of cycles to failure in Fig. 2.14, the conventional fatigue limit is not affected by hydrogen for 304 stainless steel. However, under fretting fatigue conditions, hydrogen noticeably lowers the fatigue limit [36]. Such data are essential for the safe design of components for hydrogen service. This fretting fatigue research enabled TOKi Engineering (Fukuoka, Japan) to commercialize a metal face seal (packing) for high-pressure hydrogen gas service (marketed as HYDROBLOCKER). This research activity also established for the first time the mechanisms governing fretting fatigue in hydrogen. The key insight derived from this study is that frictional contact during fretting fatigue removes the material surface oxide, promoting hydrogen uptake as well as adhesion between the contacting surfaces [37]. The combined impact of enhanced hydrogen uptake into the material and adhesion-intensified cyclic plastic strain leads to more severe hydrogen-induced degradation. *This achievement satisfies the short-term milestone in Project 1 of the Hydrogen Materials Compatibility division.*

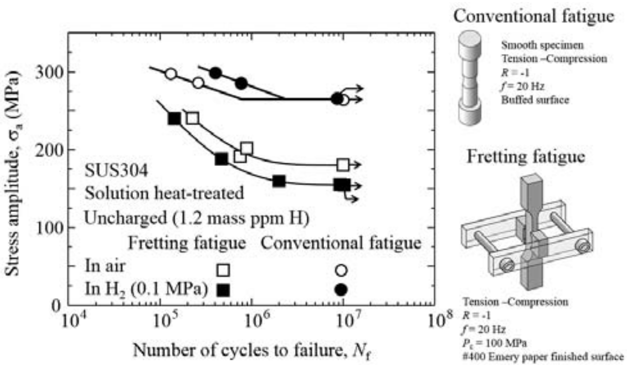


Figure 2.14. Effect of hydrogen on fatigue strength measured from conventional and fretting fatigue tests.

*18) **Hydrogen station deployment (Energy Analysis Division)**
The objective of this study was to develop an effective model for domestic hydrogen station deployment and identify prospective areas for hydrogen stations locations to meet future refueling demands of fuel cell vehicles (FCV). Two deployment models using GIS (geographic information system) were used to consider user convenience and FCV penetration phases. The models assumed that the potential initial 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 (Figure 2.15). The study also identified gaps between existing and planned stations, and the suggested station sites. This gap analysis identified certain cities, particularly prefectural capital cities, in need of coverage [38]. The results were directly reported to Ministry of Economy, Trade and Industry and shared with hydrogen station stakeholders to support hydrogen deployment policy and planning in Japan.

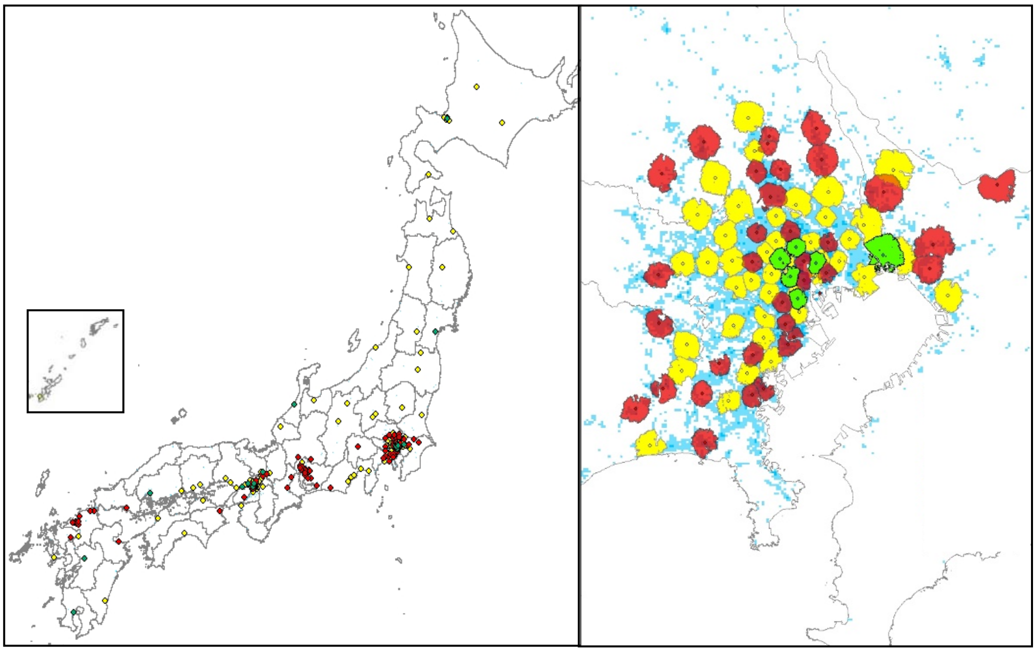


Figure 2.15. Red dots and red areas show existing/planned station sites and their 10 minute driving radiuses. The additional stations that will be created, bringing the total of initial stations to 100, are indicated by green dots (10 minute driving radiuses indicated by green areas). The additional stations (initial 100 to 200 stations) and their 10 minute driving radiuses are indicated by yellow dots and yellow areas. The initial 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.

19) **Applied math analysis of social systems (New initiative by Prof. Murata)**
The large-scale and harmonious implementation of renewable energy technologies that are under development at I²CNER will require a thorough and quantitative understanding of how energy generation, demand, and storage interact with the electric grid. Patterns of energy (electricity) consumption are of utmost importance in the emerging Smart Grid, a tightly integrated network of electricity generation, transmission and distribution, overlaid with a computing and communication system. While in the past, the demand and supply were decoupled in the control loop, the modern vision is a network where they are tightly integrated. Prof. Murata focuses on the residential energy consumption, and, in particular, his research addresses the dual goal of i) developing a flexible yet not over-fitted model for the customer, and ii) the optimization of the customer's behavior using the incentives as the control mechanism. The modeling is based on the reinforced learning approach, where the customer's behavior is described as a Markov chain with time dependent transition probabilities, depending on the instant price of the electricity (including the controllable incentives) and the consumption utility function (incorporating delayed satisfaction). The preliminary results indicate the general validity of the consumer model (the model was tested against empirical observation of electricity elasticity) [39].

*20) **Applied math analysis of geomaterials (New initiative by Prof. Shirai and PI Tsuji)**
Mathematical models of flow through porous rocks are critically important in CO_2 storage in rock formations. However, the structure of porous materials is notoriously difficult to describe and to model. This initiative deploys mathematical tools from two areas: classical random walks in heterogeneous media and very novel persistent homology theory to characterize the properties of porous materials. The random walk approach is used to model rock mineralization processes, where the rock pore evolution in the simulation grid is identified with the probability of mineral precipitation and dispersion degree. Persistent homology (PH) theory allows one to quantify in a rigorous and principled way the notions of higher connectivity at different scales of objects in Euclidean space. The notion of a "hole" is essentially topological, i.e. scale-invariant. Only recently, the theory of PH provided for the language to adequately describe the scale-dependent notions of higher connectivity. In this study, persistent homology was applied to describe heterogeneous natural rock geometries

obtained through X-ray microcomputed tomography and the appearance and disappearance of the topological features were captured by the relevant persistence diagram showing the characteristics of the rock. *These efforts address the short-term milestone of Project 2 in the CO_2 Storage division's roadmap* [40].

2-2. Research environment including facilities and equipment

Describe the degree to which the Center has prepared a research environment appropriate for a world premier international research center, including facilities, equipment and support systems, and describe the functionality of that environment.

I²CNER provides a rich platform for its researchers to pursue transformative research in non-traditional and highly multi-disciplinary environments. Specific details of the I²CNER environment are:

I²CNER Building 1

In order to continue developing a research environment befitting a top world-level research institute, and to promote collaboration and fusion research, I²CNER building 1 (approximately 4,873 m^2) was completed at the end of November 2012. All the Institute's members moved "under one roof" into I²CNER building 1 in January 2013. In fact, the building itself was designed in this spirit—it is home to several common laboratories which are available for use by any I²CNER researcher. The first floor lobby features a spacious lounge with a high ceiling and electronic black boards in order to encourage impromptu meetings and exchange of scientific views among I²CNER members. Facility equipment such as fume foods and pneumatic piping has been installed in I²CNER Building 1.

I²CNER Building 2

A second I²CNER building which has 4 stories and a total floor space of 5,000 m^2 was built. The building includes 8 large-scale labs, 2 open offices, and 1 administrative office, with the majority of rooms being designed as open, common experimental spaces in order to promote interdisciplinary research. This building was funded by the FY 2012 supplementary budget from the Japanese government. Construction of I²CNER building 2 was completed at the end of February 2015.

Six main apparati in I²CNER

i) *Complex Fatigue Testing System*
The small complex fatigue testing system is capable of monitoring slip bands, micro cracks, and others on the specimen surface while the fatigue test is underway. The system is designed for combined use with the scanning electron microscope.

ii) *Imaging Raman Spectroscopy system*
Raman spectroscopy provides information about molecular vibrations that can be used for sample identification and quantitation. This system generates a 2D image of wavelength and intensity of the sample.

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

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

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

vi) UNHT (Ultra Nanoindentation Tester)

The UNHT, ultra-high resolution nanoindenter, is used to examine the mechanical properties of a material at the nanoscale. The UNHT virtually eliminates the effect of thermal drift and compliance due to its unique patented active surface referencing system. Therefore, it is perfectly suited for long-term measurements on all types of materials, including polymers, very thin layers, and soft tissues.

2-3. Competitive and other funding

Describe the results of the Center's researchers to date in securing competitive and other research funding.

・ In Appendix 2-2, describe the transition in acquiring research project funding, and note any external funding that warrants special mention.

I^{2}CNER researchers leverage the established infrastructure, research culture, and international visibility of the Institute to aggressively pursue funding. By way of example, some new major I^{2}CNER research programs are: i) The JST-CREST Grant awarded to Profs. M. Yamauchi and N. Nakashima at a level of ~ 180 million JPY from FY15 to FY19; ii) the Research Center for Next Generation Refrigerant Properties (Next-RP) awarded to Profs. Y. Takata and S. Koyama at a level of 58 million JPY/year from FY16 to FY17; 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 from FY15 to FY19 (4.5 million USD at an exchange rate of 110 JPY); iv) the Kakenhi Grant-in-Aid awarded to Profs. Ishihara and Sakai at a level of ~385 million JPY from FY15 to FY19; v) the JSPS Core-to-Core Grant for an advanced research network to Prof. Matsumoto and collaborators at a level of 90 million JPY from FY17 to FY21; vi) The Center for Small Molecule Energy (CSME) awarded to Prof. Ogo at a level of 99 million JPY from FY14 to FY18; vii) the "International Research Center of Giant Straining for Advanced Materials (IRC-GSAM) awarded to Prof. Horita from FY15 to FY20 with funding so far at the level of ~ 3 million JPY; and viii) the JSPS Grant-in-Aid for Specially Promoted Research awarded to Prof. Ogo from FY2014 to FY2018 at a level of ~440 million JPY.

Additional resources are being secured through projects sponsored by industrial partners within the newly established Industrial Research Division. This division has been created for the purpose of advancing technology transfer with corporations which are funding projects that have a clear association with I^{2}CNER's research, and which agree to have one of their employees immersed in I^{2}CNER laboratories as WPI visiting professor. The first such project is "mobile energy storage for low-carbon society" sponsored by Mazda Motor Corporation at a level of 71 million JPY for the next three years. Details for a second project that the IHI Corporation agreed to sponsor at a level of 3 million JPY in FY2017 are currently being finalized.

Additional resources have 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 Profs. M. Kubota and Alex Staykov, JFE Steel Corporation's support of Prof. M. Kubota).

The Director's vision is that I^{2}CNER can remain strong and agile by developing a core of embedded centers and securing industrial projects that will last beyond the WPI funding period.

2-4. State of joint research

Describe the results of joint research conducted with other research organizations both in and outside Japan.

National Fuel Cell Research Center (NFCRC)

To bridge science to practical application on SOFC/SOEC cathodes using proton conducting oxides and challenges related to hydrogen compatibility with materials, scientists from I^{2}CNER and the NFCRC at the University of California, Irvine exchanged visits and participated in respective center events.

Air Resources Board of the State of California (CARB)

To reinforce the idea of Green Innovation, CARB reviewed all I^{2}CNER's division roadmaps and evaluated I^{2}CNER's research on materials reliability and life prediction and fuel cells with regard to the implementation of hydrogen infrastructure technology. At the same time, CARB became familiar with I^{2}CNER's mission-driven science for carbon-neutral energy technologies.

Norwegian University of Science and Technology (NTNU) and SINTEF

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

Sandia National Laboratories in Livermore, CA and Southwest Research Institute in San Antonio, Texas

From inception through March 2016, I^{2}CNER interacted strongly with Sandia National Laboratories at Livermore, CA, specifically, with Dr. Brian Somerday, who was a distinguished member of the technical staff and the Division Lead PI of I^{2}CNER's Hydrogen Materials Compatibility Division. In FY 2016, Dr. Somerday accepted a new position at the Southwest Research Institute (SwRI) in San Antonio, TX. The Institute has established a relationship with SwRI in order to ensure that the Institute's interaction with Dr. Somerday can continue. Dr. Somerday will continue leading the Hydrogen Materials Compatibility Division from his new post. These interactions have allowed I^{2}CNER to stay informed about hydrogen-related technologies in the US and development of codes and standards for hydrogen materials compatibility.

Oxford University

The Director serves on the Strategic Advisory Panel of HEmS (Hydrogen in Metals—From Fundamentals to the Design of New Steels) at Oxford University, which is a multi-million dollar program funded by the British government. These interactions help the administration to stay apprised of relevant research being carried out in the UK.

2-5. Appraisal by society and scientific organizations

Describe how society and/or scientific organizations in and outside Japan have recognized the Center's research achievements.
・ In Appendix 2-3, list the awards received and invitational lectures given by the Center's researchers.

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

Identified I^{2}CNER as a prime example of successful cooperation between DOE and Japanese researchers.

Recognition from National and International Organizations

PI Akiba

Prof. Etsuo Akiba has been playing an important role in an international network for research and development of hydrogen storage materials as an expert adviser of Tasks 22 and 32 for the Hydrogen Implementing Agreement in the International Energy Agency. Within Japan, he is acting as the project leader for basic research on compact and energy efficient hydrogen storage systems, such as the NEDO project "Advanced Hydrogen Storage Materials" (FY2007-FY2011), R & D for on-board hydrogen storage systems for fuel cell vehicles, and Hydrogen Utilization Technology Development (FY2013-FY2017). Prof. Akiba was the chairman of the committee for roadmap development for hydrogen storage materials for the NEDO project "Survey and Study of Hydrogen Storage Materials for Fuel Cell Vehicles" (FY2012).

PI Sasaki

Prof. 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. Prof. Sasaki is one of three participating members from academia.

PI Tsuji

PI T. Tsuji is member of the Ministry of Economy, Trade, and Industry (METI) committee for the evaluation of the geological formations around the Japanese island and the specifications for new vessels for geological survey. He is also a member of the committee of RITE (of 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 was a member of the committee on the "International Ocean Discovery Program" (US NSF).

Interactions with US Department of Energy (DOE)

As a result of his renowned technical expertise and ability to manage productive projects, Dr. Somerday, the Division Lead PI of the Hydrogen Materials Compatibility Division, was invited by the US DOE to assume a leadership role in a high-profile project titled H2FIRST (Hydrogen Fueling Infrastructure Research and Station Technology), which emphasizes public-private cooperative R&D to stimulate the development of hydrogen fueling stations in the U.S. Other former US DOE Energy employees who worked with I^{2}CNER are: Mark Paster, analyst and key contributor to the Energy Analysis Division; Jeffrey Miller, former Energy Attaché of the US Embassy in Tokyo; and Ross Matzkin-Bridger, current Energy Attaché of the US Embassy in Tokyo. Lastly, Director Sofronis has been serving as reviewer in the Annual Merit Review and Peer Evaluation Meeting for the Hydrogen and Fuel Cells Program.

Sample of Prestigious Recognition from National and International Organizations

US Department of Energy Hydrogen and Fuel Cells Program Research and Development Awards
In 2011, PIs Robertson and Sofronis won the US Department of Energy Hydrogen and Fuel Cells Program Research and Development Award. In 2014, PI Somerday also won the same award.

The 2012 Somiya Award (awarded biennially to scientists who collaborated across two continents)
PIs Kilner, Tuller, and Ishihara were part of a group of scientists who earned this prestigious award.

2012-2013 Hydrogen Student Design Contest
Students from Kyushu University, including team members from I^{2}CNER, won the 2012-2013 Hydrogen Student Design Contest, which was sponsored by the US DOE, the National Renewable Energy Laboratory, Mercedes-Benz, and Toyota.

JST Breakthrough Report 2013
PI Ogo's research was featured in this important publication of JST.

International Society of Solid State Ionics Officers
PI Tuller serves as the President of the society and PI Ishihara serves as Treasurer.

Order of Culture Award, 2014 and Kyoto Prize, 2015
Prof. T Kunitake

Medal with Purple Ribbon, 2015
PI. Z. Horita

Commendation for Science and Technology by MEXT, 2015
PI T. Tsuji and Prof. S. Ida

Daiwa Adrian Prize 2016
PIs Ishihara and Kilner, and Profs. Staykov, Druce, and Tellez

Commendation for Science and Technology by MEXT, 2016; The Society of Polymer Science, Japan, 2016 for outstanding achievements
PI N. Nakashima

3. Feeding research outcomes back into society (within 2 pages)

3-1. Applications of research results

Describe the applications created from research results, their effect in spawning innovation, intellectual properties (IPs) obtained, and joint research activities conducted with corporations, etc. Also, describe center's research achievement, vision and scenario of transition that contributes to a low-carbon society.

The relevance of the I^{2}CNER research efforts and objectives toward enabling the green innovation initiative of the government of Japan is demonstrated by the large number (81) of collaborative projects in which its researchers are involved with industry. A total of 33 projects resulted in technology transfer events. Since inception, I^{2}CNER filed for 178 patents and was granted 46 patents.

The following are representative examples for each division: i) PI Ishihara's transfer of dual carbon battery technology for energy recovery from automobiles to Ricoh Co. Ltd., ii) PI 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) PI 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) PI Yamauchi's synthetic method for the preparation of atomically well mixed Fe-Ni nanoalloys has been transferred to Daido Steel, vi) PI Fujikawa's functional nanomembrane technology for gas separation has been transferred to Nanomembrane Technology Inc. for upscale development, vii) PI Tsuji's innovative continuous CO_2 monitoring system in collaboration with the Japan Oil, Gas and Metals National Corporation (JOGMEC) has been transferred and deployed in the ongoing CO_2 sequestration project in Saskatchewan, Canada, viii) PI Sugimura's studies of diamond-like carbon (DLC) coatings in collaboration with Kitz corporation on the wear of candidate coatings in the presence of hydrogen contributed to the development of 100 MPa hydrogen flow valve, which is now in practical use in hydrogen refueling stations; ix) The results of Prof. Itaoka's investigation on the hydrogen refueling stations and supply infrastructure for Japan discussed in the preceding section have been submitted to the Ministry of Economy, Trade and Industry of Japan in the form of 73-page report in February 2017. In FY 2016, I^{2}CNER filed for 23 patents, and was granted 14, bringing the total of patent applications since inception to 178 and patents awarded since inception to 46.

As part of its efforts to pursue relationships with industry and government programs in order to identify mission-oriented basic science that supports technology implementation in industry, I^{2}CNER established the Industrial Research Division, wherein industry liaisons are embedded in I^{2}CNER working on exploratory research projects and technology transfer. Such projects are established after exploratory workshops (usually a full day) have been held with corresponding industries to identify converging interests. In FY 2016, the first such project with Mazda Motor Corporation was established and a second one with IHI Corporation will be established in FY 2017. In addition, I^{2}CNER just established the Industrial Advisory Board, whose members are prominent executives from industry, government agencies, and national laboratories that will advise I^{2}CNER on opportunities for interactions with industry and technology transfer.

3-2. Achievements of Center's outreach activities

If the Center has conducted its own unique outreach activities, describe those worthy of special mention.
・ In Appendix 2-4, list and describe media coverage, press releases, and reporting.

I^{2}CNER carried out numerous outreach activities to attract the attention and participation of Japanese and international citizens, high school students, academic faculty, national laboratory scientists, and industry and government officials. Some outstanding examples of our outreach efforts are:

I^{2}CNER Kick-off Symposium on February 1, 2011

The event provided an ideal opportunity for researchers from KU, the University of Illinois at Urbana-Champaign, and the Institute's other international partners to converge and begin exchanging ideas and engaging in debate about carbon-neutral energy issues. Among the participants were Dr. Anne Emig, Head, National Science Foundation (NSF) Tokyo Regional Office; and Dr. Toshio Kuroki, WPI Program Director.

I^{2}CNER Satellite Kick-off Symposium, March 6-7, 2012

The symposium was attended by WPI Program Director Toshio Kuroki, KU President Setsuo Arikawa, and UIUC Provost Richard Wheeler. Day 1 of the symposium featured lectures by many prominent researchers, including Sam Baldwin, Chief Science Officer, Office of Energy Efficiency &

Renewable Energy, U.S. Department of Energy. A total of 30 researchers from Kyushu University travelled to Illinois to participate in this event.

I²CNER Annual Symposia

Since the Institute's inception, the I²CNER Annual Symposium has evolved from an annual event that celebrates the current research achievements of its thematic research areas (divisions) to an exploratory forum that focuses on a single research topic that is highly relevant in I²CNER's research portfolio and the international community (i.e., computation, applied math, etc.) The objective of this series of international symposia is to identify the current state-of-the-art in a research area, establish where I²CNER's research is in comparison with the state-of-the-art, identify the roadblocks and needed advances in the field, and to set new or update existing I²CNER targets accordingly. Each year, the symposium also features more specific workshops organized by each division. These workshops provide a forum for brainstorming, which allows for opportunities to identify strengths and weaknesses in our research portfolio, and explores how we might best accomplish critical growth in our thematic research areas. For specific details and examples, please see Section 5-2 below.

I²CNER in Tokyo Symposium

The hosting of the Tokyo Symposium, which is sponsored by the U.S. Embassy in order to bring I²CNER research activities to the attention of the energy stakeholders in the capital of Japan and the international community, is another growing I²CNER tradition. So far, two symposia were hosted in 2012 and 2014, both of which were attended by the US Ambassador to Japan and high-ranking government officials from MEXT, DOE, and other US government agencies.

Hello! I²CNER/Energy Outlook

The Institute publishes two outreach publications, Hello! I²CNER (for high school students) and Energy Outlook (for industrial stakeholders), three times per year. We regularly receive requests from local high schools who are familiar with Hello! I²CNER and who want to participate in the "Science Café" section in upcoming issues. Energy Outlook features interviews with industry executives and world renowned energy researchers.

I²CNER Promotion Video

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. The video remained on the MRS website through FY2016 in order to increase our international visibility. On average, these videos receive about 60,000 hits.

4. Interdisciplinary Research Activities (within 3 pages)

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

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 by the Internal Programs Review Committee (IPRC), and the funding is reallocated based upon this assessment.

After careful consideration of the progress that was made in projects that were selected in FY 2012-FY 2014 (only 3 publications that were published as a result of these projects were truly interdisciplinary), the Director has awarded competitive funds only to those researchers who make a truly exceptional proposal. Moreover, the Director has generally awarded the funds in slightly larger "chunks" to fund overall fewer projects per year, the idea being that an increase in funding will help the projects be more productive.

In FY2015 and FY2016, the I²CNER Director utilized the competitive fund to support the Institute's new initiative on Applied Math for Energy. The competitive funding 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 I^2CNER's Applied Math Initiative. The Institute received several proposals in response to the call, including joint proposals between I^2CNER-KU faculty and a few by KU faculty outside of I^2CNER. After rigorous screening by the IPRC, 5 applications were selected in FY2015 and 2 in FY2016 as "seed projects," the idea being to foster close, ongoing collaboration between I^2CNER 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, FY2015.

ii) Prof. J. Murata, "Design of Demand Response Programs Using Inverse Optimization," Department of Electrical Engineering, FY2015.

iii) Prof. T. Tsuji, "Characterization of heterogeneous rock pore structure using persistent homology: Insight into scale dependence of hydrological and elastic properties," I^2CNER. (In collaboration with PI Christensen, University of Notre Dame), FY2015.

iv) Prof. D. Triadis, "Anomalous diffusion in realistic pore-scale simulations of two-phase flow for geologic CO_2 sequestration" IMI, Australia Branch, Trobe University, FY2015.

v) Prof. R. Nishii, "Statistical analysis of global gene expression data and applications to plant growth," IMI, FY2015.

vi) Prof. K. Matsue, "Characterization of dynamic events in flame fronts in turbulent combustion," IMI and I^2CNER, FY2016.

vii) Prof. K. Hirose, "Statistical analysis of energy consumption," IMI and I^2CNER, FY2016.

The progress of the interdisciplinary projects seeded in FY 2015 was assessed carefully by the IPRC in FY 2015 and improvements and adjustments were made through a review/rebuttal process administered by the Director. All projects that were funded in FY 2015 continued in FY 2016. Upon initiating their projects in FY 2016, tenure-track Assistant Professors Matsue and Hoa traveled to the Illinois Satellite in Spring 2017 in order to initiate collaborations with Satellite faculty.

I^2CNER's annual symposia are used as platforms to explore fusion of disciplines and come up with action plans for nurturing new cross-cutting interdisciplinary research directions and guiding new faculty hires. By way of example, major outcomes of the 2016 and 2017 symposia is that they helped in the establishment of computational science and applied math as integral components of I^2CNER's research portfolio. An additional result of the 2016 symposium is that 2 female postdoctoral researchers in computational materials science were hired in Fall 2016. Finally, plans are in place to hire a PI whose area of expertise is computation.

In October 2016, we hired Dr. Chapman, who holds a PhD in socio-environmental energy science from Kyoto University, as an Assistant Professor in order to increase the EAD's capability to analyze research projects through the lens of the societal aspects of generation and utilization of renewable energy on an international scale. Dr. Chapman has already started interactions with the technical divisions of I^2CNER and the "Kyudai interdisciplinary colloquium" to advance work on I^2CNER's need for collaboration with social scientists in terms of understanding the social components of behavior, choice, and the influence of user preferences on the future energy system. The colloquium has been established by KU to promote better exchange amongst faculty and students working in different faculties, especially in social science and humanities fields.

The importance of interdisciplinary research is emphasized consistently in the communications of the Director with all I^2CNER members. In addition, all I^2CNER faculty know that interdisciplinary research is a requirement for promotion and tenure within the Institute, a fact that is clearly stated in the Institute's governing document on Faculty Promotion.

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

Coffee and Collaboration (CO^2)

The I^2CNER building brought our researchers under the same roof and this instigated collaborations across the disciplines. In particular, informal social events, such as the I^2CNER-sponsored "Coffee and Collaboration (CO^2)," has led to a number of collaborations among I^2CNER researchers. One example is the collaboration between PI Tatsumi Ishihara, PI John Kilner, former Satellite Faculty Angus Rockett, and Profs. Druce and Tellez. While exchanging ideas at CO^2, the team initiated an effort that enabled the discovery of the fundamentals of the oxygen transport kinetics in solid oxide fuel cells and electrolyzers, which permits the engineering design of next generation electrodes. The collaboration combines materials physics (Kilner), inorganic chemistry (Ishihara), and materials science (Rockett).

Division Retreats

Beginning in Fall 2013, each research division of the Institute hosts a semi-regular division retreat at a location away from KU so that each research division can consider carefully its research themes and revisit its project roadmaps. Examples of the interdisciplinary collaborations which emerged at these division retreats are: i) The collaboration between PI Sakai and Satellite Faculty Martin on high-efficiency hybrid organic/inorganic photocatalysis systems. This work stands at the forefront of advanced materials science and chemistry, ii) The collaboration between Profs. Hagiwara and Staykov, PI Ishihara, and Satellite Faculty Ertekin on a hybrid molecular switch for ultra-efficient photocatalytic charge separation." This work is fusion of solid state photocatalysis with molecular chemistry.

IISS Presentations

Since its inception, young researchers have been giving presentations at the Institute Interest Seminar Series (IISS) with the goal of initiating cross-division collaborations. In FY 2016, a total of 32 speakers presented at 17 Institute Interest Seminars. Since the inception of the Institute, a total of 182 speakers presented at 103 Institute Interest Seminars. Examples of collaborations which have emerged from these seminars are: i) The collaboration between Profs. M. Nishihara and A. Staykov, which resulted in a joint journal publication in the Journal of Polymer Science Part B: Polymer Physics (2014), 52, 293–298. This project fuses polymer chemistry, solid state materials science, computational chemistry, and electrochemistry, ii) Molly Jhong (Illinois graduate student) from the group of Satellite Faculty Kenis presented her research before the groups of PIs Nakashima and Sasaki. I²CNER Prof. Lyth approached Ms. Jhong after the presentation to suggest that she try some of his N-doped carbon materials for CO_2 conversion. A joint collaboration on materials synthesis and electrochemistry was produced.

Unofficial Seminars on "Computational Materials Science"

In October 2013, young faculty, led by Prof. Aleksandar Staykov, put forward a new, unofficial initiative on "Computational Materials Science" in order to advance exchange and collaboration in molecular and materials chemistry across division boundaries. The effort, which involves informal seminar presentations and discussion, gives researchers from molecular chemistry and materials chemistry the opportunity to meet and exchange ideas, and share computational techniques and experience in the emerging interdisciplinary field of organic/inorganic interface chemistry, as well as in surface chemistry and material interfaces. These meetings have led to collaborations that resulted in joint publications between members of the Electrochemical Energy Conversion, Molecular Photoconversion Devices, and Hydrogen Materials Compatibility.

Workshops organized by young faculty

A joint I²CNER-AIMR workshop was organized by Prof. Staykov at I²CNER on Sept. 2, 2015. The purpose of the workshop was 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 ideas on the synthesis, application, catalysis, and development of novel experimental and theoretical techniques. 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). Dr. Staykov and Dr. Packwood are working on the organization of a similar workshop in FY 2017 which will focus on the interaction of mathematics with theoretical chemistry, again targeting young researchers.

4-3. Results of research in fused research fields

Describe the Center's record and results by interdisciplinary research activities.

- In Appendix 3, list the main papers published (up to 20 papers) on the Center's interdisciplinary research and provide a description of each of their significance.

I²CNER's approach to research bridges multiple spatial, molecular to miles, and temporal scales, nanoseconds to decades, but it also necessitates bringing together scientists and engineers from disparate disciplines: chemistry, physics, materials science, mechanics, geoscience, and biomimetics. In other words, I²CNER's research activities and goals are by nature interdisciplinary and are carried out across division boundaries and international borders. A representative sample of I²CNER results that reflects the fused nature of I²CNER are as follows:

<u>Molecular Photoconversion Devices:</u> In a collaborative effort between Ida (Kyushu) and Ertekin and Rockett (Illinois), an I²CNER-developed combination of finite-element analysis and first-principles

theoretical approach was used to design materials for photoelectrochemical water splitting. Experimental testing with Earth-abundant $CaFe_2O_4$ combined with a thin layer of TiO_2 demonstrated water splitting without an external power source and the most positive onset potential among the oxide photocathodes ever reported (*chemical synthesis, atomic resolution microscopy, first-principles, and continuum modeling*). By designing a new "pyridyl anchor" scheme, PI Sakai demonstrated that it produces an exceptionally strong bond of an organic dye molecule to inorganic TiO_2 while retaining high rate electron transport across the interface. The result is superior to previous approaches and has the potential to significantly improve the stability of hydrogen production by photoelectrochemical organic devices (*photochemistry, electrochemistry, and inorganic-organic hybrid materials chemistry*).

Hydrogen Storage: The collaboration of PI Akiba with PI Horita led to the discovery of the defect activation mechanism for hydrogen absorption of TiFe intermetallics by High Pressure Torsion, a promising system for renewable stationary energy storage (*synthetic chemistry, crystallography, spectroscopy, mechanical metallurgy, and electrochemistry*).

Catalytic Materials Transformations: The group of PI Ogo developed the first synthetic analog of the active site of the [NiFe] hydrogenase that oxidizes hydrogen by catalyzing electron and hydride transfer from H_2. The investigation of the crystal structure of the type 2 [NiFe]-hydrogenase from a new bacterium, *Citrobacter sp. S-77*, which has a novel functional mechanism having O_2-tolerant and high H_2-activation potential, by PI Ogo is the first in the world. The hydrogenase enzyme obtained from this organism is more active than platinum, fully recovers from poisoning by carbon monoxide, and opens new pathways to the design of new synthetic model catalysts having both O_2 tolerance and high H_2-activation potential. These results will help accelerate low cost hydrogen fuel cell technology, and emphasize the dramatic progress of hydrogen activation using non-precious metal catalysts (*microbiology*, *bioinorganic chemistry, coordination chemistry, electrochemistry*).

Thermal Science and Engineering: The focus of Prof. Miljkovik (Illinois) research on novel micro/nanostructures for coalescence induced droplet jumping and adsorbent nanomaterials has led to transformational efficiency enhancements in energy applications by fundamentally manipulating heat-fluid-surface interactions across multiple length and time scales. Specifically, the discovery of these novel nanomaterials and coatings has immense technological impact on renewable and non-renewable power generation and thermal management (*Synthetic Chemistry, Surface Science, Thermal Science, Fluid Mechanics, Thermodynamics, Optics, Spectroscopy, Organic Chemistry, Polymer Science*). PI Saha's foundational studies on solid-vapor adsorption phenomena for the rational design of high-uptake adsorbent materials have led to the discovery of highly porous (> 3000 m^2/g) MOFs with ultra-high water and ethanol uptake. Our interdisciplinary accomplishments are re-writing the foundational knowledge base in the field of surface science by quantifying the environmental effects on sample wettability and adsorption (*Synthetic Chemistry, Crystallography, Surface Science, Self-Assembly, Thermal Science, Thermodynamics, Organic Chemistry*).

Electrochemical Energy Conversion: Understanding complex chemo-mechanical relationships is crucial for understanding and avoiding failures in any solid-oxide-cell-based electrochemical devices. Electro-chemo-mechanics studies at I^2CNER and MIT by PI Tuller and Profs. Perry and Bishop have identified the atomistic origins of chemical expansion and discovered factors that can be used to tailor it. This has led to rational design of energy conversion materials with enhanced durability and innovation of new characterization techniques (*surface science, optical spectroscopy, crystallography, high temperature electrochemistry, and computational materials science*). The widespread use of fuel cells is currently limited by the lack of efficient and cost-effective catalysts for the oxygen reduction reaction (ORR). PI Gewirth shows how to control proton availability and in doing so shows for the first time how changes in this availability can alter the products of the reaction. This way he achieved 100% selectivity for the four electron reduction of O_2 to H_2O without generating harmful partially reduced O_2 species. Further, ORR catalysts that do not contain precious metals are the future of low temperature fuel cells. Gewirth's work developed for the first time a detailed understanding of the composition of one of these catalysts, showing that it was a carbon-encapsulated superparamagnetic iron nanoparticle (*Chemistry, physics, material science, biomimetic chemistry, electrochemistry, spectroscopy*).

CO_2 Storage: The complex relationship between hydrologic (CO_2 saturation) and elastic (seismic velocities) properties of real rock geometries has been investigated by the group of PI Tsuji through numerical simulations coupling hydrology and geophysics. The study led to the development of a new method for quantitative monitoring of CO_2 storage sites. This is the first *continuous* seismic monitoring system for CO_2 leakage and is currently deployed in an ongoing CO_2 sequestration project at a coal-fired power plant in Saskatchewan, Canada (*Earthquake science (seismology) and* *exploration geophysics*).

Hydrogen Materials Compatibility: For the first time, a study combining experiments and modeling has revealed the physics governing inhibition of H_2-accelerated fatigue crack growth by ppm-levels of O_2. A predictive analytical model was formulated that accurately quantifies how key variables (e.g. O_2 concentration and load) affect the onset of accelerated crack growth H_2 gas containing trace O_2 concentrations. In parallel, first-principles density functional theory (DFT) modeling by Prof. Staykov revealed the characteristics of hydrogen-oxygen competitive co-adsorption on iron surfaces that impede hydrogen uptake into steel (*materials science, solid mechanics, gas physics, and theoretical chemistry*).

5. International Research Environment (within 4 pages)

5-1. International Circulation of Best Brains

5-1-1. Center's record of attracting and retaining top-world researchers from abroad

Describe the participation of top-world researchers as PIs and the residing of joint researchers at the Center.

・ In Appendix 4-1, give the number of overseas researchers among all the Center's researchers, and the yearly transition in their numbers.

Participation of Overseas PIs and Researchers

All 9 of our overseas Principal Investigators are top-world researchers who are actively involved in I^2CNER's research operations. They spend between one to seven weeks at Kyushu and participate in events and exchange opinions on collaborative research projects with their Kyushu counterparts. By way of example, Prof. Kilner, an international authority in the field of ionic and mixed conducting ceramics, spent 7 weeks in I^2CNER during FY2016. Jointly with Kyushu faculty, he won international awards and research program grants, e.g. core-to-Core, and hosted one assistant professor from I^2CNER at Imperial College London for 2 months. Prof. Tuller, Distinguished Life Member of the American Ceramic Society and Senior Member of the Institute of Electrical Electronics Engineers (IEEE), spends between 2 and 4 weeks a year at I^2CNER and hosts assistant professors and postdocs from I^2CNER at MIT for multiple months every year. Dr. Somerday is a leading scientist in the area of mechanical metallurgy. He visits I^2CNER for 3 weeks a year on average and, even while at Southwest Research Institute, participates in his division's activities via videoconference. Profs. Robertson, Gewirth, and Christensen play a crucial role in management of the Satellite Institute's research activities, serving as Chief Science Advisor to the Director (Robertson), members of the IPRC (Profs. Gewirth and Christensen), and the Satellite Advisory Committee (all three). All three researchers come to I^2CNER several times every year. Aside from PIs, I^2CNER hosts WPI Professors, WPI Visiting Professors, and a WPI Associate Professor from overseas on a regular basis. An extensive list of distinguished researchers from abroad can be provided upon request.

5-1-2. Employment of young researchers at the Center and their job placement after leaving the Center

Describe the Center's employment of young researchers, including postdoctoral researchers, and the positions they acquire after leaving the Center.

・ In Appendix 4-2~4, enter the following:
- The state of international recruitment for postdoctoral researchers, applications received, and selections made
- The percentage of postdoctoral researchers from abroad
- The positions that postdoctoral researchers acquire after leaving the Center

To date, a large number of I^2CNER postdocs have leveraged their appointments at the Institute to advance their professional careers. By way of example, I^2CNER postdoctoral researcher, Dr. Yuki Naganawa, accepted a position as an Assistant Professor at Nagoya University beginning June 1, 2012. I^2CNER postdoctoral researcher, Dr. Takeshi Matsumoto, accepted an Assistant Professor position at Chuo University beginning April 1, 2014. I^2CNER EAD postdoctoral researcher, Dr. Seiichiro Kimura, left the Institute to become an associate at the Matsushita Institute of Government and Management. Beginning April 1, 2014, Dr. Kimura's appointment in the Institute changed to WPI Visiting Scholar. In FY 2015, Dr. Limin Guo accepted a faculty position at Huazhong University of Science and Technology, China. Dr. Fei Jiang accepted a position at Yamaguchi University beginning April 1, 2016.

5-1-3. Overseas satellites and other cooperative organizations

・ In Appendix 4-5, describe the state of the Center's agreements concluded with overseas satellites and other cooperative organizations.

The Satellite Institute at the University of Illinois at Urbana-Champaign facilitates cooperative research activities and personnel exchanges. In addition to conducting Institute related research, the Satellite serves as the base for identifying and engaging key research programs and faculty at universities and institutions nationally and internationally. The ongoing relationships between the faculty of Kyushu University and the University of Illinois at Urbana-Champaign are having a transformative impact upon I^{2}CNER's overall research culture. Some of the efforts undertaken at the Satellite to promote the mission of I^{2}CNER 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 I^{2}CNER research activities at Kyushu, and they are continually re-assessed based upon their relevance to the overall I^{2}CNER vision and roadmap. As of March 31, 2017, there are 7 UIUC Faculty and 1 WPI Principal Investigator participating at the Illinois Satellite. 1 member of I^{2}CNER'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 I^{2}CNER in some capacity: Prof. Ian Robertson, Dean of the College of Engineering, University of Wisconsin-Madison (WPI Principal Investigator); Prof. Ken Christensen, Assistant Dean of Faculty Department, University of Notre Dame (WPI Principal Investigator), Prof. Angus Rockett, Metallurgical and Materials Engineering Department Head, Colorado School of Mines (WPI Professor, member of I^{2}CNER's IPRC).

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 I^{2}CNER affiliation in publications, etc. Indeed, the signing of the MRA can serve as a model for the entire WPI Program.

Visiting Graduate Students

As of March 31, 2017, the Institute has hosted a total of 31 graduate/undergraduate students from Illinois and other collaborating institutions overseas since its inception. The numbers of visiting students are 5 (FY 2011), 4 (FY 2012), 8 (FY 2013), 2 (FY 2014), 4 (FY 2015), and 8 (FY 2016), of which, 3, 1, 3, 0, 3, and 8, respectively, stayed for more than a month at KU.

I^{2}CNER Undergraduate Exchange Program

The "Agreement on Academic Cooperation" between KU and Illinois helps the two universities to promote mutual understanding and strengthen their relationship. A "Student Exchange Program Agreement" between KU and Illinois was signed on October 24, 2014. The numbers of KU undergraduate students who visited UIUC are 5 (FY 2013), 6 (FY 2014), 6 (FY 2015), and 6 (FY 2016). FY2015 was a milestone year for this program because the first 2 female students visited UIUC in this year's group. During their monthly visit, the students observe and assist with research in Illinois laboratories under the supervision of Satellite faculty and graduate students, participate in group meetings, complete weekly "check-ins" with the Director, take tours of local engineering companies, and interact with the Center for East Asian and Pacific Studies (CEAPS) to enhance their cultural experience of the university, including lunches and activities with Illinois undergraduate student "buddies". At the end of their stay, the KU students give presentations on their research and cultural experiences at Illinois in a mini-workshop.

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 Illinois 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 FY 2015 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 an 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 FY 2016, the researchers began the tradition of hosting an Annual PIRE Meeting to update one another on their latest research results and to plan their activities for the following year. In FY 2015, 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 visited Kyushu from June 1-July 31, 2016. In FY 2017, 5 American students will travel to Kyushu from June 11-August 13, 2017.

5-2. Center's record of holding international symposia, workshops, research meetings, training meetings and others

・ In Appendix 4-6, describe the main international research meetings held by the Center.

- Since the Institute's inception, I²CNER has held a symposium an annual basis, which evolved over time from an event that celebrates the current research achievements of its thematic research areas (divisions) to an exploratory forum that focuses on a single research topic that is highly relevant in I²CNER's research portfolio and the international community (i.e., computation, applied math, etc.). The objective of this series of international symposia is to identify the current state-of-the-art in a research area, establish where I²CNER's research is in comparison with the state-of-the-art, identify the roadblocks and needed advances in the field, and to set new or update existing I²CNER targets accordingly. Each year, the symposium also features more specific workshops organized by each division. These workshops provide a forum for brainstorming, which allows for opportunities to identify strengths and weaknesses in our research portfolio, and explores how we might best accomplish critical growth in our thematic research areas.

- The 2017 I²CNER Annual Symposium, which was titled "Applied Math Challenges in Energy & the Next-Generation Electric Grid", was held on February 1, 2017 and was attended by more 166 scientists, including 86 participants from overseas. This symposium brought together experts from the mathematics and engineering communities to discuss and converge upon the development of necessary new tools and explore new ways of thinking to solve complex and multi-scale energy problems. The symposium included a keynote lecture entitled"Renewable Resource Integration in the Smart-Grid Environment: the Grand Challenges and the Key Opportunities Towards a Sustainable Energy Future" by Prof. George Gross, Department of Electrical and Computer Engineering, University of Illinois at Urbana-Champaign; an invited lecture entitled"The Energy Challenge - A UK Perspective" by Prof. Martin Freer, Director of the Birmingham Energy Institute, University of Birmingham; 8 Presentations; and a plenary lecture called"Mathematical and Numerical Modeling Requirements for Large-scale CCS" by Prof. Michael A. Celia, Department of Civil and Environmental Engineering, Princeton University.

- 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 focus 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 were compiled into a "Basic Needs" report on computation in I²CNER, which will be used to guide future initiatives/investments in the area of computation, and which will be published in the near future. 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.

- The I²CNER Annual Symposium 2015: "Fuel Generation and Use for the 21st Century" was held on February 2, 2015 and was attended by 141 scientists. Leaders of the international scientific community came together and discussed interdisciplinary approaches to tackle key themes of I²CNER's roadmap: polarization in relation to the defect structure of the material components; the catalytic activity dependence on the surface structure and grain boundary species diffusion; dependence of the oxygen reduction reaction on proton transfer in non-precious catalysts; molecular design and dopant effects on stability for thermally activated delayed fluorescence; and the suggestion by Prof. Kunitake that we could consider amorphous membranes for fuel cells.

- On January 30, 2014, co-organized the "I²CNER & ACT-C Joint Symposium 2014" with the Advanced Catalytic Transformation program for Carbon utilization (ACT-C) of the Japan Science and Technology Agency (JST). The symposium was attended by 177 people, including many international guests.

- 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 were the organizers of the 2012 and 2016 International Hydrogen Conference at the Jackson Hole, Wyoming (USA). This International Hydrogen Conference series, which is held about every four years, is the premier topical meeting worldwide on hydrogen effects in materials.

- Associate Director Takata PI Takata was the chair of the First Pacific Rim Thermal Engineering Conference (PRTEC2016), Hawaii, held March 13-17, 2016. The conference is co-organized by the Japan Society of Mechanical Engineers (JSME), Korean Society of Mechanical Engineers (KSME) and American Society of Thermal and Fluids Engineering.

- Associate Director Ishihara was the organizer of the International Conference on Hydrogen Production 2014 (ICH2P-2014) in Fukuoka (Japan). ICH2P-2014 is a multi–disciplinary international conference on the production of hydrogen through various methods as well as its use in various systems, including fuel cells.

5-3. System for supporting the research activities of overseas researchers

Describe the Center's preparations to provide an environment conducive for overseas research to concentrate on their work, including for example living support in various languages or living support for their families.

Administrative Support for Foreign Researchers' Transition into Japanese Society

The I²CNER Administrative Office is in close communication with the existing KU International Student and Researchers Support Center, and offers full-time support to overseas researchers in the invitation procedures, including visa application processing and accommodations on campus. To help overseas researchers adapt smoothly into the new culture and research environment, the Administrative Office i) offers additional training and workshop opportunities, ii) introduced an English version of various application forms, guidelines, and university regulations, and iii) introduced an English version of the Web Safety Training Module, which all new I²CNER members are required to complete prior to conducting experiments in the laboratory. Additionally, the Administrative Office provides extensive living assistance with medical checkups, off-campus accommodations, travel arrangements for family members, and introduction to the Japanese social insurance system.

For invited international researchers, university accommodation facilities are available, or arrangements are made for fully furnished private apartments with easy access to Kyushu University. "Ito Guest House," an on-campus housing accommodation for short-stay researchers from overseas, was built and opened on April 6, 2012 in the Center Zone of Ito campus, where I^2CNER is located.

5-4. Others

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

Collaborative Foreign Exchange Program

In July 2013, I^2CNER established the "Collaborative Foreign Exchange Program" in order to encourage young researchers, especially Japanese, to visit our overseas collaborating institutions. So far, 11 young researchers (8 Japanese, 3 non-Japanese) had their proposals approved, and 9 of them visited the Illinois Satellite for the extended period between one and nine months. In FY 2016, one young Japanese researcher stayed at the Illinois Satellite for 9 months through this program. In 2014, one young female researcher spent 6 months at Sandia National Laboratories, Livermore, CA.

6. Organizational Reforms (within 3 pages)

6-1. Decision –making system in the center

Describe the strong leadership that the director is giving the Center's operation and its effect, and the division of roles and authority between the Center and its host institution.

Kyushu University regulations and rules give the authority for the I^2CNER operations to the Institute Director, and the appointment/dismissal of the Institute Director is authorized by the President of the host institution. The Director is assisted by two Associate Directors.
The 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. I^2CNER is in line with the mid-term goal and plans of Kyushu University, and organized directly under the President of Kyushu University.

6-2. Arrangement of administrative support staff and effectiveness of support system

Describe the assignment of the Center's administrative support staff who have English language and other specialized skills, effort made in establishing the support system, and the system's effectiveness.

Administrative Director

Since April 1, 2015, Mr. Shunichi Masuda has been the I^2CNER Administrative Director, which includes responsibility for the oversight of the Administrative Office and other duties as assigned by the Director, with a mandate to execute President Kubo's vision toward the goal of realizing the WPI mission within KU. Mr. Masuda has extensive experience working in industry, both in the US and Japan.

Composition of Administrative Staff

As of March 31, 2017, the administrative office consists of 20 staff members including the

Administrative Director and the Associate Administrative Director (Head of Administration), and is divided into four groups:

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

These four groups act as a support system to the Institute's researchers and administration under the supervision of the Administrative Director and the Associate Administrative Director. The Administrative Staff has a good command of English (one member is trilingual). 6 members belong to the administrative bureau of Kyushu University and have technical knowledge of either general affairs and human resources, or accounting and budget management. The KU members' broad experience and deep understanding of the university's system contribute to the smooth operation of the Institute within Kyushu University. At the same time, the international work environment of I^2CNER significantly helps the KU employees to strengthen their English language skills and acquire international experiences from interacting with foreign scientists.

6-3. System reforms advanced by WPI program and their ripple effects

Concisely itemize the system reforms made to the Center's research operation and administrative organization, and describe their background and results. Describe the ripple effects that these reforms have on the host institution. (Describe the ripple effects on other institutions.)

In order to ensure smooth management of the Institute, the I^2CNER Director has requested that the Kyushu University administration work for flexible implementation, adjustment, and modification of the university's internal systems. In response to this, the Executive Vice President in charge of Research has been working to explore and implement cross appointments, improve the intra-university faculty transfer system, and identify ways for I^2CNER 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 KU, the KU Administration institutionalized a cross-appointment employment system in March 2015. The KU Administration views this system as an excellent way to hire elite young faculty/researchers from the private sector (industry) and other universities and institutes, both foreign and domestic. By way of example, I^2CNER and the Institute of Mathematics for Industry (IMI) have already utilized this system for jointly hiring 2 tenure track assistant professors. In implementing this system, KU aims to execute the WPI goals to further promote internationalization of research and education, and increase its visibility around the world. The US-Japan IAME will immediately apply this system for its new faculty. Specifically, under this system, a US faculty member who has a 9-month contract of employment with his/her "home" university can be hired by KU for the remaining three months within a year. The total duration of the employment contract shall be of 3-5 years.

Intra-University Faculty Transfer System

Kyushu University's "Intra-University Faculty Transfer System" was implemented on December 1, 2012 to enable flexibility in allocating faculty within the University for the purpose of improving the standards of education and research conducted at KU. I^2CNER has been utilizing this system since FY 2013, and in FY 2016, 9 senior-level faculty were transferred to I^2CNER and served as the core Kyushu-based PIs of I^2CNER. After having utilized this system for the past 4 years, the KU Administration is working together with I^2CNER to assess the effectiveness of the system and explore ways in which the system could be improved.

I^2CNER Faculty Involvement with Teaching

I^2CNER faculty are involved with teaching in three new "Education and Research Fields," which were established in Summer 2013, in collaboration with 1) the School of Engineering, 2) the Graduate School of Engineering, and 3) the Graduate School of Integrated Frontier Sciences. All three fields are engaged in research areas which overlap with those of I^2CNER. Kyushu University views this involvement as essential to the revitalization of its programs, because it brings faculty into the classroom who have international experiences with cutting-edge research.

I²CNER's Merit-based Salary System / KU's New Merit-based Annual Salary System
In view of the effectiveness of the I²CNER's Merit-based Salary System, Kyushu University adopted and introduced this system across all units. As of April 1, 2017, 339 Kyushu University faculty (16.4%) are 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
When inviting renowned researchers from overseas, I²CNER has established a practice of handling their travel expenses flexibly where appropriate. Beginning April 1, 2014, this became an approved/common practice across all units of Kyushu University.

Director as a Fukuoka City Ambassador
On February 24, 2016, Director Sofronis was appointed by the Mayor of the City of Fukuoka as a city Ambassador. His duties include the advancement of the international image of Fukuoka and the organization of international conferences in the city.

6-4. Support by Host Institution

The following two items concern the support that the host institution provides the Center, including those items of support that it committed to at the time of the initial project proposal submittal or in its revised commitment following the project's interim evaluation. Describe the functional measures that the host institution has taken to sustain and advance the Center's project.

6-4-1. Record of host institution support and its effects

・ In Appendix 5-1, describe the concrete measures being taken by the host institution.

I²CNER's Permanent Position within Kyushu University
Effective April 1, 2013, with the revision of the "Regulations of Kyushu University," I²CNER's position is clearly defined as a permanent Research Institute of Kyushu University without regard to the length of the WPI Program.

President Kubo's Vision Regarding Tenured Faculty and PIs
President Kubo envisions that by 2020, I²CNER will employ 20-25 PIs, including 10 tenured PIs organically in the Institute (3 to 4 of which will be non-Japanese). Following this vision, Kyushu University has allotted a total of more than 10 tenured faculty positions (Professor and Associate Professor level) to I²CNER. As of April 1, 2017, I²CNER has filled a total of 3 Associate Professor and 5 Full Professor positions, with 3.55 points (approximately 3 positions) left to fill in FY2017. Academic units of KU can obtain points for faculty hires through an annual internal competition.

With regard to the 10-15 PI positions which are not "tenured and organic in I²CNER," they will be filled through either: i) the Intra-University Transfer System (i.e., faculty transfer from other units of KU), ii) cross-appointments between I²CNER and other units of KU (e.g. economics, sciences, mathematics, life sciences, etc.), or iii) cross-appointments between I²CNER and its international partner institutes and industry.

IMI-I²CNER Tenure-Track Positions in Applied Math for Energy
The Institute of Mathematics-for-Industry (IMI) and I²CNER hired jointly 2 tenure-track assistant professors in Fall 2016 after submitting a joint proposal to KU's newly initiated tenure-track faculty program. These two faculty will work to foster the I²CNER applied math for energy research initiative and strengthen the ties and interaction between I²CNER and IMI.

6-4-2. Position of the Center within the host institution's mid-term plan

・ To Appendix 5-2, attach the cover sheets of the host institution's "Mid-term objectives" and/or "Mid-term plan" and parts of these documents related to the WPI Center.

Kyushu University's Mid-term Plan
I²CNER is at the center of Kyushu University's 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 (I^2CNER)."

Kyushu University Platform of Inter/Transdisciplinary Energy Research (Q-PIT)
In order to promote the concept of I^2CNER as the model project for internationalization of research and education in the University, and integrate research efforts and education on energy across its various units, KU established the "Kyushu University Platform of Inter/Transdisciplinary Energy Research (Q-PIT)" as of October 1, 2016. I^2CNER is expected to play a central role in this new organization by helping to catalyze and cross-pollinate 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 in areas of energy relating to social sciences, economics, law, and political sciences. Director Sofronis is a member of the Q-PIT strategic and faculty recruiting committees.

6-5. Others

Describe efforts advanced to foster young researchers (e.g., start-up funding, autonomous research environment) and to enlist female researchers.
・ In Appendix 5-3, give the transition in the number of female researchers.

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

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

Director's Discretionary Funding
The "I^2CNER Competitive Funding" initiative has mainly been used by young faculty and postdocs. In addition, the Director's discretional funds are also available to assist young faculty when need arises on matters such as travel, conference registration, etc.

General Start-up Research Funding
The amounts allocated to newly hired I^2CNER full-time researchers to develop their research environment are, 22 (FY 2011), 56 (FY 2012), 52 (FY 2013), 26 (FY 2014), 27 (FY 2015), and 29 (FY 2016) million JPY.

SRA Program
I^2CNER instituted the "Super Research Assistants (SRA)" Program in order to recruit and support excellent graduate students to carry out PhD thesis work under the supervision of our faculty within the various divisions of the Institute. These SRAs who are supported by the WPI fund are carefully selected from a large pool of KU graduates and are supervised by young faculty. This helps our young faculty develop educational and research supervision skills.

Skill Building Seminars for Young Researchers
In its early years and on a regular basis, the Institute holds special seminars by senior faculty to help young researchers improve their proposal-writing skills. In FY 2015 and 2016, such skill-building was administered on an individual basis. It is an established tradition in the Institute that I^2CNER's full-time researchers with a proven record of winning KAKENHI grants provide advice/consultation to young researchers. Lastly, on February 5, 2014, the Institute hosted a special seminar given by Dr. Vincent Dusastre, the Chief Editor of Nature Materials, on what it takes to write an article that can attract an editor's attention.

Efforts to Hire Female Researchers
It is a priority within the Institute to hire and retain excellent female researchers. The Director specifically reviews every female applicant for any postdoc or faculty position. As a result, the

number of female researchers in I^{2}CNER has been 4 (FY 2010), 7 (FY 2011), 9 (FY 2012), 12 (FY 2013), 11 (FY 2014), 11 (FY 2015), and 10 (FY 2016). These numbers, although not at the desired level, they are certainly larger than corresponding totals in the other sciences, math, and engineering units of KU. In addition, as recommended in the FY 2016 Follow-up and the Site Visit Reports, the Director has started a concentrated effort to make I^{2}CNER more attractive to female researchers. After attending a lecture entitled "Still Too Slow: the Advancement of Women" at Illinois by Virginia Valian, a distinguished professor at the Hunter College and CUNY Graduate Center on Sept. 7, 2016, where he learned some best practices for hiring female researchers, the Director has decided to require all members of the FRC to complete "unconscious bias training" in order to make our hiring process more inclusive of women. The Institute may also implement a required minimum number of female applicants in any given applicant pool before the hiring and interview process can proceed. Director Sofronis has also been working closely with PI Yamauchi to gather input as to what changes may make I^{2}CNER more attractive to female applicants. Our female PI, Prof. Miho Yamauchi, was hired through the Faculty Excellence Program, which expedites the normal hiring process for candidates with international acclaim and a proven record that they can bring about transformational change across division boundaries. Among the 13 newly hired faculty and postdocs in FY2016, 1 was a female Associate Professor and 2 were female postdocs. As of March 31, 2017, I^{2}CNER employs a total of 23 female researchers: 10 at KU, 6 at Illinois, and 7 at other international partner institutions.

7. Others

・In addition to the above 1-6 evaluation items, only if there is anything else that deserves mention regarding the center project's progress, please note it.

Internal Programs Review Committee (IPRC)

The Internal Programs Review Committee (IPRC) is an important standing committee of the Institute which is called by the Director whenever necessary to review individual programs within the Institute. The members of the IPRC and the Chair of the Committee are appointed by the Director. Once the review(s) are complete, the IPRC provides the Director with a written advisory report. The final decision about what action to take regarding any individual research program is the responsibility of the Director. In FY 2016, Professor Angus Rockett, Metallurgical and Materials Engineering Department Head at the Colorado School of Mines, joined the committee, bringing additional expertise in the area of photovoltaics and energy photoconversion. The rest of the committee members are: PIs Gewirth (UIUC), Christensen (Notre Dame), Ogo (KU), and Takata (KU). In FY2016, the IPRC completed a "deep dive" review of all individual research efforts in the Institute which resulted in individual feedback to researchers and related rebuttals, a review of each individual project of all divisions, assisted with the screening and progress reviews of the seed projects in applied math for energy, and reviewed the research plans of newly hired researchers.

NEXT-RP (Center for Next Generation Refrigerant Properties)

The Research Center for Next Generation Refrigerant Properties (NEXT-RP) was awarded to Profs. Y. Takata and S. Koyama at a level of 58 million JPY/year from FY 2016 to FY 2017 by the New Energy and Industrial Technology Development Organization (NEDO). This is a unique center throughout the world because it is a focused effort on behalf of NEDO to help coordinate the efforts of the international community toward the development of next generation refrigerants. More specifically, the objectives of the Center are: accurate evaluation of thermophysical properties and fundamental performance of heat exchange and air conditioning and refrigeration (ACR) cycles for zero-ODP (ozone depletion potential) and low-GWP (global warming potential) refrigerants; organize 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 I^{2}CNER researchers involved in the project are PI B.B. Saha and WPI Professor M. Kohno.

Asian Pacific Innovation Conference

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

8. Center's Response to Results of FY2016 Follow-up (including Site Visit Results)

* Describe the Center's Response to Results of FY2016 Follow-up. Note: If you have already provided this information, please indicate where in the report.

1. Feeding research outcomes back into society: There have been a number of technology transfers from I²CNER to various companies. The number of patent applications and patent awards is also significant. However, it seems that the center does not have a firm plan or strategy for feeding back its results to society in a more concerted way, so there is room for improvement.
   Please see the last paragraph of Section 3-1.

2. Interdisciplinary research: The research activities of the Energy Analysis Division (EAD) will require further collaboration, especially with economists, social scientists, government agencies and other stakeholders.
   As mentioned in Section 6-4, I²CNER is expected to play a central role in the newly established Q-PIT organization of KU, including the process of new faculty hiring. In close interaction with Q-PIT, I²CNER plans to capitalize on opportunities to broaden and enrich its energy portfolio in areas relating to social sciences, economics, law, and political sciences.
   Regarding the role of EAD for further collaboration, please look at the penultimate paragraph of Section 4-2.

3. Efforts toward Sustainability: More comprehensive planning is required, including the provision of administrative support, research infrastructure, and other financing.
   The establishment of Q-PIT by President Kubo provides I²CNER with the institutional setting to maintain and expand its momentum in energy research and education. More specifically, I²CNER now has state-of-the-art facilities (Section 2-2) for its research mission, a powerful support structure for PI and faculty staffing, such as cross-appointments, intra-university faculty transfer, etc. (Section 6-3), a large number of tenured faculty positions (Section 6-4-1), and an effective administrative support system (Section 5-3, 6-2).

4. Advice/Recommendations: It will be important to clearly identify which of the achievements of I²CNER can be considered truly significant and thereby determine which avenues of research should continue to be allocated the center's considerable resources.
   In this year's report, we summarized the significance of our research achievements by inserting statements into our report of the type "The estimated device lifetime of 4,000 hrs (Figure 2.1) is one of the longest ever reported," "to our knowledge, our work is the first direct comparison of measured activity across a spectrum of dopant species to computational predictions," "a finding that was previously not recognized," etc. Also, we have made an extra effort to stress the importance of our research results in Section 4-3. Lastly, an indirect indicator of the importance of our research results is their association with technology transfer, as described in the 2nd paragraph of Section 3-1.
   As stated in the beginning of Section 2-1, I²CNER's research achievements are all addressing milestones and targets in the project roadmaps that have been established through a close collaboration/interaction between the technical divisions and the EAD. In FY2017, the EAD will execute a comprehensive assessment of how I²CNER's current research results are impacting the deployment and penetration of the technologies related to I²CNER's roadmaps, including an evaluation of CO_2 emissions percent reduction and a comparison to the Institute's reduction target for 2050 of 70-80% compared to 1990 levels. This will make clear what new work will be required to meet the target and help I²CNER to focus on its most effective research efforts and redirect resources as needed.

5. Advice/Recommendations: The Internal Program Review Committee (IPRC) and Energy Analysis Division should continually monitor the overall direction of the Institute and the roadmap of each division.
The Internal Programs Review Committee (IPRC) is an important standing committee of the Institute and continuously helps the Director to review all division projects and all individual research efforts. It has been particularly active in FY2016 and its activities are described in detail in Section 7. The EAD is continuously interacting with the technical divisions for the continuous revision of all project roadmaps. The EAD has already started to execute an evaluation of the entire research portfolio of I^2CNER against the target for CO_2 emissions reduction as described in the response to Item 4 above.

6. Advice/Recommendations: To increase the number of female researchers, it is recommended that external advice be sought from women in senior positions of relevant fields.
Please see last Item in Section 6-5-1.

World Premier International Research Center Initiative (WPI)
Appendix 1-1 FY 2016 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 FY2016> Principal Investigators Total: 27

Name (Age)	Affiliation (Position title, department, organization)	Academic degree specialty	Working hours (Total working hours: 100%) Work on center project: Research activities	Work on center project: Other activities	Others: Research activities	Others: Other activities	Starting date of project participation	Status of project participation (Describe in concrete terms)	Contributions by PIs from overseas research institutions
Center director Petros Sofronis (59)	Prof., International Institute for Carbon-Neutral Energy Research, Kyushu University	Ph.D., Micromechanics of materials, Environmental degradation of materials	10%	80%	5%	5%	2010, Dec.1st	・Directs and Administers the Institute ・Travels to Kyushu University to participate in events and engage with researchers (50.9% time) ・Promotes I^2CNER’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.	・Manages and directs I^2CNER’s operations
Tatsumi Ishihara (55)	Prof., International Institute for Carbon-Neutral Energy Research, Kyushu University	Dr. of Eng., Catalyst and solid state electrochemistry	90%	10%	0%	0%	2010, Dec.1st	・Located at I^2CNER ・Participates in research/events as Associate Director, Lead PI of Molecular Photoconversion Devices Division	
Chihaya Adachi (53)	Prof., Department of Applied Chemistry, Kyushu University	Dr. of Eng., Materials science and device physics	60%	20%	10%	10%	2010, Dec.1st	・Located at I^2CNER ・Participates in research/events	
Atsushi Takahara (61)	Prof., Institute for Materials Chemistry and Engineering, Kyushu University	Dr. of Eng., Surface and Interface Characterization	60%	20%	10%	10%	2010, Dec.1st	・Located at I^2CNER ・Participates in research/events	
Seiji Ogo (53)	Prof., International Institute for Carbon-Neutral Energy Research, Kyushu University	Dr. of Science, Green Chemistry	90%	10%	0%	0%	2010, Dec.1st	・Located at I^2CNER ・Participates in research/events as Lead PI of Catalytic Materials Transformations Division	

Zenji Horita (63)	Prof., International Institute for Carbon-Neutral Energy Research, Kyushu University	Ph.D., Dr. of Eng., Materials Science	90%	10%	0%	0%	2010, Dec.1st	・Located at I^{2}CNER ・Participates in research/events	
Naotoshi Nakashima (65)	Prof., International Institute for Carbon-Neutral Energy Research, Kyushu University	Ph.D., Nanocarbon science, Supramolecular science	85%	15%	0%	0%	2010, Dec.1st	・Located at I^{2}CNER ・Participates in research/events	
Kazunari Sasaki (52)	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.1st	・Located at I^{2}CNER ・Participates in research/events	
Etsuo Akiba (65)	Prof., International Institute for Carbon-Neutral Energy Research, Kyushu University	Dr. of Science, Materials science	70%	30%	0%	0%	2010, Dec.1st	・Located at I^{2}CNER ・Participates in research/events as Lead PI of Hydrogen Storage Division	
Harry L. Tuller (71)	Prof., Department of Materials Science and Engineering, Massachusetts Institute of Technology, USA	Eng. Sc. D., Functional electroceramic materials	35%	5%	45%	15%	2010, Dec.1st	・Primarily located at partner institution ・Participates in research ・Visited I^{2}CNER for two weeks to participate in events and work on collaborative research projects ・Discussion via Internet	Hosts Assistant Professors and Postdocs from I^{2}CNER at MIT for mulitiple months per year
John A. Kilner (70)	Prof., Department of Materials, Imperial College, London, UK	Ph.D., Materials for solid oxide fuel cells and electrolysers	50%	5%	45%	0%	2010, Dec.1st	・Primarily located at partner institution ・Participates in research ・Visited I^{2}CNER for seven weeks to participate in events and work on collaborative projects ・Regular discussion via Internet	
Joichi Sugimura (59)	Prof., International Institute for Carbon-Neutral Energy Research, Kyushu University	Dr. of Eng., Tribology and Machine Design	70%	30%	0%	0%	2010, Dec.1st	・Located at I^{2}CNER ・Participates in research/events	
Yasuyuki Takata (60)	Prof., International Institute for Carbon-Neutral Energy Research, Kyushu University	Dr. of Eng., Thermal Engineering	70%	30%	0%	0%	2010, Dec.1st	・Located at I^{2}CNER ・Participates in research/events as Associate Director, Lead PI of Thermal Sciences and Engineering Division	

Xing Zhang (55)	Prof., Department of Engineering Mechanics, Tsinghua University, China	Ph.D., Thermal Science	10%	10%	45%	35%	2010, Dec.1st	・Primarily located at partner institution ・Participates in research/events ・Visited I²CNER for four weeks to participate in events and work on collaborative projects ・Discussion via Internet	
Brian P. Somerday (48)	Dr., South West Research Institute, USA	Ph.D., Materials Science and Engineering	15%	10%	45%	30%	2010, Dec.1st	・Primarily located at partner institution ・Participates in research as Lead PI of Hydrogen Materials Compatibility Division ・Visited I²CNER for four weeks to participate in events and work on collaborative projects ・Participates in meetings/events via videoconference system	
Setsuo Takaki (64)	Prof., International Institute for Carbon-Neutral Energy Research, Kyushu University	Dr. of Eng.	90%	10%	0%	0%	2011, Apr.1st* (*revised in the final version)	・Located at I²CNER ・Participates in research/events	
Reiner Kirchheim (73)	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, Apr.1st* (*revised in the final version)	・Primarily located at partner institution ・Participates in research ・Visited I²CNER for two weeks to participate in events and work on collaborative projects ・Discussion via Internet	
Miho Yamauchi (43)	Associate Prof.* (*revised in the final version), International Institute for Carbon-Neutral Energy Research, Kyushu University	Dr. of Science, Chemistry	100%	0%	0%	0%	2012, Jan.1st	・Located at I²CNER ・Participates in research/events	
Ken Sakai (55)	Prof., Department of Chemistry Faculty of Sciences, Kyushu University	Ph.D., Inorganic Chemistry	80%	10%	0%	10%	2012, Jan.16th	・Located at I²CNER ・Participates in research/events	
Ian Robertson (59)	Prof., Dean of Engineering, University of Wisconsin-Madison, USA	Ph.D., Metallurgy	10%	5%	25%	60%	2012, April.1st	・ Primarily located at partner institution ・ Participates in research/events as Chief Science Advisor to the Director ・ Visited I²CNER for two weeks to participate in events and work on collaborative projects ・ Discussion via Internet	

Andrew A. Gewirth (57)	Prof., Department of Chemistry, University of Illinois at Urbana Champaign, USA	Ph.D., Chemistry	20%	5%	60%	15%	2012, April.1st	・Primarily located at partner institution ・Participates in research ・Serves as a member of the Illinois Satellite Advisory Committee and IPRC ・Visited I^2CNER for two weeks to participate in events and work on collaborative projects ・Discussion via Internet	Hosts students, post-docs, & young faculty from I^2CNER at UIUC for long periods of stay
Kenneth T. Christensen (43)	Prof., Assistant Dean of Faculty Development, College of Engineering, University of Notre Dame, USA	Ph.D., Theoretical and Applied Mechanics specializing in experimental fluid mechanics	20%	5%	60%	15%	2012, April.1st	・Primarily located at partner institution ・Participates in Research ・Serves as a member of the Illinois Satellite Advisory Committee and IPRC ・Visited I^2CNER for one week to participate in events and work on collaborative projects ・Discussion via Internet	
Shigenori Fujikawa (46)	Associate Prof., International Institute for Carbon-Neutral Energy Research, Kyushu University	Dr. of Eng., Nanoscience and engineering	100%	0%	0%	0%	2013, June.1st	・Located at I^2CNER ・Participates in research/events as Lead PI of CO_2 Capture and Utilization Division	
Takeshi Tsuji (37)	Associate Prof., International Institute for Carbon-Neutral Energy Research, Kyushu University	Dr. of Science, Earth and Planetary Science, Resource engineering, Space exploration	85%	5%	0%	10%	2013, June.1st	・Located at I^2CNER ・Participates in research/events as Lead PI of CO_2 Storage Division	
Hiroshige Matsumoto (50)	Prof., International Institute for Carbon-Neutral Energy Research, Kyushu University	Dr. of Eng.	80%	20%	0%	0%	2010, Dec.1st	・Located at I^2CNER ・Participates in research/events as Lead PI of Electrochemical Energy Conversion Division	
Bidyut B. Saha (51)	Prof., International Institute for Carbon-Neutral Energy Research, Kyushu University	Dr. of Eng.	80%	15%	0%	5%	2010, Dec.1st	・Located at I^2CNER ・Participates in research/events	
Thomas Lippert (54)	Prof., Department of Chemistry and Applied Biosciences, Laboratory of Inorganic Chemistry, Swiss Federal Institute of Technolgy Zurich, and Paul Scherrer Institut, Thin Films & Interfaces Group, Villigen-PSI, Switzerland	Dr. of Science, Physical Chemistry	10%	15%	30%	45%	2016, Aug.1st	・Primarily located at partner institution ・Participates in research/events ・Visited I^2CNER for two weeks to participate in events and work on collaborative projects ・Discussion via Internet	

World Premier International Research Center Initiative (WPI)
Appendix 1-1 attachment
FY 2016 Biographical Sketch of a New Principal Investigator

Name (Age)	Thomas Lippert (54)
Current affiliation (Position title, department, organization)	Professor and Head of Group, Thin Films & Interfaces Group at Paul Scherrer Institut, and Laboratory of Inorganic Chemistry, ETH Zurich, Switzerland
Academic degree, specialty	Dr. of Science, Physical Chemistry

[Research and education history]

(Research)

2016-present Principal Investigator of the Molecular Photoconversion Devices Division, International Institute for Carbon-Neutral Energy Research, Kyushu University, Japan

2013-present Professor (titulary), Department of Chemistry and Applied Biosciences, Laboratory of Inorganic Chemistry, Swiss Federal Institute of Technolgy (ETH) Zurich, Switzerland

2013-present Member of the Paul Scherrer Institute (PSI) Research Committee, Switzerland

2005-present Laser Subject Matter Expert at PSI, Switzerland

2002-present Group leader of the Thin Films & Interfaces Group (formerly *Materials*) which (as of November 2014) consist of 1 senior scientist (senior lecturer), 1 scientist, 3 postdocs, and 6 PhD students (one with LEC) at the PSI, Switzerland.

2002-2012 Senior Lecturer (Privatdozent), ETH Zurich, Switzerland; Habilitation thesis in Physical Chemistry (2002)

1999-2001 Senior Scientist in the Materials Development and Characterization Group at the PSI, Switzerland.

1998-1999 Technical Staff Member (TSM) at Los Alamos National Laboratory, USA.

1995-1998 Director's Postdoctoral Fellow at Los Alamos National Laboratory, USA

1994-1995 Japan Science and Technology Agency (JST) / Alexander v. Humboldt (AvH) Postdoctoral Fellow: National Institute of Materials and Chemical Research (NIMC), Tsukuba, Japan.

1993-1994 Postdoctoral fellow: Wacker Chemistry, Burghausen.

(Education)

1993 Ph.D. in Chemistry, University of Bayreuth, Germany.

1990 Diploma (~MSc) in Chemistry, University of Bayreuth

1983-1990 Studies of Chemistry, University of Bayreuth

[Achievements and highlights of past research activities]

(Describe qualifications as a top-caliber researcher if he/she is considered to be ranked among the world's top researchers.)

- M. Pichler, H. Téllez, J. Druce, E. Fabbri, M. El Kazzi, M. Döbeli, A. Wokaun, D. Pergolesi, T. Lippert, *Oxynitride thin films as model systems for photocatalysis,* Adv. Funct. Mat., invited feature article, in press.

- W. Si, D. Pergolesi, F. Haydous, A. Wokaun, T. Lippert, *Understanding the behaviour of various co-catalysts on $LaTaON_2$ photoanode*, Phys. Chem. Chem. Phys. 19, 656 (2017).

- S. E. Temmel, E. Fabbri, D. Pergolesi, T. Lippert, T. J. Schmidt, *Investigating the Role of Strain towards the Oxygen Reduction Activity on Model Thin Film Pt Catalysts*, ACS Catal. 6, 7566 (2016).

- A. Palla Papavlu, T. Mattle, U. Lehmann, A. Hintennach, A. Grisel, S. Temmel, A. Wokaun, T. Lippert, *Highly sensitive SnO_2 sensor via reactive laser-induced transfer*, Sci. Rep 6, 25144 (2016).

- A. Fluri, D. Pergolesi, V. Roddatis, A. Wokaun, T. Lippert, *Stress observation in thin oxide films: tensile stress aids oxygen ion migration*, Nature Commun. 7:10692 (2016).

[Achievements]

(1) International influence

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

- 147 invited presentations (as presenting author).
- Over 220 talks or posters at international conferences (partly as co-author).

b) Holder of a prestigious lectureship,

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

- President of the Senate of the European-Materials Research Society (E-MRS) (from 1/2016 to 2/2017).
- President of the European-Materials Research Society (E-MRS) (from 1/2014 to 12/2015).
- Vice-President of the European-Materials Research Society (E-MRS) (from 6/2011 to 12/2013).
- Member of the E-MRS Executive Committee (from 2008).
- Member of the Program/Scientific Committee of > 55 international conferences.
- Member of the Nomination Committee for the *Kyoto Prize* and *Japan Prize* (both with ca. 420 kCHF as prize money).
- Co-chair of 9 international conferences/symposia (including General Co-chair of the E-MRS spring meetings in 2010 and 2012 with more than 2500 attendees, the MRS Fall Meeting in 2012 with over 6000 attendees, and of the COLA conference in 2007). Coming: COLA conference in 09/2017 in Marseille France.
- Evaluation committee member or expert for:
  a. SNF (Swiss National Science Foundation).
  b. ESF (European Science Foundation).
  c. NSF (National Science Foundation, USA).
  d. NSERC (Natural Sciences and Engineering Research Council of Canada).
  e. RPF (Research Promotion Foundation, Cyprus).
  f. Czech Academy of Science.
  g. Czech Science Foundation.
  h. DFG (German Research Foundation)-"Schwerpunktprogramm" and "Forschung."
  i. AERES (agence d'évaluation de la recherche et de l'enseignement supérieu) France.
  j. FONDECYT (National Commission for Scientific & Technological Research), Chile.
  k. Romanian National University Research Council (CNCSIS).
  l. Luxembourg National Research Fund (FNR).

m. US-DOE (Department of Energy, USA), proposal and project.
n. ANR (French National Research Agency).
o. Danish Council for Strategic Research (DSF).
p. National Council for Research and Development for Partnership Programme - Joint Applied Research Projects, Romania.
q. EU-FP7 Research Projects.
r. Aristeia Research Programme for Research and Technology of Greece.
s. Technology Foundation STW of The Netherlands.
t. UEFISCIDI, Romania-declined, second time accepted
u. Macquarie University Fellowships, Australia
v. A*star, Singapore.
w. OKTA-EPR, Hungarian Scientific Research Fund, Hungary, declined, twice.
x. Croatian Science Foundation, declined.
y. EU research projects or Marie Curie Action (declined several times).
z. EU, Laserlab (Integrated Initiative, 7th framework program), several times.
aa. ISL (Israel Science Foundation).

d) Recipient of an international award(s) ,

2014 Dr. *honoris causa,* University of Bucharest, Romania.

e) Editor of an influential journal etc.

2017-present Editor-in-Chief of *Applied Physics A: Materials Science & Processing.*
2016-present Editorial Board of *npj 2D Materials and Applications,* (npj = Nature Partner Journals).
2012-2016 Editor of *Applied Surface Science.*
2008-2014 Editorial Board of *Materials.*
2006-2013 Co-Editor of *Journal of Laser Micro/Nanoengineering* .
2006-2011 Associate Editor of *Laser Chemistry.*

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

Swiss National Science Foundation (SNF):

- **<u>Current project</u>** (with N. Marzari) *Theory and experiment synergy for artificial photosynthesis* within the SNF National Centre of Competence in Research (NCCR) MARVEL (Materials' Revolution: Computational Design and Discovery of Novel Materials) (from 07/2015 for 2 years, 212 kCHF)
- **<u>Current project</u>** (with N. Marzari)**:** *The search for low temperature super protonic conductivity* (from 09/2015 for 3 years, 448 kCHF).
- Previous project (with J. Rupp)**:** *Influence of Strain and Interfaces on the Properties of Ion Conducting Thin Films for micro-Solid-Oxide-Fuel-Cells* (from 08/2013 for 3.5 years, 420 kCHF).
- Previous project (with PI Alexander Wokaun)**:** *Positive or negative? Selecting the charge state of ions during pulsed laser deposition of thin films* (from 04/2011 for 3 years, 260 kCHF).
- Previous project (with M. Dinescu, Romania)**:** *Small band-gap nanostructured perovskite materials for photovoltaic and photocatalytic hydrogen generation applications* (from 01/2013 for 3 years, 328 kCHF)

CRUS.CH (Rektorenkonferenz der Schweizer Universitäten): Scientific Exchange Programme-NMS (Sciex-NMS)

- Previous project (with A. Palla-Papavlu): *Application of laser-induced forward transfer for the fabrication of a flexible carbon nanotube sensor array-ALECSA* (from 2/2013 for 1 year, 100 kCHF).
- Previous project (with M. Filipescu): *NANO-Sens: Laser Printing of nanocomposite chemiresistors* (from 9/2014 for 6 month, 50 kCHF).

Kommission für Technologie und Innovation (KTI):

- Previous project**:** *Processing of low power integrated gas sensors with functionalized carbon nanotubes as sensitive layers deposited by a laser based technique* (start 5/2015, for 18 months 210 kCHF).

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

1. T. Lippert*, J. T. Dickinson, *Chemical and spectroscopic aspects of polymer ablation- special features and novel directions*, invited review, Chem. Rev. 103, 453 (2003).
   Cited 221
2. T. Lippert*, *Laser Applications of Polymers*, chapter in *Polymers and Light*, Ed. T. Lippert, Springer: Adv. Polym. Sci. 168, 51-246 (2004).
   Cited 99
3. V.-M. Graubner, R. Jordan, O. Nuyken, B. Schnyder, T. Lippert*, R. Kötz, A. Wokaun, *Photochemical modification of crosslinked poly(dimethylsiloxane) by irradiation at 172 nm,* Macromolecules 37, 5936 (2004).
   Cited 92
4. B. Schnyder, T. Lippert, R. Koetz, A. Wokaun, V.-M. Graubner, O. Nuyken, *UV-irradiation induced modification of PDMS films investigated by XPS and spectroscopic ellipsometry*, Surf. Sci. 532-535, 1067 (2003).
   Cited 92
5. Doraiswamy, R. Narayan, T. Lippert, L. Urech, A. Wokaun, M. Nagel, B. Hopp, M. Dinescu, R. Modi, R. Auyeung, D. Chrisey, *Excimer Laser Forward Transfer of Mammalian Cells using a Novel Triazene Absorbing Layer*, Appl. Surf. Sci. 252, 4743 (2006).
   Cited 89
6. R. Fardel, M. Nagel, F. Nüesch, T. Lippert*, A. Wokaun, *Fabrication of organic light-emitting diode pixels by laser-assisted forward transfer*, Appl. Phys. Lett. 91, 061103 (2007).
   Cited 87
7. R. Phipps, M. Birkan, W. Bohn, H.-A. Eckel, H. Horisawa, T. Lippert, M. Michaelis, Yu. Rezunkov, A. Sasoh, W. Schall, S. Scharring, J. Sinko, *Laser ablation propulsion,* J. Prop. Power 26, 609 (2010).
   Cited 79
8. T. Lippert*, *Interaction of Photons with Polymers: From Surface Modification to Ablation*, invited review for Plasma Process. Polym. 2, 525 (2005).
   Cited 75
9. R. Stöckle, P. Setz, V. Deckert, T. Lippert, A. Wokaun, R. Zenobi, *Nanoscale atmospheric pressure laser ablation- mass spectrometry,* Anal. Chem. 73, 1399 (2001).
   Cited 70
10. T. Lippert, A. Wokaun, J. Stebani, O. Nuyken, J. Ihlemann, *Excimer laser ablation of novel triazene polymers-influence of the structure on ablation characterics*, J. Phys. Chem. 97, 12297 (1993).
    Cited 66
11. G. Kopitkovas, T. Lippert*, C. David, A. Wokaun, J. Gobrecht, *Fabrication of Microoptical Elements in Quartz by Laser Induced Backside Wet Etching*, Microelectron. Eng. 67-68, 438 (2003).
    Cited 65
12. G. Kopitkovas, T. Lippert*, C. David, A. Wokaun, J. Gobrecht, *Surface Micromachining UV-transparent Materials,* Thin Solid Films, 453-454, 31 (2004).
    Cited 56
13. Weidenkaff, S. G. Ebbinghaus, T. Lippert, *$Ln_{1-x}A_xCoO_3$ (Ln = Er, La) (A= Ca, Sr) / carbon nanotube*

composite materials applied for rechargeable Zn/air batteries, Chem. Mat. 14, 1797 (2002).
Cited 55

14. L. S. Bennett, T. Lippert, H. Furutani, H. Fukumura, H. Masuhara, *Laser induced microexplosion of a photosensitive polymer,* Appl. Phys. A 63, 327 (1996).
Cited 55
15. M. Nagel, R. Hany, D. Rentsch, M. Molberg, F. Nüesch, T. Lippert, *Aryltriazene Photopolymers for UV-Laser Applications: Improved Synthesis and Photodecomposition Study,* Macromol. Chem. Phys. 208, 277 (2007).
Cited 54
16. T. Lippert*, M. Hauer, C. Phipps, A. Wokaun, *Fundamentals and applications of polymers designed for laser ablation,* Appl. Phys. A 77, 259 (2003).
Cited 53
17. H. Furutani, H. Fukumura, H. Masuhara, T. Lippert, A. Yabe, *Laser-induced decomposition and abaltion dynamics studied by nanosecond interferometry (I) a triazenopolymer film,* J. Phys. Chem. A 101, 5742 (1997).
Cited 53
18. H. V. Brand, R. L. Rabie, D. J. Funk, I. Diaz-Acosta, P. Pulay, T. Lippert, *Theoretical and experimental study of the vibrational spectra of the* α, β, *and* δ *phases of octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX),*J. Phys. Chem. B 106, 10594 (2002).
Cited 52
19. U. Gurudas, D. M. Bubb, S. Heiroth, T. Lippert, A. Wokaun, *Saturable and reverse saturable absorption in silver nanodots at 532 nm using picoseconds laser pulses*, J. Appl. Phys. 104, 073107 (2008).
Cited 51
20. T. Lippert, R. Webb, S. C. Langford, J. T. Dickinson, *Dopant induced ablation of PMMA at 308 nm,* J. Appl. Phys. 85, 1838 (1999).
Cited 49
21. S. Heiroth, R. Frison, J. L. M. Rupp, T. Lippert*, E. Barthazy, E. Müller, M. Döbeli, K. Conder, A. Wokaun, L. J. Gauckler, *Crystallization and grain growth characteristics of yttria-stabilized zirconia thin films grown by pulsed laser deposition*, Solid State Ionics 191, 12 (2011).
Cited 48
22. T. Lippert*, A. Yabe and A. Wokaun, *Laser ablation of doped polymer systems,* review article, Adv. Mater. 9, 105 (1997).
Cited 48
23. S. Heiroth, R. Ghisleni, T. Lippert*, A. Wokaun, J. Michler, *Optical and mechanical properties of amorphous and crystalline YSZ coatings prepared by pulsed laser deposition,* Act. Mat. 59, 2330 (2011).
Cited 47
24. R. Fardel, M. Nagel, T. Lippert*, F. Nüesch, A. Wokaun, *Laser forward transfer using a sacrificial layer: influence of the material properties*, Appl. Surf. Sci. 254, 1322 (2007).
Cited 47
25. F. Raimondi, S. Abolhassani, R. Brütsch, F. Geiger, T. Lippert*, J. Wambach, J. Wei, A. Wokaun, *Quantification of Polyimide Carbonization after Laser Ablation,* J. Appl. Phys. 88, 3659 (2000).
Cited 47
26. G. Kopitkovas, S. Canulescu, C. David, J. Gobrecht, T. Lippert*, A. Wokaun, *Fabrication of micro-optical elements in UV-transparent materia*ls, J. Photochem. Photobiol. A Chem. 166, 135 (2004).
Cited 45
27. T. Lippert, A. Wokaun, J. Stebani, O. Nuyken, J. Ihlemann, *Dopant induced ablation of PMMA at 308nm, influence of the molecular weight of PMMA and the photochemical activity of added chromophors,* Angew. Makromol. Chem. 213, 127 (1993).
Cited 45
28. T. Lippert, A. Wokaun, J. Stebani, O. Nuyken, J. Ihlemann, *Triazene polymers designed for excimer laser ablation*, Angew. Makromol. Chem. 206, 97 (1993).
Cited 45
29. W. Schneider, M. Esposito, I. Marozau, K. Conder, M. Doebel[1], Y. Hu, M. Mallepell, A. Wokaun, T. Lippert *, *The origin of oxygen in oxide thin films - role of the substrate,* Appl. Phys. Lett. 97, 192107 (2010).

Cited 44

30. Weidenkaff, R. Robert, M. Aguirre, L. Bocher, T. Lippert, S. Canulescu, *Development of thermoelectric oxides for renewable energy conversion technologies*, Renewable Energy 33, 342 (2008).
Cited 44
31. S. Heiroth, T. Lippert*, A. Wokaun, M. Döbeli, J. L. M. Rupp, B. Scherrer, L. J. Gauckler, *Yttria-stabilized zirconia films by laser ablation: microstructural and compositional control,* J. Europ. Ceram. Soc. 30, 489 (2010).
Cited 43
32. R. Phipps, J. R. Luke, T. Lippert, M. Hauer, A. Wokaun, *Micropropulsion Using a Laser Ablation Jet*, J. Prop. Power 20, 1000 (2004).
Cited 43
33. T. Lippert, A. Wokaun, D. Lenoir, *Surface reactions of brominated arenes as a model for the formation of chlorinated dibenzodioxins and -furans in incineration. Inhibition by ethanolamine*, Environ. Sci. Technol. 25, 1485 (1991).
Cited 43
34. J. Xu, J. Liu, D. Cui, M. Gerhold, A. Y. Wang, M. Nagel, T. Lippert, *Laser-assisted forward transfer of multi-spectral nanocrystal quantum dot emitters,* Nanotechnology 18, 025403 (2007).
Cited 42
35. J. Stebani, O. Nuyken, T. Lippert, A. Wokaun, *Preparation of novel triazene polymers*, Makromol. Chem. Rapid Commun. 14, 365 (1993).
Cited 42
36. J. Wei, T. Lippert*, N. Hoogen, O. Nuyken, A. Wokaun, *Novel laser ablation resists for excimer laser ablation lithography. Influence of photochemical properties on ablation,* J. Phys. Chem. B 105, 1267 (2001).
Cited 37
37. E. Ortelli, F. Geiger, T. Lippert*, J. Wei, A. Wokaun, *UV-laser induced decomposition of Kapton: an ex-situ Infrared Spectroscopy Study*- Macromolecules 33, 5090 (2000).
Cited 37
38. R. Phipps, J. Luke, D. Funk, D. Moore, J. Glownia, T. Lippert, *Laser Impulse Coupling at 130 fs*, Appl. Surf. Sci. 252, 4834 (2006).
Cited 36
39. T. Lippert*, C. David, M. Hauer, T. Masubuchi, H. Masuhara, O. Nuyken, C. Phipps, J. Robert, T. Tada, K. Tomita, A. Wokaun, *Novel applications for laser ablation of photopolymers,* invited paper for special issue of Appl. Surf. Sci. 186, 14 (2002).
Cited 36
40. M. Hauer, D. J. Funk, T. Lippert*, A. Wokaun, *Time Resolved Study of the Laser Ablation Induced Shockwave,* Thin Solid Films, 453-454, 584 (2004).
Cited 35
41. R. Phipps, J. R. Luke, G. G. McDuff, T. Lippert, *Laser-driven micro-rocket*, Appl. Phys. A 77, 193 (2003).
Cited 34
42. T. Lippert*, D. J. Funk, Th. Gerber, M. Goto, H. Fukumura, A. Wokaun, *Single pulse nm-size grating formation in polymers using UV laser ablation,* Appl. Phys. Lett. 75, 1018 (1999).
Cited 34
43. K. Kaur, R. Fardel, T.C. May-Smith, M. Nagel, D.P. Banks, C. Grivas, T. Lippert, R.W. Eason, *Shadowgraphic studies of triazene assisted laser-induced forward transfer of ceramic thin films*, J. Appl. Phys. 105, 113119 (2009).
Cited 33
44. S. Heiroth, Th. Lippert*, A. Wokaun, M. Döbeli, *Microstructure and electrical conductivity of YSZ thin films prepared by pulsed laser deposition*, Appl. Phys. A 93, 639 (2008).
Cited 33
45. R. Phipps, J. R. Luke, T. Lippert, *Laser Ablation of Organic Coatings as a basis for Micropropulsion*, Thin Solid Films, 453-454, 573 (2004).
Cited 32
46. V.-M. Graubner, M. Hauer, R. Jordan, T. Lippert*, O. Nuyken, B. Schnyder, A. Wokaun, *Incubation and ablation behaviour of polydimethylsiloxane for 266 nm irradiation,* Appl. Surf. Sci. 197-198, 786 (2002).

Cited 32

47. T. Lippert*, L. S. Bennett, T. Nakamura, H. Niino, A. Ouchi, A. Yabe, *Comparison of the transmission behavior of a triazeno-polymer with a theoretical model,* Appl. Phys. A 63, 257 (1996).
Cited 32
48. R. Fardel, M. Nagel, F. Nüesch, T. Lippert*, A. Wokaun, *Laser-induced forward transfer of organic LED building blocks studied by time-resolved shadowgraphy*, J. Phys. Chem. C 114, 5617 (2010).
Cited 31
49. David, J. Wei, T. Lippert, A. Wokaun, *Diffractive grey-tone phase masks for laser ablation lithography,* Microelectron. Eng. 57-58, 453 (2001).
Cited 31
50. F. Zimmermann, T. Lippert, C. Beyer, A. Wokaun, *N=N vibrations frequencies and fragmentation patterns of substituted 1-aryl-3,3-dialkyltriazenes- Comparison with other high nitrogen compounds*, Appl. Spectrosc. 47, 986 (1993).
Cited 31

Career Summary:

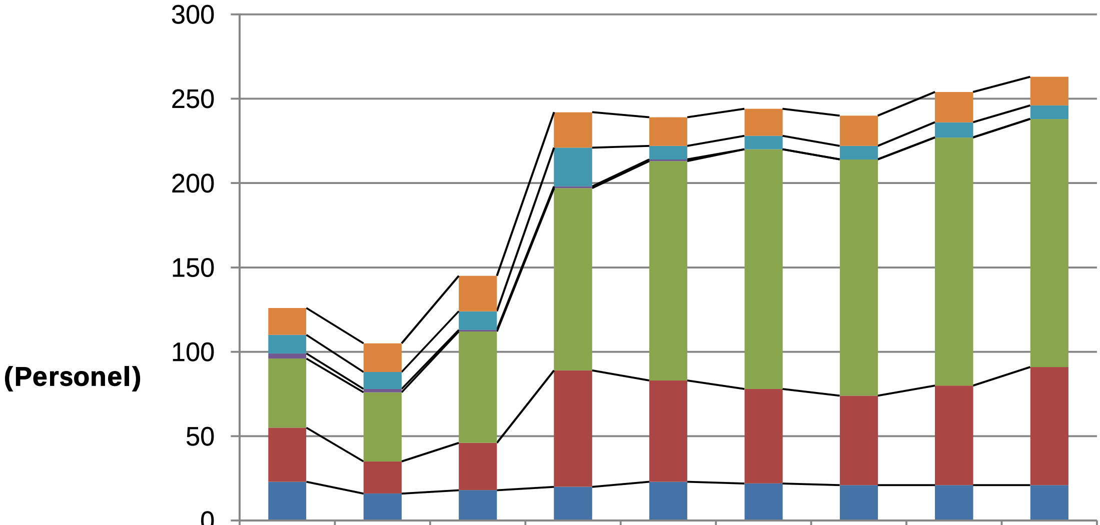
Total Number of Citations:	**5012**
Total Number of Papers:	**245**
Average Citations per Item:	**20**
h-index:	**37**

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

World Premier International Research Center Initiative (WPI)
Appendix 1-2 Annual Transition in the Number of Center Personnel

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

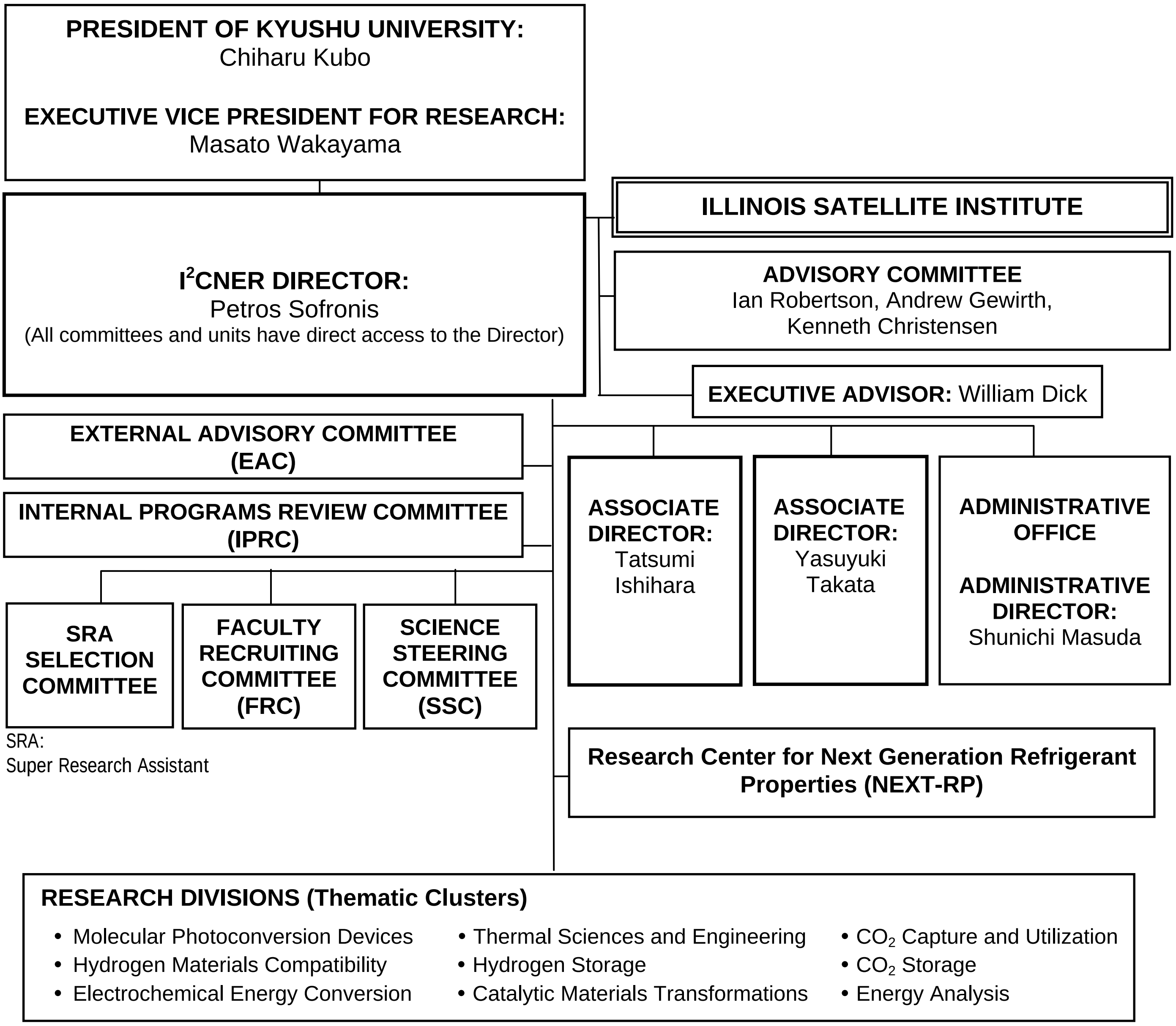
Number of Center Personnel



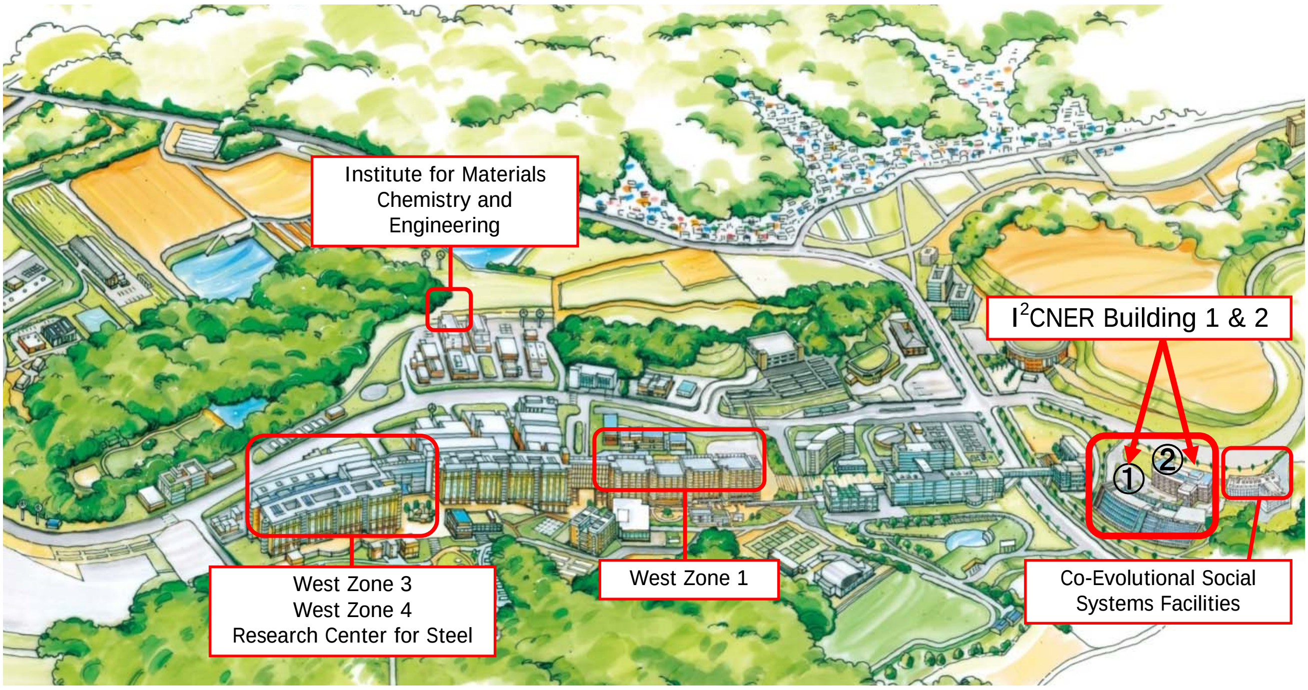
	(At beginning)	FY2010	FY2011	FY2012	FY2013	FY2014	FY2015	FY2016	(Final goal) FY 2020
PI：Researchers from within host institution	16	17	21	21	17	16	18	18	17
PI：Foreign researchers invited from abroad	11	10	11	23	8	8	8	9	8
PI：Researchers invited from other Japanese institutions	3	2	1	1	1	0	0	0	0
Other researchers	41	41	66	108	130	142	140	147	147
Research support staffs	32	19	28	69	60	56	53	59	70
Administrative staffs	23	16	18	20	23	22	21	21	21

World Premier International Research Center Initiative (WPI)
Appendix 1-3 Diagram of Management System

I^2CNER ORGANIZATIONAL STRUCTURE
(As of March 31, 2017)



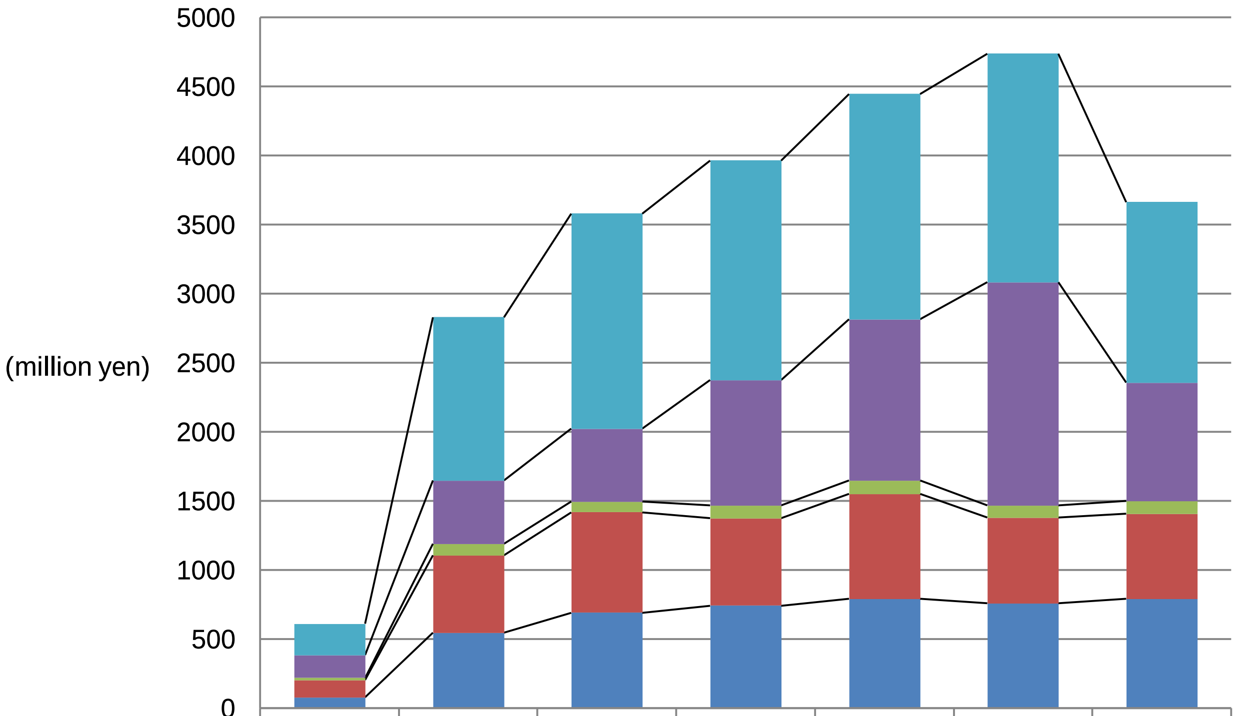
World Premier International Research Center Initiative (WPI)
Appendix 1-4　Campus Map



World Premier International Research Center Initiative (WPI)
Appendix 1-5 Annual Transition in the Amounts of Project Funding

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

Amounts of Project Funding



	FY2010	FY2011	FY2012	FY2013	FY2014	FY2015	FY2016
Research projects	230	1184	1561	1593	1630	1655	1310
Equipment	163	458	527	907	1170	1619	858
Travel	18	84	77	92	95	87	91
Project activities	121	559	726	631	759	618	614
Personnel	81	547	693	744	793	761	793

World Premier International Research Center Initiative (WPI)

Appendix 1-6 FY2016 Project Expenditures

1) Overall Project Funding

(Million Yen)

Cost Items	Details	Costs
Personnel	Center director and Administrative director	21
	Principal investigators (no. of persons):17	237
	Other researchers (no. of persons):80	363
	Research support staff (no. of persons):29	67
	Administrative staff (no. of persons):27	105
	Total	793
Project activities	Gratuities and honoraria paid to invited principal investigators (no. of persons):76	7
	Cost of dispatching scientists (no. of persons):0	0
	Research startup cost (no. of persons):33	46
	Cost of satellite organizations (no. of satellite organizations):1	183
	Cost of international symposiums (no. of symposiums):1	4
	Rental fees for facilities	254
	Cost of consumables	30
	Cost of utilities	33
	Other costs	57
	Total	614
Travel	Domestic travel costs	15
	Overseas travel costs	50
	Travel and accommodations cost for invited scientists (no. of domestic scientists):58 (no. of overseas scientists):59	22
	Travel cost for scientists on secondment (no. of domestic scientists):2 (no. of overseas scientists):7	4
	Total	91
Equipment	Depreciation of buildings	81
	Depreciation of equipment	777
	Total	858
Other research projects	Projects supported by other government subsidies, etc.	154
	Commissioned research projects, etc.	938
	Grants-in-Aid for Scientific Research, etc.	218
	Total	1,310
Total		3,666

(Million Yen)

WPI grant	1,245
Costs of establishing and maintaining facilities	1
Establishing new facilities (0m²)	0
Repairing facilities (Building 2) (5,000m²)	1
Others	0
Cost of equipment procured	280
(CD spectrometer) No. of units:1	15
(High-Performance Computing Cluster) No. of units:1	16
Others	249

2) Costs of Satellites and Partner Institutions

(Million Yen)

Cost Items	Details	Costs
Personnel	Principal investigators (no. of persons):2	
	Other researchers (no. of persons):8	
	Research support staff (no. of persons):20	
	Administrative staff	
	Total	114
Project activities		49
Travel		16
Equipment		4
Other research projects		0
Total		183

World Premier International Research Center Initiative (WPI)

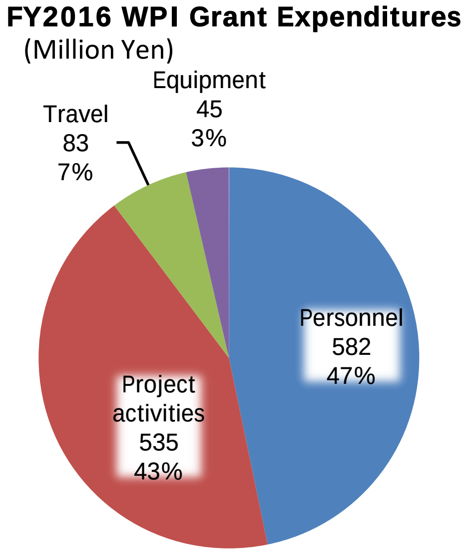
Appendix 1-7 FY2016 WPI Grant Expenditures

1) Overall Expenditures

* Describe a circle graph for cost items.

(Million Yen)

Cost Items	Details	Costs
Personnel	Center director and Administrative director	21
	Principal investigators (14)	195
	Other researchers (47)	247
	Research support staff (29)	67
	Administrative staff (18)	52
	Total	582
Project activities	Gratuities and honoraria paid to invited principal investigators (75)	7
	Cost of dispatching scientists (0)	0
	Research startup cost (33)	29
	Cost of satellite organizations (1)	183
	Cost of international symposiums (1)	4
	Rental fees for facilities	254
	Cost of consumables	21
	Cost of utilities	6
	Other costs	31
	Total	535
Travel	Domestic travel costs	12
	Overseas travel costs	47
	Travel and accommodations cost for invited scientists (domestic scientists: 53) (overseas scientists: 52)	20
	Travel cost for scientists on secondment (domestic scientists: 2) (overseas scientists: 7)	4
	Total	83
Equipment	Cost of equipment procured	45
	Total	45
Total		1,245



2) Costs of Satellites and Partner Institutions

Cost Items	Details	Costs (Million Yen)
Personnel	Principal investigators (2)	
	Other researchers (8)	
	Research support staff (20)	
	Administrative staff	
	Total	114
Project activities		49
Travel		16
Equipment		4
Total		183

World Premier International Research Center Initiative (WPI) Appendix 2-1 List of Papers Underscoring Each Research Achievement

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

1) Extended stability in hybrid perovskite photovoltaics (PI Adachi)

1. C. Qin, T. Matsushima, T. Fujihara, W.J. Potscavage, C. Adachi (2016) Degradation Mechanisms of Solution-Processed Planar Perovskite Solar Cells: Thermally Stimulated Current Measurement for Analysis of Carrier Traps, *Advanced Materials*, 28(3), 466-471.

Organic-inorganic perovskite materials are very promising as light absorbers in solar cells because of their efficient solar power conversion (a certified efficiency surpassing 20%) along with excellent film processability. However, the long-term stability of perovskite solar cells is still problematic and needs to be improved. In this paper, we found that degradation of perovskite solar cells occurs by the formation of carrier traps in the perovskite film and that the source of carrier traps is metallic lead generated by decomposition of the perovskite compound in the presence of water and oxygen under solar irradiation. We reduced the content of oxygen and water into the perovskite solar cells by fabricating the perovskite films in a high purity nitrogen atmosphere, enhancing lifetime (LT-80) to around 570 h by a factor of 2.5 compared with perovskite solar cells fabricated in air.

2. C. Qin, T. Matsushima, T. Fujihara, C. Adachi (2017) Multifunctional benzoquinone additive for efficient and stable planar perovskite solar cells, *Advanced Materials*, 29(4), 1603808.

Although we could improve the stability by fabricating the perovskite solar cells in nitrogen as mentioned in paper 1 the perovskite solar cells fabricated in nitrogen and degraded under continuous solar irradiation still contain a small amount of metallic lead. Therefore, we introduced benzoquinone (BQ) into a precursor solution used for fabrication of the perovskite films. This suppresses the formation of metallic lead, and improves device stability. The estimated device lifetime reached 4,000 h, one of the longest ever reported.

2) Visualization of the active site of a photocatalyst (PI Ishihara)

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

In many systems designed for photocatalytic water splitting, the hydrogen evolution half-reaction exhibits slow kinetics and can often be the limiting factor to good performance. To overcome this limitation, it is common to include "co-catalysts"—typically metallic nanoparticle clusters—to accelerate the reaction. However, the working mechanism of a co-catalyst and the minimum particle size has not been well-understood in the past. In this paper, a combined experimental and computational effort was able to show that single atomic sites can effectively serve as co-catalysts to promote hydrogen evolution in rhodium-doped titania nanosheets. Atomic scale visualization through high-resolution electron microscopy demonstrated the incorporation of the dopants into the two-dimensional nanosheet, and the hydrogen production rate for optimally doped systems was found to increase by a factor of ten over undoped systems. Corresponding first-principles simulations and modelling show that the presence of the dopants can reduce the thermodynamic energy barrier for molecular water adsorption, believed to be rate-limiting. The work carried out gives new clear fundamental insights to the working mechanism of co-catalytic species and will be useful in the continued design and development of photocatalytic water splitting.

3) Activation of TiFe by HPT for hydrogen storage (PIs Akiba and Horita)

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

This is the first report on the activation of TiFe, which normally needs conditions above 673K and over 30 bar hydrogen atmosphere to start hydrogenation, using the high pressure torsion (HPT) method. TiFe is one of the promising candidates for stationary hydrogen storage but it has not been applied because of difficulty in activation. This paper suggests the research direction to solve the problem.

*5. K. Edalati, H. Shao, H. Emami, H. Iwaoka, Z. Horita, E. Akiba (2016) Activation of titanium-vanadium alloy for hydrogen storage by introduction of nanograins and edge dislocations using high-pressure torsion, *International Journal of Hydrogen Energy*, 41(21), 8917-8924.

Ti-V binary alloys are the model alloy of Ti-based multi-element body-centered cubic hydrogen storage alloys, which are one set of the candidates for on-board hydrogen storage for fuel cell vehicles. The authors applied the high-pressure torsion (HPT) method to the Ti-V model alloy and investigated the behaviors of initial activation of the alloy. They found that grains and edge dislocations play an important role for easy activation of the alloys. The authors applied the HPT method to various hydrogen storage materials and reported defects introduced by the HPT method are effective to improve reaction kinetics of hydrogen and materials.

*6. T. Hongo, K. Edalati, M. Arita, J. Matsuda, E. Akiba, Z. Horita (2015) Significance of grain boundaries and stacking faults on hydrogen storage properties of Mg_2Ni intermetallics processed by high-pressure torsion, *Acta Materialia*, 92, 46-54.

Mg_2Ni can accommodate hydrogen up to 4 wt %, but its reaction rate needs improvement before it can be used in most hydrogen storage applications. In particular, the kinetics of hydrogen release are very slow. This paper shows importance of the role of defects such as grain boundaries and stacking faults generated by the high-pressure torsion method in the acceleration of the hydrogen release reaction rate.

4) A functional [NiFe]hydrogenase mimic that catalyzes electron and hydride transfer from H2 (PI Ogo)

*7. S. Ogo, K. Ichikawa, T. Kishima, T. Matsumoto, H. Nakai, K. Kusaka, T. Ohhara (2013) A Functional [NiFe]Hydrogenase Mimic That Catalyzes Electron and Hydride Transfer from H_2, *Science,* 339(6120), 682-684.

This paper reports the first evidence of hydrogen activation utilizing a functional [NiFe]-based model complex inspired by natural [NiFe]-hydrogenase. This complex heterolytically activates hydrogen to form a hydride complex that is capable of reducing substrates by an electron transfer or a reaction with a hydride. These results will help accelerate hydrogen fuel cell technology, involving the research theme of division "H_2-catalyst for low cost and highly efficient practical application."

5) A high-valent iron(IV) peroxo core derived from O2 (PI Ogo)

*8. T. Kishima, T. Matsumoto, H. Nakai, S. Hayami, T. Ohta, S. Ogo (2016) A High-Valent Iron(IV) Peroxo Core Derived from O_2, *Angewandte Chemie International Edition*, 55(2), 724–727.

Together with the previous studies of the first functional biomimetic iron-nickel hydrogen-splitting catalyst reported in paper 4, we worked on producing a catalyst for the complementary oxygen-splitting cathode side of the cell. The catalyst for O_2-activation is a model for studying O_2-tolerant [NiFe]-hydrogenases. This result is the benchmark of the first biomimetic model catalyst of O_2-tolerant [NiFe]-hydrogenase, forming the first example of a side-on iron (IV) peroxo complex.

*9. T. Matsumoto, T. Ando, Y. Mori, T. Yatabe, H. Nakai, S. Ogo (2015) A $(Ni\text{-}SIr)_I$ Model for [NiFe]hydrogenase, *Journal of Organometallic Chemistry*, 796(1), 73-76.

Understanding the reaction mechanism of O_2-activation is very important in the industrial chemical process and also in fuel cell technology to develop an O_2-reduction cathode catalyst. This study is the first example of the development of O_2 activation using the organic metal complex, elucidating the reaction mechanisms of O_2-activation. The complex can be easily modulated by changing the coordinated metal ligand, resulting in the synthesis of new efficient catalysts.

6) CO2-free electric power circulation via direct charge and discharge using the glycolic acid/oxalic acid redox couple (PI Yamauchi)

*10. R. Watanabe, M. Yamauchi, M. Sadakiyo, R. Abe, T. Takeguchi (2015) CO_2-free electric power circulation via direct charge and discharge using the glycolic acid/oxalic acid redox couple, *Energy & Environmental Science*, 8(5), 1456-1462.

Efficient electronic power storage and distribution are indispensable for the realization of sustainable society driven by renewable energy. This paper describes the first ever reported of an electric power circulation method that does not emit CO_2 and is based on the glycolic acid (GC)/oxalic acid (OX) redox couple.

7) Fundamental understanding of coalescence-induced droplet jumping (PI Takata)

*11. H. Cha, C. Xu, J. Sotelo, J.M. Chun, Y. Yokoyama, R. Enright, N. Miljkovic (2016) Coalescence-Induced Nanodroplet Jumping, *Physical Review Fluids*, 1, 064102.

This paper was the first study to experimentally show and theoretically explain the coalescence induced droplet jumping of nanodroplets. This is important because prior to this work, previous studies had shown that the minimum droplet departure size was 10 microns, which was accepted by the community as the theoretical minimum. The efficiency of droplet jumping is directly related to the size of departing droplets, with smaller jumping droplets having greater performance. The experimental and theoretical elucidation that nanodroplet jumping is indeed possible and the surface structure design guidelines developed to achieve nanodroplet jumping are very important for the enhancement of condensation heat transfer, anti-icing, self-cleaning, and anti-microbial performance.

*12. J. Oh, P. Birbarah, T. Foulkes, S.L. Yin, M. Rentauskas, J. Neely, R.C.N. Pilawa-Podgurski, N. Miljkovic (2017) Jumping-Droplet Electronics Hot-Spot Cooling, *Applied Physics Letters*, 110, 123017.

This paper was the first demonstration of active jumping droplet electronics hot spot cooling. The use of electric field condensation was instrumental to achieve for the first time active thermal routing and temperature equalization of a multi Gallium Nitride semiconductor device, allowing us to achieve the highest power densities ever recorded in academia (290 W/cm^3). This paper is very important not only due to its broad implementation potential as a next generation thermal management schemes in future high power density ultra-efficient power electronics applications (>98%), but also for the enabling of thermal routing and thermal diode technologies, which have been difficult to achieve to date.

*13. H. Cha, J.M. Chun, J. Sotelo, N. Miljkovic (2016) Focal Plane Shift Imaging for the Analysis of Dynamic Wetting Processes, *ACS NANO*, 10(9), 8223–8232.

This paper details the development of a single-camera technique capable of providing 3D information on droplet-surface interactions through the use of focal plane manipulation (FPSI). This is an important development because up until this study, obtaining accurate 3D analysis for the study of droplet-surface interactions was not possible. The FPSI technique developed here overcomes prior limitations and has broad implications in the utilization for the study of sprays, droplets, and droplet-surface interactions. As a technique, the powerful FPSI technique is to the study of liquid-droplet interactions as confocal microscopy is to optical microscopy

8) Development of novel functionalized adsorbents for HVAC applications (PI Saha)

*14. I.I. El-Sharkawy, K. Uddin, T. Miyazaki, B.B. Saha, S. Koyama, J. Miyawaki, S.H. Yoon (2014) Adsorption of ethanol onto parent and surface treated activated carbon powders, *International Journal of Heat and Mass Transfer*, 73, 445-455.

The discovery of super-efficient new adsorbents for ethanol uptake is reported and proved that surface properties of adsorbents can be fine-tuned for improved sorption performance. The concept is demonstrated using three activated carbon samples with different oxygen contents for ethanol uptake where the strong interaction between the hydroxyl group of ethanol molecules and the oxygen-containing surface functional group is ingeniously exploited. The results provided new research dimension and possibilities of controlling surface properties of activated carbons toward significant improvement of adsorption heat pump performance.

*15. K. Uddin, I.I. El-Sharkawy, T. Miyazaki, B.B. Saha, S. Koyama, H.S. Kil, J. Miyawaki, S.H. Yoon (2014) Adsorption characteristics of ethanol onto functional activated carbons with controlled oxygen content, *Applied Thermal Engineering*, 72, 211-218.

The equilibrium characteristics of three samples with different oxygen content were analyzed in detail. Adsorption isotherm equations for the three samples were made by approximation of measured data. In addition, the heat of adsorption was evaluated by using the isotherm equations, and it was represented as a function of adsorption uptake for the three samples. The data obtained by the analysis were fundamentals of adsorption heat pump design.

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

The development of the adsorbent with record-breaking sorption uptake is reported in this article. The new activated carbon was synthesized from spherical phenol resin with the high specific surface area of

~3,000 m^2/g where a slightly larger pore width of 1.6 nm in average is designed in contrast to a conventional activated carbon with 1.1 nm. With tailor-made pore level design, the new adsorbent sets the current record for ethanol uptake.

9) Air electrodes in high temperature electrochemical devices: An atomistic study of composition and mechanisms (PI Kilner)

*17. J. Druce, H. Tellez, M. Burriel, M.D. Sharp, L.J. Fawcett, S.N. Cook, D.S. McPhail, T. Ishihara, H.H. Brongersma, J.A. Kilner (2014) Surface termination and subsurface restructuring of perovskite-based solid oxide electrode materials, *Energy & Environmental Science*, 7(11), 3593-3599.

Degradation processes in high temperature electrochemical devices for energy conversion and storage present a substantial hurdle to their commercialization. One major source of degradation is the deterioration of oxygen exchange properties of the catalytically active transition metal containing complex oxides used as air electrodes. This paper reported on an international collaborative investigation, using the novel technique of Low Energy Ion Scattering, capable of detecting the outermost atomic composition of these ceramic materials, and showed that contrary to expectations, after exposure to simulated operational conditions, there is a surprising absence of the catalytically active transition metals, previously thought to be the active sites for oxygen exchange. The study went on to show how quickly and comprehensively the surfaces can be further degraded by the segregation of the additives used to promote mixed ionic electronic conductivity, such a Sr, leading to a SrO dominated surface. This paper was the first to show the detailed changes in the outermost surface chemistry of the air electrodes under operating conditions and thus provide strategies for ameliorating degradation.

*18. T. Akbay, A. Staykov, J. Druce, H. Tellez, T. Ishihara, J.A. Kilner (2016) The interaction of molecular oxygen on LaO terminated surfaces of La2NiO4, *Journal of Materials Chemistry A*, 4(34), 13113-13124.

In this paper, our multidisciplinary team investigated the surface of some newer, additive free, transition metal complex oxides that were known to be active for surface oxygen exchange but puzzlingly did not show the presence of oxygen vacancies. These materials have similar transition metal free surfaces under operating conditions; a typical example is the LaO surface. By using similar methods to those in our earlier papers [17,19], the team was able to show that, unlike the SrO surface, the LaO surface is active for oxygen exchange: an entirely new concept that runs contrary to the accepted view that the La cation is catalytically inert. This finding has provided the key to understanding many previous experimental results and has spawned a series of investigations of the catalytic role of the large rare earth atoms in oxide materials.

*19. A. Staykov, H. Tellez, T. Akbay, J. Druce, T. Ishihara, J. Kilner (2015) Oxygen Activation and Dissociation on Transition Metal Free Perovskite Surfaces, *Chemistry of Materials*, 27(24), 8273-8281.

The recognition that air electrode materials with the common additive Sr give an effectively SrO dominated surface at device operating temperatures led to the investigation of the interaction of molecular oxygen gas with this surface in a model air electrode material. An interdisciplinary and cross-divisional team was formed to perform theoretical calculations, with experimental back-up, based on first principle quantum mechanical methods, on surfaces found in operational air electrodes. These showed that the SrO surface was present in the model system and was essentially inactive to the exchange of oxygen with the molecules in the gas, validating the earlier finding that Sr segregation is detrimental to air electrode performance. Further calculations answered a very long-standing question as to what are the active sites for oxygen exchange in these materials by showing that locations missing oxygen atoms in the SrO surface layer (surface oxygen vacancies) are highly active for the exchange process, and thereby provided insight suitable for further optimization of performance.

10) Novel electrocatalyst based on polymer-wrapping of carbon nanotubes (PI Nakashima)

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

This paper summarized the advancement of our unique polymer-wrapped approach for the development of the PEFC electrocatalyst materials. This method has attracted strong attention, since it allow us to use carbon nanotubes as supporting materials for Pt nanoparticle without oxidizing the nanotube surface, which results in a highly durable polymer electrolyte fuel cell.

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

Reports, 3, 1764.

Improvement of the durability of the polymer electrolyte fuel cell (PEFC) above 100 ºC is one of the targets of the fuel cell industry. This paper reported the most durable PEFC at 120 ºC under non-humidified condition (single cell test: >500,000 cycles), in which the carbon nanotube (CNT) was used as the catalyst supporting material instead of conventional carbon black. The key was to use CNTs without oxidizing the surface prior to Pt loading using our polymer-wrapping approach, in which polybenzimidazole (PBI) was used to functionalize the surface of CNTs for Pt loading.

*22. Z. Yang, I. Moriguchi, N. Nakashima (2015) Durable Pt Electrocatalyst Supported on a 3D Nanoporous Carbon Shows High Performance in a High-Temperature Polymer Electrolyte Fuel Cell, *ACS Applied Materials & Interfaces,* 7(18), 9800-9806.

This paper is the first report describing the use of 3D nanoporous carbon for polymer electrolyte fuel cell (PEFC) cathode, in which the polymer-wrapping approach was used to immobilize the Pt nanoparticle onto the 3D nanoporous carbon. By applying the polymer-wrapping approach to the 3D nanoporous carbon, low cost and durable PEFC cathode electrocatalyst was fabricated.

11) Intermediate temperature steam electrolysis (PI Matsumoto)

*23. Y. Okuyama, K. Isa, Y.S. Lee, T. Sakai, H. Matsumoto (2015) Incorporation and Conduction of Proton in $SrCe_{0.9-x}Zr_xY_{0.1}O_{3-\delta}$, *Solid State Ionics*, 275, 35-38.

This paper deals with the proton conductivity of strontium-based zirconate-cerate solid solution that is the key material for intermediate solid oxide cells. We found so far that x being 0.5, corresponding to Zr/Ce fraction to be 5/4, is the best for the proton conductivity. This paper elucidated why this composition has the best performance, concluding that the hydration of oxide ion vacancy is almost fully complete at this composition.

*24. K. Leonard, Y.S. Lee, Y. Okuyama, K. Miyazaki, H. Matsumoto (2017) Influence of dopant levels on the hydration properties of SZCY and BZCY proton conducting ceramics for hydrogen production, *International Journal of Hydrogen Energy*, 42(7), 3926-3937.

This paper deals with barium-based proton conductor and demonstrated high proton conductivity, which is the highest level of proton conductivities reported so far and is higher than any other solid electrolyte at temperatures of 500 °C or lower. The magic fraction of Zr/Ce=5/4 does work for Ba-based composition and lower grain-boundary resistivity was found to bring us such a high proton conductivity.

*25. Y. Matsuzaki, Y. Tachikawa, T. Somekawa, T. Hatae, H. Matsumoto, S. Taniguchi, K. Sasaki (2015) Effect of proton-conduction in electrolyte on electric efficiency of multi-stage solid oxide fuel cells, *Scientific Reports*, 5, 12640.

The use of proton conductors as the electrolyte for solid oxide cells is advantageous in comparison with oxide-ion conductors not only by the opportunity of lowering operation temperature but also by changing the electrode reaction and, therefore, relying on a different mass transport process. This paper elucidated quantitatively that the choice of proton conductor increases the hydrogen fuel cell efficiency by about 10% from that of oxide-ion-conductor-based fuel cell, due to essential avoidance of fuel dilution.

12) Inertial effects in liquid CO2-water flow behavior for CO2 storage (PI Christensen)

*26. F. Kazemifar, G. Blois, D.C. Kyritsis, K.T. Christensen (2016) Quantifying the flow dynamics of supercritical CO_2–water displacement in a 2D porous micromodel using fluorescent microscopy and microscopic PIV, *Advances in Water Resources*, 95, 352-368.

This work represents the first quantitative study of liquid CO_2-water flow in a porous micromodel at reservoir-relevant conditions. This work clarified the importance of inertial forces during CO_2 bursts through the rock and also the occurrence of flow within trapped water ganglia that could promote enhanced dissolution of CO_2 into the resident brine. Thus, pore-scale models of liquid CO_2 migration must be modified to account for such dynamic flow processes that can greatly alter macroscale migration of CO_2 in geologic reservoirs.

*27. Y. Li, F. Kazemifar, G. Blois, K.T. Christensen (2017) Micro-PIV measurements of multiphase flow of water and liquid/supercritical CO_2 in 2D heterogeneous porous micromodels, *Water Resources Research*, submitted.

This work represents the first quantitative study of liquid CO_2-water flow in a heterogeneous micromodel whose pore structure was generated from reservoir sandstone. These experiments confirmed the cooperative nature of CO_2 displacement of water in real rock, with correlated flow occurring across large neighborhoods of pores, in contrast to most pore-scale models that assume pore-filling events are uncorrelated from pore to pore. Furthermore, this work confirmed the occurrence of dynamic CO_2 bursts through the pore structure at speeds well above that for which inertial effects can be safely ignored.

*28. Y. Chen, A. Valocchi, Y. Li, K.T. Christensen (2017) Comparison of the Lattice Boltzmann simulation and experiment of pore-scale flow interactions between water and supercritical CO_2 in 2D heterogeneous micromodels at reservoir conditions, *Journal of Contaminant Hydrology*, submitted.

This study involved careful comparison of lattice Boltzmann simulations of liquid CO_2-water flow in a heterogeneous porous micromodel inspired by real reservoir roach with experiments at reservoir conditions. Strong qualitative agreement in liquid CO_2 invasion patterns between simulation and experiment were observed; however, the formation of secondary CO_2 pathways observed in the experiments was not observed in the simulations. Further investigation revealed that enhanced viscosity of the fluids in the simulations to enhance numerical stability (though correct viscosity ratio between the phases) suppressed inertial forces and thus the formation of these secondary CO_2 pathways. Thus, this work confirms that it is not sufficient to match the viscosity ratio and capillary number of the flow of liquid CO_2 and water (a common assumption in both simulations and experiments), rather the absolute magnitudes of these viscosities must be matched.

13) Develop continuous and accurate monitoring system for injected CO_2 (PI Tsuji)

*29. T. Tsuji, T. Ikeda, T.A. Johansen, B.O. Ruud (2016) Using seismic noise derived from fluid injection well for continuous reservoir monitoring, *Interpretation*, 4(4), SQ1-SQ11.

We developed a monitoring method to estimate the temporal variation of seismic velocity using ambient noise which overcomes limitations in current methods related to high cost and difficulties to continuously monitor the injected CO_2. Since this method constructs virtual source signals from ambient noise, we can conduct a time-lapse survey and extract subsurface information using only passive seismometer data. The low cost of this approach makes it particularly attractive for long-term monitoring of geologic CO_2 storage and it is being applied to seismometer data acquired during CO_2 injection.

*30. T. Ikeda, T. Tsuji, T. Watanabe, K. Yamaoka (2016) 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.

We developed a novel seismic monitoring system that, unlike existing systems, can detect leaked CO_2 using a continuous and controlled seismic source device under the support of the Ministry of Environment. Our field experiments show that hourly-variation of seismic velocity can be monitored with better than 1% accuracy. This temporal stability has possibility to detect changes in seismic velocities associated with CO_2 leakage through fault zones. This is the first continuous seismic monitoring system of CO_2 leakage.

*31. T. Ikeda, T. Tsuji, M. Takanashi, I. Kurosawa, M. Nakatsukasa, A. Kato, K. Worth, D. White, B. Roberts (2017) Temporal variation of the shallow subsurface in the Aquistore CO_2 storage site associated with environmental influences using a continuous and controlled seismic source, *Journal of Geophysical Research: Solid Earth*, 122, doi:10.1002/2016JB013691.

We developed a novel monitoring system based on a continuous and controlled seismic source that is cost-effective, with high temporal resolution and high accuracy to monitor geologically-stored CO_2. We applied this monitoring technique in the ongoing CCS project in Saskatchewan, Canada, and clearly found seasonal variation (i.e., freezing of formation water) in shallow sediments which decrease the monitoring accuracy in deep CO_2 injection reservoirs. Therefore, our monitoring system contributes to accurate monitoring of injected CO_2 by considering the influence of shallow seismic velocity variation, which is not feasible in existing monitoring systems.

14) A novel approach for CO_2 capture through nanometer membranes (PI Fijikawa)

*32. S. Fujikawa, M. Ariyoshi, E. Shigyo, C. Fukakusa, R. Selyanchin, T. Kunitake (2017) Preferential CO_2 separation over nitrogen by a free-standing and nanometer-thick membrane, *Energy Procedia*, accepted.

The reported free-standing membranes comprised of polymeric materials exhibit preferential CO_2 separation over N_2, despite having a thickness of less than 100 nm (no serious defects or pin-holes). To the best of our knowledge, this is the first example of gas separation by a free-standing nanomembrane with the thickness of a few tens of nanometers.

15) Bimetallic Cu-Pd catalyst with different mixing patterns for the electroreduction of CO2 (PI Yamauchi)

*33. S. Ma, M. Sadakiyo, M. Heima, R. Luo, R.T. Haasch, J.I. Gold, M., Yamauchi, P.J.A. Kenis, (2017) Electroreduction of carbon dioxide to hydrocarbons using bimetallic Cu-Pd catalysts with different mixing patterns, *Journal of the American Chemical Society*, 139, 47–50.

This paper presents a novel approach to developing electroreduction catalysts with high hydrocarbon selectivity. Nanoengineering of Cu-Pd bimetallic particles allows tuning of the selectivity, and produces higher selectivities than possible with simple copper systems. A new insight is presented that geometric effects in the particles are more important than electronic effects. This can potentially be leveraged into other bimetallic systems. This paper combines materials chemistry, electrochemistry, analytical chemistry, and chemical engineering.

16) Next-generation high-strength, low-cost alloy for hydrogen service (PI Takaki)

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

This article demonstrates that grain refining is an excellent method to obtain high yield strength and retain acceptable ductility (elongation > 30%) in stainless steel after hydrogen exposure. One unique result is that the mechanism of hydrogen-induced degradation depends on grain size: with hydrogen exposure, larger-grain stainless steel shows intergranular fracture, while finer-grain stainless steel shows only ductile fracture. The technological implication of these results is that ultra-fine grain (UFG) stainless steels are attractive alternatives to the benchmark (i.e. SUS316 stainless steel), since cost savings can be realized without compromising hydrogen compatibility.

*35. A. Macadre, K. Tsuboi, N. Nakada, T. Tsuchiyama, S. Takaki (2014) Ultra-Grain Refinement Effect on Tensile and Phase Transformation Behaviour in a Metastable Austenitic Steel Charged in Hydrogen Gas, *Procedia Materials Science*, 3, 350-356.

Producing ultra-fine grain (UFG) stainless steels relies on the tendency of these materials to form strain-induced martensite, which can also have adverse effects on hydrogen compatibility. One significant outcome from this study was to demonstrate that grain size and low hydrogen (~25 wppm) contents have no effect on strain-induced martensite formation, thus the UFG process does not compromise hydrogen compatibility. Demonstrating the hydrogen compatibility of UFG stainless steels is essential to promoting these alloys as alternatives to the benchmark (i.e. SUS316 stainless steel).

17) Mechanism of fretting fatigue in hydrogen (PI Somerday)

36. M. Kubota, K. Kuwada, Y. Tanaka, Y. Kondo (2011) Mechanism of Reduction of Fretting Fatigue Limit Caused by Hydrogen Gas in SUS304 Austenitic Stainless Steel, *Tribology International*, 44, 1495-1502.

This is the first report on the fretting fatigue in hydrogen gas aimed to contribute to the development of hydrogen energy systems. This paper clearly shows that fretting fatigue is one of the most important issues in the design of hydrogen energy systems in terms of safety, because the fretting fatigue strength of an austenitic stainless steel was significantly reduced in hydrogen gas. The mechanism that caused the reduction in the fretting fatigue strength was clarified based on the detailed observation of phenomena at the contacting surfaces. In particular, adhesion between contacting surfaces was promoted in hydrogen gas, and it resulted in nucleation of small cracks.

*37. R. Komoda, M. Kubota, J. Furtado (2015) Effect of Addition of Oxygen and Water Vapor on Fretting Fatigue Properties of an Austenitic Stainless Steel in Hydrogen, *International Journal of Hydrogen Energy*, 40, 16868-16877.

A significant reduction in the fretting fatigue strength of an austenitic stainless steel was caused by addition of water vapor and ppm-level oxygen as impurities to hydrogen gas. These first-time experimental results were only possible because a unique system enabling controlled ppm-level oxygen contents in hydrogen gas was developed. These unexpected results were attributed to the repeated abrasion and reforming of the surface oxide layer, which led to fretting wear and associated stress conditions that drove crack initiation on the specimen surface. The observation that trace oxygen concentrations can exacerbate the detrimental effect of hydrogen on fretting fatigue strength has technological implications, since ppm-level oxygen impurities are expected in hydrogen gas for the consumer market.

18) Hydrogen station deployment (Energy Analysis Division)

*38. K. Itaoka, K. Hirose, S. Kimura, Y. Kikuchi, T. Higuma, K. Honda, K. Simokawa (2017) Basic research on development of hydrogen supply facilities (research on deployment of new hydrogen stations), submitted to Ministry of Economy, Trade and Industry Japan through the Next Generation Vehicle Promotion Center in February 2017, 73 pp., contract file number 28-0366.

This report analyzed optimum geographical deployment of new hydrogen stations using mathematical model and large computing power finding a gap between the existing and planned stations and the suggested station sites of the stations from the analysis. This report is important in terms of policy influence of I2CNER's research because the research was supported by the Ministry of Economy, Trade and Industry (METI) and the results were directly reported to the METI and shared with hydrogen station stakeholders including energy companies and automobile companies, consequently influencing hydrogen deployment policy and planning in Japan.

19) Applied math analysis of social systems (New initiative by Prof. Murata)

39. M. Murakami, R. Funaki, T. Matsumura, J. Murata (2016) Modeling of consumer behaviors and incentive design in demand response programs, *Symposium on Systems and Information*, Otsu City, Shiga Prefecture, Japan, Dec. 6-8, 2016, Technical Division of Systems and Information, Society of Instrument and Control Engineers, Paper No. GS01-13.

An incentive design method was developed for incentive-based demand response programs that are used to change electrical power consumption behaviors of consumers. A type of consumer model was proposed which is the first one that considers the dynamical changes in consumer behaviors. Unlike other studies on demand response programs that primarily rely on empirical data and observations, this study uses a mathematical technique, inverse optimization, with theoretical proofs to determine appropriate incentive schema. The study, however, does not deny or contradict the empirical studies, but gives theoretical foundations for them.

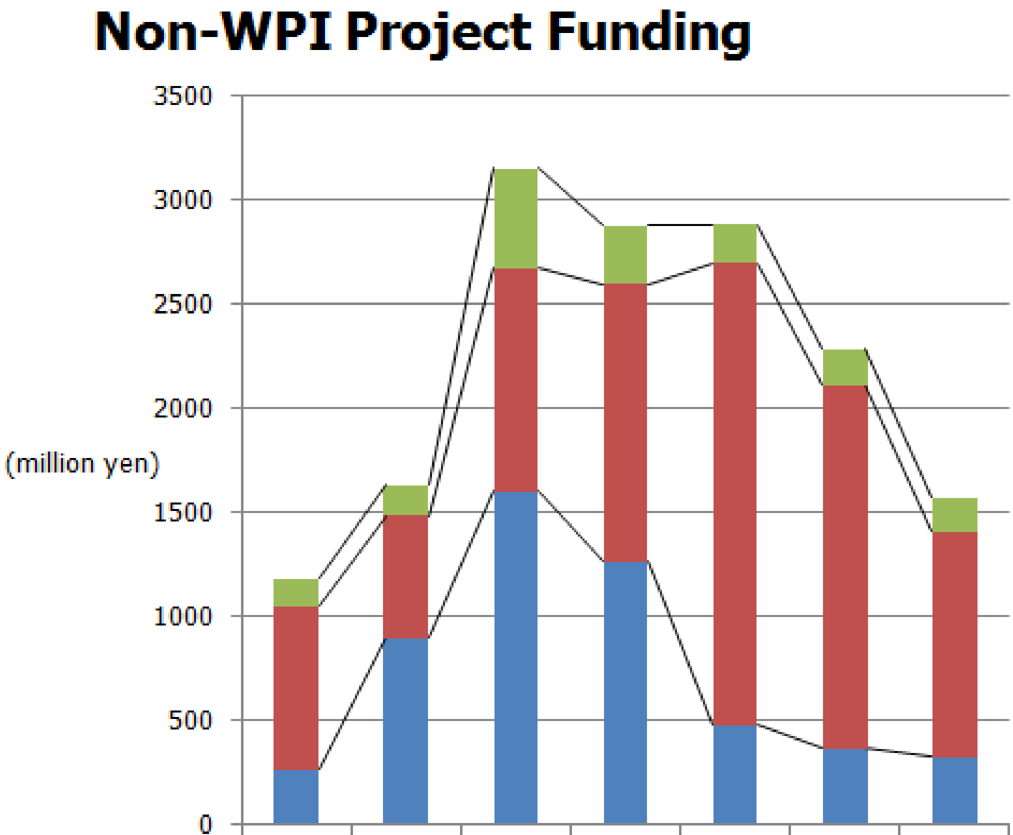
20) Applied math analysis of geomaterials (New initiative by Prof. Shirai and PI Tsuji)

*40. T. Tsuji, F. Jiang, A. Suzuki, T. Shirai (2017) Mathematical modeling of rock pore geometry and mineralization: Applications of persistent homology and random walk, *In: Agriculture as a metaphor for creativity in all human endeavors, Proceedings of Forum Math-for-Industry 2016*, Queensland University of Technology, Brisbane, Australia, Eds. B. Anderssen, Y. Fukumoto, M. Simpson, I. Turner, Springer 2017.

Mathematical methods used to model heterogeneous pore geometry of natural rocks and their temporal evolution (mineralization) are explored. Using persistent homology, we successfully characterized rock pore features for estimation of their hydraulic properties. We further applied random walk to model rock mineralization processes, and successfully calculated temporal variation of hydraulic properties due to rock mineralization. The mineralization parameter in random walk can be flexibly changed and a short computation time. Thus, this approach is practical when simulating rock evolution processes such as long-term chemical reactions.

World Premier International Research Center Initiative (WPI)
Appendix 2-2 Annual Transition in Non-WPI Project Funding (Grants)

*Make a graph of the annual transition in non-WPI project funding (grants). Describe external funding warranting special mention.



	FY2010	FY2011	FY2012	FY2013	FY2014	FY2015	FY2016
Projects supported by other government subsidies, etc.	131	150	480	276	184	173	164
Commissioned research projects, etc.	788	585	1077	1340	2217	1743	1084
Grants-in-Aid for Scientific Research, etc.	267	901	1599	1261	483	371	327

[External funding warranting special mention]

- Funding Program for World-Leading Innovative R&D on Science and Technology (from JSPS) FY2010: 648,397,800 JPY (acquired by Chihaya Adachi)
- Funding Program for World-Leading Innovative R&D on Science and Technology (from JSPS) FY2011: 654,296,000 JPY (acquired by Chihaya Adachi)
- Fundamental Research Project on Advanced Hydrogen Science (from NEDO) FY2011: 265,454,000 JPY (acquired by Saburo Matsuoka)
- Funding Program for World-Leading Innovative R&D on Science and Technology (from JSPS) FY2012: 761,772,570 JPY (acquired by Chihaya Adachi)
- Fundamental Research Project on Advanced Hydrogen Science (from NEDO) FY2012:

381,004,000 JPY (acquired by Saburo Matsuoka)

- Installation Project for Base as a Mediator of Technology (from METI) FY2012:
  717,659,000 JPY (Including KU budget of 239,220,000 JPY) (acquired by Kazunari Sasaki)
- Funding Program for World-Leading Innovative R&D on Science and Technology (from JSPS) FY2013:
  112,273,000 JPY (acquired by Chihaya Adachi)
- Installation Project for International Scientific Innovative Base (from MEXT) FY2013:
  704,958,503 JPY (acquired by Chihaya Adachi)
- R&D Project on Useful Technology of Hydrogen (from NEDO) FY2013:
  382,612,000 JPY (acquired by Joichi Sugimura)
- R&D Project on Useful Technology of Hydrogen (from NEDO) FY2014:
  828,346,000 JPY (acquired by Joichi Sugimura)
- ERATO, Exploratory Research for Advanced Technology (from JST) FY2014:
  253,800,000 JPY (acquired by Chihaya Adachi)
- KAKENHI Specially Promoted Research (from JSPS) FY2014:
  174,800,000 JPY (acquired by Seiji Ogo)
- The Center of Innovation (COI) Program (from MEXT) FY2014:
  126,960,000 JPY (acquired by Kazunari Sasaki)
- CREST, Core Research for Evolutionary Science and Technology (from JST) FY2012-15:
  94,959,000 JPY (acquired by Miho Yamauchi)
- R&D Project on Useful Technology of Hydrogen (from NEDO) FY2015:
  393,537,000 JPY (acquired by Joichi Sugimura)
- ERATO, Exploratory Research for Advanced Technology (from JST) FY2015:
  228,996,000 JPY (acquired by Chihaya Adachi)
- KAKENHI Specially Promoted Research (from JSPS) FY2015:
  117,300,000 JPY (acquired by Seiji Ogo)
- Demonstration Research on a Hydrogen-based Society through Collaboration among Industry, University, Government and Local Community (from MEXT) FY2015:
  108,542,000 JPY (acquired by Kazunari Sasaki)
- CREST, Core Research for Evolutionary Science and Technology (from JST) FY2015-FY2016:
  29,650,000 JPY (acquired by Miho Yamauchi)
  **Amount requested in the proposal (ACCEPTED): 180,000,000 JPY for FY2015-2019*
- Development of Small and Medium-sized Air-conditioning Equipment with High Efficiency, Low GWP Refrigerants (from NEDO) FY2016:
  44,936,560 JPY (acquired by Shigeru Koyama)

- ERATO, Exploratory Research for Advanced Technology (from JST) FY2016:
  214,373,700 JPY (acquired by Chihaya Adachi)
- Demonstration Research on a Hydrogen-based Society through Collaboration among Industry, University, Government and Local Community (from MEXT) FY2016:
  107,131,000 JPY (acquired by Kazunari Sasaki)

World Premier International Research Center Initiative (WPI)
Appendix 2-3
Major Awards, Invited Lectures, Plenary Addresses (etc.) (within 2 pages)

1. Major Awards

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

1) Reiner Kirchheim, Foreign affiliate of the United States National Academy of Engineering, 2017
2) Tatsumi Ishihara, John A Kilner, Helena Tellez-Lozano, Aleksandar T. Staykov, Daiwa Adrian Prize, 2016.
3) Atsushi Takahara, Fellow, The Royal Society of Chemistry, 2016
4) John A Kilner, Imperial College Medal, 2016
5) Naotoshi Nakashima, The Commendation for Science and Technology by MEXT, 2016
6) Helena Tellez-Lozano, 9th Shiseido Female Researcher Grant Award, 2016
7) Harry L. Tuller, Distinguished Life Membership in American Ceramic Society, 2016
8) Takeshi Tsuji, The Young Scientists' Prize by MEXT, 2016
9) Yasunori Kikuchi, The Society of Chemical Engineers, JP Award for Outstanding Young Researcher, 2016
10) Zenji Horita, Medal of Honor with Purple Ribbon, Government of Japan, 2015
11) Shigenori Fujikawa, The Nanotechnology Prize by ISIT, 2015
12) Toyoki Kunitake, The Kyoto Prize, 2015
13) Takeshi Tsuji, Ozawa Yoshiaki Award, 2015
14) Ian Robertson, 2014 Edward DeMille Campbell Memorial Lecture ASM International, 2015
15) Toyoki Kunitake, Order of Culture, 2014
16) Hellena Téllez-Lozano, John Druce, Ju, Y.-W., Tatsumi Ishihara, and John Kilner, Christian Friedrich Schonbein Contribution to Science Medal, 2014
17) Brian Somerday, DOE Hydrogen and Fuel Cells Program Achievement Award, 2014
18) Harry Tuller, Fellow, Electrochemical Society, 2014
19) Robert O. Ritchie, David Turnbull Award by Materials Research Society, 2013
20) Atsushi Takahara, The Society of Rheology, Japan Award, 2013
21) Seiji Ogo, The Commendation for Science and Technology by MEXT, 2013
22) Zenji Horita, The Japan Institute of Metals Distinguished Contribution Award, 2013
23) Chihaya Adachi, Outstanding achievement award from JP Society of Organic Electroluminescence, 2013
24) Seiji Ogo, The 30th Chemical Society of Japan Award, 2013
25) Harry L. Tuller, Helmholtz Intl. Fellow Award from the Helmholtz Association of German Research Centers, 2013
26) Tatsumi Ishihara, John A. Kilner and Harry L. Tuller, Somiya Award, 2012
27) Ian Robertson, Petros Sofronis, US Department of Energy Hydrogen and Fuel Cells Program Research and Development Award, 2011
28) Zenji Horita, The Commendation for Science and Technology by MEXT, 2011

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

*List up to 20 main presentations in order from most recent.
*For each, write the lecturer/presenter's name, presentation title, conference name and date(s)

1) Tatsumi Ishihara, "New Technology for Carbon Neutral Energy," 8th International Conference on Materials Science and Technology MSAT-8, Bangkok, Thailand, Dec. 15, 2014. (Plenary)
2) Chihaya Adachi, "Current Status of High Efficiency OLEDs Based on Delayed Fluorescence," ICSM2016, Guang Zhou, China, Jul. 1, 2016 (Invited)

3) 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)
4) 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)
5) Naotoshi Nakashima, "Design and Creation of Advanced Nanomaterials Based on Soluble Carbon Nanotubes," 2014 MRS Spring Meeting & Exhibit, San Francisco, CA, USA, Apr. 23, 2014. (Invited)
6) Harry L. Tuller, "Electro-Chemo-Mechanics – Applications to Solid State Ionic Materials," The 19th International Conference of Solid State Ionics, Kyoto, Japan, Jun. 5, 2013. (Invited)
7) Xing Zhang, "Thermophysical characterization methods for individual nanoscale materials," International Heat Transfer Symposium 2016, Nottingham, UK, Jun. 26-29, 2016. (Plenary)
8) Yasuyuki Takata, "Wettability Effects in Boiling Heat Transfer," The 8th International Conference on Multiphase Flow (ICMF2013), Jeju, Korea, May 29, 2013. (Plenary)
9) Zenji Horita, et al., "Severe Plastic Deformation under High Pressure: Scaling-up of high-pressure sliding for grain refinement and enhanced mechanical properties," Engineering Mechanics Institute Conference (2016EMI-IC), Metz, France, Oct. 25-27, 2016. (Keynote)
10) Etsuo Akiba, Kyushu University Hydrogen Project: Challenges to realize a hydrogen society," The Road to a Hydrogen Society: Prospects for Developing Zero-Emission Fuel and Outlook for U.S.-Japan Cooperation, Washington D.C., USA, Apr. 21, 2016. (Plenary)
11) Takahiro Matsumoto, "Hydrogenase and its Mimics for Fuel Cell Electrodes," 42nd International Conference on Coordination Chemistry (ICCC–42), Brest, France, Jul. 5, 2016. (Invited)
12) Miho Yamauchi, "Catalyst Development For the Realization of Carbon-Neutral Energy Cycles," The International Chemical Congress of Pacific Basin Societies 2015 (Pacifichem2015), Honolulu, HI, USA, Dec. 16, 2015, (Invited)
13) Seiji Ogo, "A significant contribution to the fundamentals and applications of chemistry: Catalytic electron and hydride transfer from H_2 by functional hydrogenase mimic," The 30th Chemical Society of Japan (CSJ) Award, Japan, Mar. 24, 2013. (Invited)
14) Shigenori Fujikawa, "Molecular separation by a free-standing and nanometer-thick membrane," The International Chemical Congress of Pacific Basin Societies 2015 (Pacifichem2015), Honolulu, HI, USA, Dec. 17, 2015. (Invited)
15) Takeshi Tsuji, "Digital rock physics: Insight into fluid flow and elastic deformation of porous media," GeoMod2014, Potsdam, Germany, Sep. 3, 2014. (Keynote)
16) Kenneth T. Christensen, "Quantitative Studies of Environmental Flows at the Micro- and Macro-Scales," 16th International Symposium on Flow Visualization, Okinawa, Japan, Jun. 27, 2014. (Keynote)
17) 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 5th Social Research Network Meeting, Cambridge, UK, Jul. 6, 2015. (Invited)
18) Yukihiro Higashi, "Measurements of Vapor Pressures, Saturated Densities, and Critical Parameters for R1224yd(Z)," 11th Asian Thermophysical Properties Conference, Yokohama, Japan, Oct. 4, 2016. (Invited)
19) Petros Sofronis (2012) Recent Advances in Experiments, Modeling and Prognosis of Hydrogen-Induced Fracture, Gordon Research Conference on Corrosion-Aqueous, Colby-Sawer College, New London, NH, July 8-13, 2012 (invited)
20) Ikuo Taniguchi, "Effort of I2CNER and the CO2 capture by membranes," New Membrane Technology Symposium 2016, Tokyo, Japan, Oct. 28, 2016. (Invited)

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Appendix 2-4 List of Achievements of Center's Outreach Activities between FY 2010 – 2016

* Using the table below, show the achievements of the Center's outreach activities from FY2010 through FY2016 (number of activities, times held).

(number of activities, times held)

Activities	FY2010	FY2011	FY2012	FY2013	FY2014	FY2015	FY2016	Total
PR brochure, pamphlet	0	4	6	5	5	5	5	30
Lectures, seminars for general public	0	3	6	11	14	12	17	63
Teaching, experiments, training for elementary, secondary and high school students	0	11	10	9	16	22	15	83
Science cafe	0	1	0	0	1	2	1	5
Open house	0	1	0	1	1	1	1	5
Participating, exhibiting in events	0	3	1	4	5	7	7	27
Press releases	0	1	7	10	14	14	8	54

World Premier International Research Center Initiative (WPI)
Appendix 2-4 List of Media Coverage of Projects carried out between FY 2010 – 2016
* Select main items of press releases, media coverage, and reports for FY 2010-2016 (especially by overseas media)

1) Japan

No.	Date	Type media (e.g., newspaper, magazine, television)	Description
1	May 7, 2011	Website	**NIKKEI.com** Web Article introducing an interview with Prof. Yukitaka Murakami, Vice Director of I^2CNER. Risk of the concentration of power stations, and proposal of dispersed power sources by the usage of hydrogen fuel cell are mentioned.
2	Jun. 5, 2011	Newspaper	**Asahi Shimbun** Newspaper featured an interview with Prof. Petros Sofronis, Director of I^2CNER, reviewing his future perspective from hiring excellent young brains worldwide to the achievement of the hydrogen society.
3	Sep., 2011	Newspaper, Website	**Yomiuri Shimbun** (Sep. 13, 2011), **Kyodo News** (Sep. 13, 2011), **Nikkan Kogyo Shimbun** (Sep. 14, 2011), **Nikkei Sangyo Shimbun** (Sep. 14, 2011), **Asahi.com** (Sep. 14, 2011) Newspaper/online article introducing a new technology, platinum-free nickel complex catalyst Fuel Cell, with the expectation of cost reduction (Seiji Ogo, Materials Transformations division)
4	Dec. 21, 2011	Television	**NHK Fukuoka Broadcasting Office** TV coverage featuring the next generation fuel cell (Kazunari Sasaki, lead of Fuel Cells division)
5	Mar. 11, 2012	Newspaper	**Nikkei Shimbun** Newspaper article introducing the latest research on solid oxide fuel cell and its unique technology (Tatsumi Ishihara, lead of Hydrogen Production division)
6	May 24, 2012	Television	**"Today's Close-up" on NHK** Television article introducing a front-line waste heat utilization technology (Tatsumi Ishihara, Hydrogen Production division)
7	Oct., 2012-Nov. 2012	Newspaper	**Nikkei Sangyo Shimbun** (Oct. 24, 2012), **Nikkan Kogyo Shimbun** (Oct. 25, 2012), **Kagaku Kogyo Nippo** (Oct. 25, 2012), **Denki Shimbun** (Oct. 25, 2012), **Kagaku Shimbun** (Nov. 2, 2012) Newspaper article introducing the reason of high oxygen permeation rate of a praseodymium nickel oxide (Tatsumi Ishihara, Hydrogen Production division)
8	Dec. 12, 2012	Newspaper	**Nikkan Kogyo Shimbun** Newspaper article introducing the success in the fabrication of dual carbon batteries with high capacity (Tatsumi Ishihara, Hydrogen Production division)

9	Feb. 2013	Newspaper	**Yomiuri Shimbun** (Feb. 8, 2013), **Asahi Shimbun** (Feb. 8, 2013), **Mainichi Shimbun** (Feb. 8, 2013), **Nikkei Shimbun** (Feb. 8, 2013), **Nishinippon Shimbun** (Feb. 8, 2013), **Science News** (Feb. 15, 2013), **Nikkei Shimbun** (Feb. 21, 2013) Newspaper article introducing the invention of a new catalyst that can release electrons from hydrogen gas (Seiji Ogo, Advanced Materials Transformations division)
10	Feb., 2013-Mar. 2013	Newspaper	**Nikkei Shimbun** (Feb. 22, 2013), **Nikkei Sangyo Shimbun** (Feb. 26, 2013), **Science News** (Mar. 15, 2013) Newspaper article introducing the development of fuel cell electrocatalyst using polybenzimidazole-modified carbon nanotubes as support materials (Naotoshi Nakashima, Fuel Cells division)
11	Feb. 2013-Mar. 2013	Website, Newspaper	**NIKKEI.com** (Feb. 26, 2013), **Yahoo Japan! News** (Feb. 26, 2013), **Optronics Web Journal** (Feb. 26, 2013), **Nikkei Shimbun** (Feb. 26, 2013), **Sustainablejapan.net** (Feb. 28, 2013), **Nanotech Japan** (Mar. 11, 2013), **Yomiuri Shimbun** (Mar. 16, 2013) Web/newspaper article introducing the development of a new manufacturing technology that can use iron titanium alloy (FeTi) for hydrogen storage (Zenji Horita, Hydrogen Storage division)
12	May 4, 2013	Newspaper, Website	**Nikkei Shimbun,** **Yomiuri Shimbun,** **Nishinippon Shimbun,** **Nikkan Kogyo Shimbun,** **Kyodo Tsushin (online),** **Shikoku Shimbun (online),** **Shizuoka Shimbun (online)** Newspaper article introducing a polymer electrolyte fuel cell, which is remarkably durable in high temperatures, based on poly(vinylphosphonic acid)-doped polybenzimidazole (Naotoshi Nakashima, Assoc. Prof. Fujigaya, Fuel Cells division)
13	May 27, 2013	Magazine	**Nikkei Business** Magazine article introducing groundbreaking organic materials (Chihaya Adachi, Hydrogen Production division)
14	Oct. 2, 2013	Newspaper	**Nikkei Business Daily** Newspaper article introducing an idea that fuel cell is expected to be downsized and solid oxide fuel cells can operate at 300℃ (Tatsumi Ishihara, Hydrogen Production division)
15	Apr. 2014, Sep. 2014	Newspaper	**Nikkei Shimbun** (Apr. 11, 2014), **Nishinippon Shimbun** (Sep. 6, 2014), **Nikkan Kogyo Shimbun** (Sep. 8, 2014), **Nikkei Sangyo Shimbun** (Sep. 9, 2014) Development of a future-generation of PEFCs using a minimal amount of Pt (Naotoshi Nakashima, Fuel Cells division)

16	May 2014-Jun. 2014	Newspaper, Website	**Nikkei Technology Online** (May 30, 2014), **Nishinippon Shimbun** (May 31, 2014), **Nikkan Kogyo Shimbun** (Jun. 2, 2014) Development of EL devices with 100% of luminous efficiency (Chihaya Adachi, Hydrogen Production division)
17	Jun. 4, 2014-Jun. 5, 2014	Television, Newspaper	**NHK,** **Yomiuri Shimbun,** **Mainichi Shimbun,** **Nikkei Shimbun** [NiFe]Hydrogenase from Citrobacter sp. S–77 Surpasses Platinum as an Electrode for H_2 Oxidation Reaction (Seiji Ogo, Catalytic Materials Transformations division)
18	Sep. 29, 2014	Newspaper	**Denki Shimbun,** **Nikkan Kogyo Shimbun,** **Nikkei Shimbun** World-first experiment on a controlled sub-seabed CO_2 leak demonstrates minimal environmental impact and rapid recovery (Kiminori Shitashima, CO_2 Storage division)
19	Oct., 2014	Newspaper	**Zaikei Shimbun** (Oct. 6, 2014), **Nikkei Sangyo Shimbun** (Oct. 8, 2014), **Nikkan Kogyo Shimbun** (Oct. 10, 2014), **Kagaku Shimbun** (Oct. 10, 2014) Semiconducting carbon nanotube sorting (Naotoshi Nakashima, Fuel Cells division)
20	Apr. 7, 2015	Newspaper	**Nihon Keizai Shimbun** Interview about usage of hydrogen (Etsuo Akiba, Hydrogen Storage division)
21	Apr. 20, 2015	Newspaper	**Nihon Keizai Shimbun** Vision and challenge of hydrogen society (Kazunari Sasaki, Electrochemical Energy Conversion division)
22	Jun. 2015, Nov. 2015	Newspaper	**Asahi Shimbun** (Jun. 20, 2015), **Nishinippon Shimbun** (Jun. 23, 2015), **Yomiuri Shimbun** (Nov. 23, 2015) Kyoto Prize (Toyoki Kunitake, CO_2 Capture and Utilization division)
23	Jul. 2, 2015	Newspaper	**Mainichi Shimbun** Mechanism of cell membrane (Toyoki Kunitake CO_2 Capture and Utilization division)
24	Jul. 29, 2015	Newspaper	**Nihon Keizai Shimbun** Increasing the efficiency of the electric power generation of fuel cells (Kazunari Sasaki, Electrochemical Energy Conversion division)

25	Oct. 1, 2015	Newspaper, Website	**Sankei Shimbun,** **Nihon Keizai Shimbun,** **Science Portal,** **excite news,** **zakzak,** **Sankei News** Found new geological formation controlling earthquake off the Kii peninsula (Takeshi Tsuji, CO_2 Storage division)
26	Oct. 20, 2015	Newspaper	**Nikkei Sangyo Shimbun** Organic Electroluminescence, Cheap But Brilliant Light (Chihaya Adachi, Molecular Photoconversion Devices division)
27	Nov. 2, 2015	Newspaper	**Nishinippon Shimbun,** **Asahi Shimbun,** **Yomiuri Shimbun,** **Nihon Keizai Shimbun** Medal with Purple Ribbon (Zenji Horita, Hydrogen Storage division)
28	Nov. 4, 2015	Newspaper	**Nikkei Sangyo Shimbun,** **Asahi Shimbun** Enzyme for both sides of fuel cells (Seiji Ogo, Catalytic Materials Transformations division)
29	Nov. 9, 2015	Newspaper	**Nihon Keizai Shimbun** Breakthrough in continuous monitoring of CO_2 leaks from storage sites (Takeshi Tsuji and Tatsunori Ikeda, CO_2 Storage division)
30	Nov. 26, 2015	Newspaper	**Nikkan Kogyo Shimbun** Durability enhancement of polymer electrolyte fuel cells (Naotoshi Nakashima, Electrochemical Energy Conversion Devices division)
31	Apr. 2016	Newspaper	**Nikkan Sangyo Shimbun** (Apr. 13, 2016), **Nikkan Kogyo Shimbun** (Apr. 28, 2016) Increasing efficiency in underground CO_2 storage: KU researchers analyze rocks to detect suitable areas (Takeshi Tsuji, CO_2 Storage division)
32	Apr. 15, 2016	Newspaper	**Nihon Keizai Shimbun** Comment on Kumamoto Earthquakes: 3rd largest number of inland earthquakes in history possibly affected by the near-surface epicenter (Takeshi Tsuji, CO_2 Storage division)
33	Jun. 6, 2016	Newspaper	**Nihon Keizai Shimbun** Successful experiment producing hydrogen with tens of times more energy efficiency by combining bacteria and photocatalyst (Tatsumi Ishihara, Yuki Honda. et al., Molecular Photoconversion Devices division)
34	Jul. 8, 2016	Newspaper	**Nikkan Kogyo Shimbun** 12 Scientists Recognized at Thomson Reuters "Japan Research Front Awards" (Chihaya Adachi, Molecular Photoconversion Devices division)
35	Jul. 11, 2016	Newspaper	**Nikkei Sangyo Shimbun** Chemically-Modified Carbon Nanotubes Emit New Near-Infrared Light (Naotoshi Nakashima, Electrochemical Energy Conversion division)

36	Sep. 15, 2016	Newspaper	**Nihon Keizai Shimbun** New support from NEDO's Strategic Core Technology Advancement Program: Collaboration with Nagano Forging Co. for practical application of high-pressure sliding process (Zenji Horita, Hydrogen Storage division)
37	Oct. 2, 2016	Newspaper	**Nihon Keizai Shimbun** CO_2 catch by ultrathin membrane (Shigenori Fujikawa, CO_2 Capture and Utilization division)
38	Nov. 20, 2016	Newspaper	**Yomiuri Shimbun** Organic electroluminescence: Next-generation lighting devices (Chihaya Adachi, Molecular Photoconversion Devices division)
39	Feb. 21, 2017	Newspaper	**Yomiuri Shimbun, others** Horizontal sliding of kilometer-scale hot spring area during the 2016 Kumamoto earthquake (Takeshi Tsuji, CO_2 Storage division)

2) Overseas

No.	Date	Type media (e.g., newspaper, magazine, television)	Description
1	May 11, 2011	Website	**U.S. Department of Energy** DOE Hydrogen and Fuel Cells Program Team Awards with special recognition for outstanding technical contributions (Petros Sofronis, Director)
2	May 12, 2011	Website	**Sandia National Laboratories** Japanese collaboration promises to put Sandia hydrogen program on global track (Brian Somerday, Hydrogen Materials Compatibility division)
3	Nov. 8, 2011	Website	**MRS Bulletin Website** Japan funds new international energy center, I²CNER, led by the University of Illinois
4	Jun. 2012-Aug. 2012	Website	**The Guardian** (Jun. 29, 2012), **Fish Update** (Jun. 29, 2012), **Planet Earth Online** (Jun. 29, 2012), **This is Cornwall** (Jun. 30, 2012), **International Business Time** (Jul. 1, 2012), **Responding to Climate Change** (Aug. 14, 2012) Web article introducing the world-first field experiment of CO_2 leakage in CCS (Kiminori Shitashima, CO_2 Storage division)

5	Jan. 17, 2013	Website	**CHEMICAL & ENGINEERING NEWS** Polymer Gets Sticky When Hit with Light (Atsushi Takahara, Hydrogen Production division)
6	Aug. 29, 2013	Webpage	**Helmholtz Zentrum Berlin** Massachusetts Institute of Technology/Materials Processing Center (Sep. 24) Interview of Prof. Harry Tuller (Fuel Cells division)
7	Nov. 21, 2013	Webpage	**Helmholtz-Zentrum Geesthacht** Web article introducing international ECOSTORE project (Etsuo Akiba, Hydrogen Storage division)
8	Feb., 2015	Newspaper	**Economist,** **Seattle Times,** **Washington Times** Wendy Schmidt Ocean Health XPRIZE: selected as Team SINDEN Japan Team Leader (Kiminori Shitashima, CO_2 Storage division)
9	Dec. 11, 2015	Television	**Bangladesh Sangbad Sangstha** Japanese Team meets DU VC (Bidyut Baran Saha, Thermal Science and Engineering division)
10	Jul. 8, 2016	Digital newspaper	**Europa Press,** **La Vanguardia,** **El Confidencial** Press release covering the 9th Shiseido Female Researcher Grant Award (Helena Téllez-Lozano, Electrochemical Energy Conversion division)
11	Jul. 8, 2016	Radio	**Cadena Sur** Interview by Spanish National Radio (Helena Téllez-Lozano, Electrochemical Energy Conversion division)
12	Jul. 13, 2016	Newspaper	**Diario Cordoba** Press release covering the 9th Shiseido Female Researcher Grant Award (Helena Téllez-Lozano, Electrochemical Energy Conversion division)
13	Aug. 7, 2016	Radio	**COPE** Interview by Spanish National Radio (Helena Téllez-Lozano, Electrochemical Energy Conversion division)

World Premier International Research Center Initiative (WPI) Appendix 3 List of Papers of Representative of Interdisciplinary Research Activities

* List **up to 20 papers** that underscoring each interdisciplinary research activity and give brief accounts (within 10 lines).
* For each, write the author name(s); year of publication; journal name, volume, page(s), and article title. Any listing order may be used as long as format is the same. If a paper has many authors, underline those affiliated with the Center.
* If a paper has many authors (say, more than 10), all of their names do not need to be listed.

1) S. Ida, K. Kearney, T. Futagami, H. Hagiwara, T. Sakai, M. Watanabe, A. Rockett, T. Ishihara (2017) Photoelectrochemical H_2 evolution using TiO_2-coated $CaFe_2O_4$ without an external applied bias under visible light irradiation at 470 nm based on device modeling, *Sustainable Energy & Fuels*, 1, 280-287.

$CaFe_2O_4$ (CFO) is a potential photocathode material for photo-electrochemical (PEC) water splitting, but is unstable by itself. Coating the material with TiO_2 improves stability, but was found to require a higher voltage to operate. Theoretical predictions based on a numerical device model and ab-initio density functional theory showed the mechanism for charge transport and predicted that removing the short wavelength light would resolve the problem. Experiments based on the prediction demonstrated dramatically improved performance. Our collaboration resulted in achieving the most positive onset potential among the oxide photocathodes ever reported, in addition to creating a PEC device that split water without an external applied bias.

Disciplines: Theoretical electrochemistry, experimental materials science

2) K. Takijiri, K. Morita, T. Nakazono, K. Sakai, H. Ozawa (2017) Highly Stable Chemisorption of Dyes with Pyridyl Anchors over TiO_2: Application in Dye-Sensitized Photoelectrochemical Water Reduction in Aqueous Media, *Chemical Communications*, 53(21), 3042-3045.

All forms of organic optical devices benefit from stable high-performance dye molecules coupled to inorganic substrates with strong linkages that transfer charge efficiently. This is particularly important when coupling organic ligands to titanium dioxide (TiO_2), which is used in many photoelectrochemical devices. In this accomplishment, a new “pyridyl anchor” scheme was designed and demonstrated that produces an exceptionally strong bond of an organic dye molecule to inorganic TiO_2 while retaining high rate electron transport across the interface. The result is superior to previous approaches and has the potential to significantly improve devices.

Disciplines: Electrochemistry, materials science, organic/inorganic chemistry

3) H. Emami, K. Edalati, A. Staykov, T. Hongo, H. Iwaoka, Z. Horita, E. Akiba (2016) Solid-state reactions and hydrogen storage in magnesium mixed with various elements by high-pressure torsion: experiments and first-principles calculations, *RCS Advances*, 6(14), 11665-11674.

This paper has two distinguished features. The first is that material development was done by a close collaboration of modeling and synthesis. It was found that the modelling can be a very powerful tool for the development of new materials. The other feature is the application of the high-pressure torsion technique to the synthesis of Mg-X alloys, which are lightweight and applicable for fuel cell vehicle on-board hydrogen storage. The HPT method has allowed the rapid synthesis of small scale alloys for research purposes.

Disciplines: Theoretical chemistry, experimental materials science and materials processing

4) K. Edalati, H. Emami, A. Staykov, D.J. Smith, E. Akiba, Z. Horita (2015) Formation of metastable phases in magnesium-titanium system by high-pressure torsion and their hydrogen storage performance, *Acta Materialia*, 99, 150-156.

Mg and Ti are immiscible, meaning that they do not form an intermetallic phase. The authors used the high-pressure torsion method to synthesize metastable Mg-Ti compounds. They were able to successfully synthesize an Mg-Ti compound with body-centered cubic structure. This paper reports that the HPT method is effective in the synthesis of alloys, opening up a new field for materials research in otherwise inaccessible alloys. This work is collaboration between modeling and materials synthesis. Modeling is critical to the development novel materials, for the selection of chemical composition of candidate materials, and interpretation of experimental results.

Disciplines: Theoretical chemistry, materials processing, metallurgy

5) T. Matsumoto, S. Eguchi, H. Nakai, T. Hibino, K.S. Yoon, S. Ogo (2014) [NiFe]Hydrogenase from Citrobacter sp. S-77 Surpasses Platinum as an Electrode for H2 Oxidation Reaction, *Angewandte Chemie International Edition*, 53(34), 8895–8898.

The fuel cell comprising [NiFe]-Hydrogenase anode isolated from I^2CNER research and Pt cathode showed a higher power density than that achievable by Pt. The enzyme electrode is also stable in air and, unlike Pt, can be recovered 100% after poisoning by carbon monoxide. Together with the previous studies of biomimetic [NiFe]-hydrogenase published in Science 2013, this result is the bench mark of the first biological fuel cells of O_2-tolerant hydrogenase, which satisfactorily accomplished the short-term target of H_2-activation.

Disciplines: Chemistry, biomimetic chemistry, fuel cell engineering

6) N.D. Muhd Noor, K. Nishikawa, H. Nishihara, K.S. Yoon, S. Ogo, Y. Higuchi (2016) Improved Purification, Crystallization and Crystallographic Study of Hyd-2-type [NiFe]-hydrogenase from Citrobacter sp. S-77, *Acta Crystallographica, Section F (Structural Biology Communications)*, F72(1), 52–58.

With this result combined with previous biochemical studies, we have achieved the initial mid-term studies of the crystal structure of O_2-tolerant [NiFe]-hydrogenase. This interdisciplinary work is based on the initial isolation of new bacterium containing new O_2-tolerant [NiFe]-hydrogenase and biochemical characterization, and protein structural analysis. This is the first crystal study of the type II O_2-tolerant [NiFe]-hydrogenase purified by I^2CNER.

Disciplines: Biology, biomimetic chemistry, crystallography

7) S. Ma, M. Sadakiyo, M. Heima, R. Luo, R.T. Haasch, J.I. Gold, M. Yamauchi, P.J.A. Kenis (2017) Electroreduction of Carbon Dioxide to Hydrocarbons Using Bimetallic Cu-Pd Catalysts with Different Mixing Patterns, *Journal of the American Chemical Society*, 139, 47-50 (2017).

In a collaboration between Kyushu University and University of Illinois groups forming the CO_2 capture and utilization division, we succeeded in developing a highly efficient CO_2 electroreduction process to produce C_2 compounds. Newly designed phase-separated-type CuPd nano-alloy catalyst was found to exhibit the highest selectivity to C_2 chemicals in electrochemical CO_2 reduction (up to 63% Faradaic efficiency, among the highest reported values for C_2 production reported in the literature). Furthermore, we proposed origins for selectivity on the nanoalloy catalysts.

Disciplines: Electrochemistry, materials science, organic chemistry

8) S. Ma, M. Sadakiyo, R. Luo, M. Heima, M. Yamauchi, P.J.A. Kenis (2016) One-step Electrosynthesis of Ethylene and Ethanol from CO_2 in an Alkaline Electrolyzer, *Journal of Power Sources*, 301, 219-228.

We prepared Cu nanocatalysts having large surface roughness and conducted CO_2 electroreduction using an alkaline electrolyzer that was constructed by Prof. Kenis. The Cu catalyst showed a combined Faradaic efficiency (46%) for the electroreduction of CO_2 to ethylene and ethanol under conditions with current densities of ~200 mA cm^{-2}, resulting in a 10-fold increase in performance achieved at much lower overpotential (only < 0.7 V) compared to prior work.

Disciplines: Electrochemistry, materials science

9) B.B. Saha, I.I. El-Sharkawy, T. Miyazaki, S. Koyama, S.K. Henninger, A. Herbst, C. Janiak (2015) Ethanol Adsorption onto Metal Organic Framework: Theory and Experiments, *Energy*, 79, 363-370.

In this interdisciplinary research article, we have reported the adsorption characteristics of newly developed Metal Organic Framework (MOF) for ethanol uptake covering both equilibrium and transient performances. Details on adsorption kinetics of such adsorbent + adsorbate pair is modelled and highlighted significant findings such as higher activation energy of MOF as compared to activated carbons and stronger dependent of adsorption time constant on the temperature.

Disciplines: Materials science, surface science, theoretical thermodynamics and kinetics

10) S. Chavan, H. Cha, D. Orejon, K. Nawaz, N. Singla, Y.F. Yeung, D. Park, D.H. Kang, Y. Chang, Y. Takata, N. Miljkovic (2016) Heat Transfer through a Condensate Droplet on Hydrophobic and Nanostructured Superhydrophobic Surfaces, *Langmuir*, 32(31), 7774-7787.

Understanding the fundamental mechanisms governing vapor condensation on nonwetting surfaces is crucial to a wide range of energy and water applications. This paper reconciles classical droplet growth modeling barriers by utilizing two-dimensional axisymmetric numerical simulations to study individual droplet heat transfer on nonwetting surfaces. Incorporation of an appropriate convective boundary condition at the liquid−vapor interface reveals that the majority of heat transfer occurs at the three phase contact line, where the local heat flux can be up to 4 orders of magnitude higher than at the droplet top. Droplet distribution theory is incorporated to show that previous modeling approaches under predict the overall heat transfer by as much as 300% for dropwise and jumping-droplet condensation. To verify the simulation results, condensed water droplet growth experiments are conducted using optical and environmental scanning electron microscopy, showing excellent agreement with the simulations. This paper demonstrates the importance of resolving local heat transfer effects for the fundamental understanding and high fidelity modeling of phase change heat transfer.

Disciplines: Mechanical engineering, thermal science, surface science

11) N.H. Perry, S.R. Bishop, H.L. Tuller (2014) Tailoring Chemical Expansion by Controlling Charge Localization: In Situ X-ray Diffraction and Dilatometric Study of (La,Sr)(Ga,Ni)$O_{3-\delta}$ Perovskite, *Journal of Materials Chemistry A*, 2(44), 18906-18916.

This paper provided the first experimental demonstration of our earlier collaborative computational predictions showing that delocalizing charge on multivalent cations is an effective route to lowering coefficients of chemical expansion for increased device durability, while maintaining excellent ionic/electronic transport and surface reactivity. It also revealed, via *in situ* structural studies, the important role of dynamic crystal symmetry in chemical expansion behavior. Thus the atomistic predictions were combined with unit cell- and macroscopic-level measurements to understand and identify means to tailor chemical expansion of perovskites. This structure is one of the most widely used in solid oxide cell electrodes and electrolytes.

Disciplines: Theoretical chemistry, crystallography, electrochemistry

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

This invited review, led by I^2CNER researchers, brought together an international experimental and computational team to provide the first comprehensive review of chemical expansion – its definition, a taxonomy of various types, its origins, examples across multiple applications and materials classes, a collection of measured and simulated coefficients, and implications for electrochemical device durability. The paper serves as a core reference defining the emerging area of chemo-mechanics and has already been cited many times.

Disciplines: Theoretical chemistry, crystallography, electrochemistry, chemo-mechanics

13) D. Marrocchelli, N.H. Perry, S.R. Bishop (2015) Understanding Chemical Expansion in Perovskite-Structured Oxides, *Physical Chemistry Chemical Physics*, 17(15), 10028-10039.

This paper resulted from a collaboration between younger experimental and computational researchers at I2CNER and MIT, providing the first detailed description of the origins of chemical expansion in the perovskite structure, used widely in solid oxide cells. The paper identifies factors which can impact chemical expansion in perovskites, provides atomistic insight into the chemical expansion process via computational simulations, introduces a new empirical model for describing pseudo-cubic lattice parameters in perovskites which is more accurate and physically reasonable than all previous models, and thereby determines the effective size of oxygen vacancies in a range of perovskite compositions. Interestingly, the work found that oxygen vacancies in perovskites are generally not much smaller than oxide ions, and therefore, unlike for the fluorite structure, focusing on the cation sub-lattice (rather than anion vacancy size) is likely to be a more effective way to tailor chemical expansion in perovskites for enhanced durability.

Disciplines: Theoretical chemistry, crystallography, materials synthesis

14) C.J. Barile, E.C.M. Tse, Y. Li, T.B. Sobyra, S.C. Zimmerman, A. Hosseini, A.A. Gewirth (2014) Proton Switch for Modulating Oxygen Reduction by a Copper Electrocatalyst embedded in a Hybrid Bilayer Membrane, *Nature Materials*, 13(6), 619-623.

What limits the performance of polymer electrolyte fuel cell is the oxygen reduction reaction (ORR). This paper reports that the oxygen reduction reaction can be switched on and off by controlling the pH of solution above the active surface. At low pH values, a proton transfer agent achieves a neutral form, which allows it to 'flop-flop' diffuse through a lipid leaflet, and this 'flop-flop' is inhibited at high pH values. Conclusively, the proton switch has general utility in connection with another finding of controlling the ORR by using light and other proton-couple electron transfer (PCET) reactions.

Disciplines: Chemistry, material science, biomimetic chemistry, electrochemistry

15) E.C.M. Tse, C.J. Barile, N.A. Kirchschlager, Y. Li, J.P. Gewargis, S.C. Zimmerman, A. Hosseini, A.A. Gewirth (2016) Proton Transfer Dynamics Control the Mechanism of O_2 Reduction by a Non-Precious Metal Electrocatalyst, *Nature Materials*, 15(7), 754-759.

In this paper, the authors developed a platform that allows strict control over the transport of protons to a Cu-based NPM ORR catalyst using a hybrid bilayer membrane (HBM) formed by appending a monolayer of lipid molecules to a self-assembled monolayer (SAM) of thiols on Au. The presence of a proton carrier in the membrane is used to modulate proton transport quantitatively to the catalyst contained in the SAM. Using this platform we observed changes in the ORR product speciation given different proton availabilities, proving the proton-coupled electron transfer (PCET) nature of the ORR on NPM catalysts. Furthermore, we demonstrated that by optimizing the rates of proton and electron transfer to the catalyst we can achieve 100% selectivity for the four electron reduction of O_2 to H_2O without generating harmful partially reduced O_2 species.

Disciplines: Chemistry, biomimetic chemistry, electrochemistry, catalysis

16) J.A. Varnell, E.C.M. Tse, C.E. Schulz, T.T. Fister, R.T. Haasch, J. Timoshenko, A.I. Frenkel, A.A. Gewirth (2016) Identification of Carbon-Encapsulated Iron Nanoparticles as Active Species in Non-Precious Metal Oxygen Reduction Catalysts, *Nature Communications*, 7, 12582.

In this paper, the authors examined iron-based non-precious metal catalysts as an alternative to state-of-the-art platinum catalysts. However, the identity of the active species in non-precious metal catalysts remains elusive, impeding the development of new catalysts. In this work, the authors demonstrated the reversible deactivation and reactivation of an iron-based non-precious metal oxygen reduction catalyst achieved using high-temperature gas-phase chlorine and hydrogen treatments. Additionally, a decrease in catalyst heterogeneity following treatment with chlorine and hydrogen was observed using Mössbauer and X-ray absorption spectroscopy. This study reveals that protected sites adjacent to iron nanoparticles are responsible for the observed activity and stability of the catalyst.

Disciplines: Chemistry, physics, material science, spectroscopy, catalysis, electrochemistry

17) H. Yamabe, T. Tsuji, Y. Liang, T. Matsuoka (2015) Influence of fluid displacement patterns on seismic velocity during supercritical CO_2 injection: Simulation study for evaluation of the relationship between seismic velocity and CO_2 saturation, *International Journal of Greenhouse Gas Control,* 46, 197-204.

Numerical simulations were conducted to evaluate the influence of CO_2 behavior within storage rock on seismic velocity and its correlation to CO_2 saturation. Doing so is critical for the use of seismic-based monitoring methods for monitoring CO_2 migration and detection of CO_2 leakage. Through the interdisciplinary combination of hydrology and geophysics, the complex relationship between hydrologic (CO_2 saturation) and elastic (seismic velocities) properties has been identified for real rock geometries and provides a new method for more quantitative monitoring of CO_2 storage sites.

Disciplines: Geophysics, hydrology, mathematics

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

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

Disciplines: Materials synthesis, organic chemistry, electrochemistry

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

By applying density functional theory (DFT) simulations, mechanistic details of oxygen-inhibited hydrogen uptake into iron were described. The DFT simulations revealed two key mechanistic insights: 1) the gas-surface attractive force is stronger for O_2 compared to H_2, and 2) the oxygen-covered iron surface inhibits H_2 dissociation on the surface. In addition to simulating the co-adsorption of H_2 and O_2, the DFT method was applied to other gas species that can compete with H_2 for surface adsorption sites, such as CO. These preliminary results for CO led to a more extensive study supported by Air Liquide for the purpose of applying chemical inhibitors to mitigate hydrogen-accelerated cracking in steels.

Disciplines: Theoretical chemistry, surface science, mechanical metallurgy

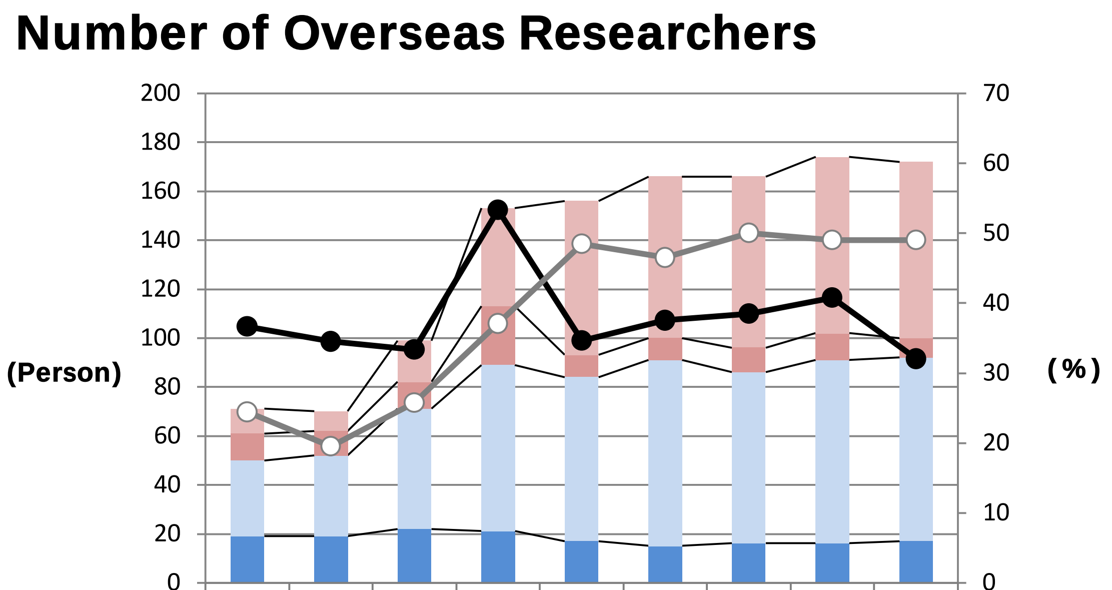
20) R. Kirchheim, B.P. Somerday, P. Sofronis (2015) Chemomechanical Effects on the Separation of Interfaces Occurring during Fracture with Emphasis on the Hydrogen-Iron and Hydrogen-Nickel System, *Acta Materialia*, 99, 87–98.

Critical to the development of predictive capabilities, the modeling of hydrogen-assisted intergranular cracking was advanced through a thermodynamic treatment of new surface creation accompanying 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. This interdisciplinary modeling effort combines material physics, solid mechanics, and mechanical metallurgy.

Disciplines: Material physics, solid mechanics, mechanical metallurgy

World Premier International Research Center Initiative (WPI)
Appendix 4-1　Number of Overseas Researchers and Annual Transition

*Make a graph of the transition in the number of overseas researchers since the application.



	(At beginning)	FY2010	FY2011	FY2012	FY2013	FY2014	FY2015	FY2016	(Final goal) FY 2020
Researchers from abroad	10	8	17	40	63	66	70	72	72
PIs from abroad	11	10	11	24	9	9	10	11	8
Japanese researchers excluding PIs	31	33	49	68	67	76	70	75	75
Japanese PIs	19	19	22	21	17	15	16	16	17
Ratio of PIs from abroad	36.7	34.5	33.3	53.3	34.6	37.5	38.5	40.7	32.0
Ratio of researchers from abroad	24.4	19.5	25.8	37.0	48.5	46.5	50.0	49.0	49.0

World Premier International Research Center Initiative (WPI)

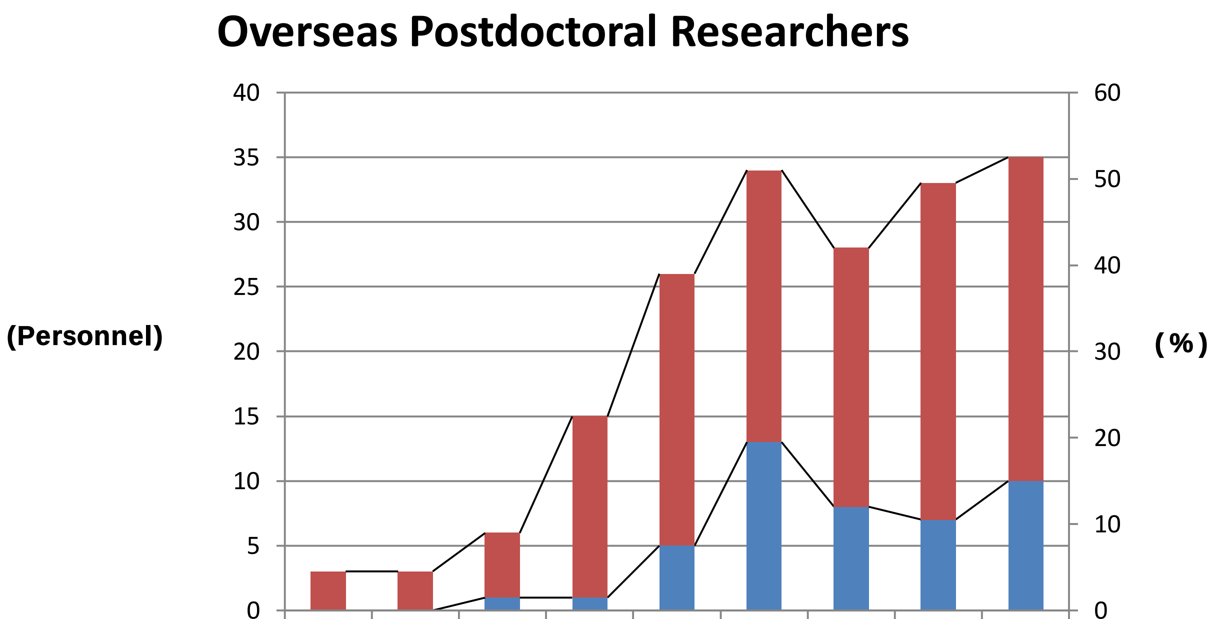
Appendix 4-2 Postdoctoral Positions through Open International Solicitations

- In the column of number of applications and number of selection, put the number and percentage of overseas researchers in the < > brackets.

Fiscal year	number of applications	number of selection
FY2010	75	1
	< 71, 95%>	< 0, 0%>
FY2011	95	2
	< 62, 100%>	< 2, 100%>
FY2012	13	3
	< 12, 92%>	< 2, 67%>
FY2013	12	2
	< 11, 92%>	< 1, 50%>
FY2014	16	2
	< 15, 93%>	< 2, 100%>
FY2015	79	2
	<72, 91 %>	<2, 100 %>
FY2016	0	0
	<0, 0%>	<0, 0%>

World Premier International Research Center Initiative (WPI)
Appendix 4-3 Number of Overseas Postdoctoral Researchers and Annual Transition

*Make a graph of the transition in the number of overseas postdoctoral researchers since the application.



	(At beginning)	FY2010	FY2011	FY2012	FY2013	FY2014	FY2015	FY2016	(Final goal) FY 2020
Overseas postdoc	3	3	5	14	21	21	20	26	25
Japanese postdoc	0	0	1	1	5	13	8	7	10
Ratio of overseas postdoc	100.0	100.0	83.3	93.3	80.8	61.8	71.4	78.8	71.4

World Premier International Research Center Initiative (WPI)

Appendix 4-4 Status of Employment of Postdoctoral Researchers at Institutions

*List each researcher in 1 line. If the list exceeds this form, please add extra pages

Japanese Postdocs

Period of project participation	Previous Affiliation Position title (Country)	Next AffiliationPosition title (Country)
Apr. 1, 2011-May. 31, 2012	PhD Student, Kyoto University (Japan)	Assistant Professor, Nagoya University (Japan)
Apr. 1, 2013-Mar. 31, 2014	Postdoc, Hokkaido University (Japan)	Assistant Professor, Chuo University (Japan)
Apr. 1, 2013-Mar. 31, 2014	PhD Student, Kyushu University (Japan)	Associate, The Matsushima Institute of Government and Management (Japan)
May 1, 2013-Mar. 31, 2014	Research Support Staff, Kyushu University (Japan)	Researcher, Iwate University (Japan)
Apr. 1, 2014-Mar. 31, 2015	Postdoc, Kyushu University (Japan)	Assistant Professor, Kyushu University (Japan)
Apr. 1, 2014-Feb. 28, 2015	Researcher, Toyota Central R&D Labs., inc. (Japan)	Researcher, National Institute of Advanced Industrial Science and Technology (Japan)
Apr. 1, 2014-Oct. 15, 2016	PhD Student, Kyoto University (Japan)	Assistant Professor, I^2CNER (Japan)
Apr. 1, 2014-Mar. 31, 2017	Postdoc, Kyushu University (Japan)	Assistant Professor, Nara Women's University (Japan)
Apr. 1, 2014-Present	PhD Student, Kindai University (Japan)	(Currently at I^2CNER)
Aug. 1, 2014-Jul. 31, 2015	Researcher, Pennsylvania State University (USA)	Postdoc, Kyushu University (Japan)
Oct. 1, 2014-Sep. 30, 2016	Postdoc, Tokyo University of Science (Japan)	Postdoc, Tokyo University of Science, Yamaguchi (Japan)
Oct. 1, 2014-Mar. 31, 2015	PhD Student, Kyushu University (Japan)	Mitsubishi Gas Chemical Company, Inc., (Japan)
Mar. 1, 2015-Dec. 31, 2016	Researcher, Tokyo Institute of Technology (Japan)	Researcher, Tohoku University (Japan)
Apr. 1, 2015-Mar. 31, 2016	PhD Student, Kyushu University (Japan)	Assistant Professor, Okayama University (Japan)
May 1, 2015-Present	Researcher, Asahi Intecc (Japan)	(Currently at I^2CNER)
Apr. 1, 2016-Mar. 31, 2017	PhD Student, Kyushu University (Japan)	ADECA CORPORATION (Japan)

Overseas Postdocs

Period of project participation	Previous Affiliation Position title (Country)	Next AffiliationPosition title (Country)	Nationality
Jan. 16, 2012-Dec. 31, 2015	Postdoc, Imperial College London (UK)	Assistant Professor, I^2CNER (Japan)	UK
Apr. 1, 2012-Present	Postdoc, Kyushu University (Japan)	(Currently at I^2CNER)	French
Sep. 1, 2012-Aug. 15, 2014	Postdoc, Northwestern University (USA)	Assistant Professor, I^2CNER (Japan)	USA
Dec. 1, 2012-Jan. 30, 2015	Postdoc, Kyushu University (Japan)	Associate Research Fellow, Wenzhou Institute of Biomaterials and Engineering (China)	Chinese
Dec. 1, 2012-Mar. 25, 2016	JSPS Postdoc, Tohoku Univesity (Japan)	Professor, Huazhing University of Science and Technology (China)	Chinese
Apr. 1, 2013-Jan. 31, 2014	PhD Student, Tokyo Institute of Technology (Japan)	Postdoc, Eindhoven University of Technology (Holland)	Chinese
Apr. 1, 2013-Nov. 30, 2014	Postdoc Researcher, JST(ERATO) (Japan)	Postdoc, Singapore University of Technology and Design (Singapore)	Burmese
Apr. 1, 2013-Mar. 31, 2015	Postdoc, Kyushu University (Japan)	Assistant Professpr, I^2CNER (Japan)	Iranian
Apr. 1, 2013-Apr. 30, 2015 Jun. 1, 2015-Jul. 17, 2015	PhD Student, Yale University (USA)	Assistant Professor, North Dakota State University (USA)	USA
Apr. 1, 2013-Mar. 30, 2016	Postdoc, Kyushu University (Japan)	Assistant Professor, Tanta University (Egypt)	Egyptian
Apr. 1, 2013-Mar. 31, 2016	PhD Student, Kyushu University (Japan)	Assistant Professor, Yamaguchi University (Japan)	Chinese
Oct. 1, 2013-Oct. 15, 2016	PhD Student, University of Edinburgh (Scotland)	Assistant Professor, I^2CNER (Japan)	Spanish
Oct. 1, 2013-Present	JSPS Postdoc, Kyushu University (Japan)	(Currently at I^2CNER)	Cameroonian
Nov. 1, 2013-Dec. 30, 2013	Lecturer, Sriwijaya University (Indonesia)	Researcher, Sriwijaya University (Indonesia)	Indonesian
Jan. 1, 2014-Present	Postdoc, University of Kitakyushu (Japan)	(Currently at I^2CNER)	Ukrainian
Feb. 1, 2014-Present	Postdoc, Kyushu University (Japan)	(Currently at I^2CNER)	Chinese
Feb. 1, 2014-Mar. 31, 2015	Research Support Staff, Hokkaido University (Japan)	Postdoc, University of Wisconsin-Madison (USA)	Chinese
Apr. 1, 2014-Apr. 15, 2015	Postdoc, Kyushu University (Japan)	Chief Operating Officer/Principal Scientist, Akron Ascent Innovations (USA)	USA
May 1, 2014-Aug. 31, 2014	Postdoc, Kyushu University (Japan)	Assistant Professor, Pukyung National University (Korea)	Korean
Nov. 1, 2014-Jul. 31, 2015	PhD Student, University of Edinburgh (Scotland)	JSPS Postdoc, Kyushu University (Japan)	Greece
Mar. 16, 2015-Present	PhD Student, National University of Singapore (Singapore)	(Currently at I^2CNER)	Indian
Apr. 1, 2015-Present	PhD Student, Kyushu University (Japan)	(Currently at I^2CNER)	Vietnamese
Dec. 1, 2015-Dec. 19, 2016	JSPS Postdoc, NIMS (Japan)	Researcher, Charles University in Prague (Czech)	Czech
Dec. 1, 2015-Present	PhD Student, University of Southampton (UK)	(Currently at I^2CNER)	Romanian
Jan. 16, 2016-Present	PhD Student, Jawaharlal Nehru Centre for Advanced Scientific Research (India)	(Currently at I^2CNER)	Indian
Mar. 1, 2016-Sep. 30, 2016	Postdoc, Kyushu University (Japan)	Assistant Professor, Nanjing Tech University (China)	Chinese
Mar. 1, 2016-Present	Researcher, Sebelas Maret Univesity (Indonnesia)	(Currently at I^2CNER)	Indonesian
Apr. 1, 2016-Present	PhD Student, Kyoto Institute of Technology, (Japan)	(Currently at I^2CNER)	Thai
May 1, 2016-Present	Postdoc, Kyushu University (Japan)	(Currently at I^2CNER)	Chinese

May 16, 2016-Present	PhD Student, Indian Institute of Science, Bangalore (India)	(Currently at I^{2}CNER)	Indian
May 16, 2016-Present	PhD Student, Imperial College London (UK)	(Currently at I^{2}CNER)	Chinese
Jun. 1, 2016-Present	Postdoc, Kyushu University (Japan)	(Currently at I^{2}CNER)	Chinese
Sep. 1, 2016-Present	Assistant Professor, Jagannath University (Bangladesh)	(Currently at I^{2}CNER)	Bangladeshi
Oct. 1, 2016-Present	Research Assistant Professor, Hangyang University (Korea)	(Currently at I^{2}CNER)	Chinese
Nov. 1, 2016-Present	Postdoc, Kyushu University (Japan)	(Currently at I^{2}CNER)	German
Nov. 16, 2016-Present	Postdoc, Norweigian University of Science and Technology (Norway)	(Currently at I^{2}CNER)	French
Dec. 1, 2016-Present	Postdoc, Kyushu University (Japan)	(Currently at I^{2}CNER)	Greece
Dec. 1, 2016-Present	Postdoc, Kyushu University (Japan)	(Currently at I^{2}CNER)	Bulgarian
Jan. 1, 2017-Present	Researcher, University of Toronto (Canada)	(Currently at I^{2}CNER)	Indian
Jan. 1, 2017-Present	PhD Student, University of Girona (Spain)	(Currently at I^{2}CNER)	Spanish

World Premier International Research Center Initiative (WPI)

Appendix 4-5 List of the Cooperative Research Agreements Outside Japan

1. Name of an Agreement

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

Dates of an Agreement

March 17, 2014

Counterpart of an Agreement

The Norwegian University of Science and Technology (NTNU)

Summary of an Agreement

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

2. Name of an Agreement

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

Dates of an Agreement

October 1, 2013

Counterpart of an Agreement

ECOSTORE beneficiaries such as Helmholtz-Zentrum Geesthacht Zentrum für Material- und Küstenforschung GmbH (HZG), Institutt for Energiteknikk (IFE), Aarhus Universitet (AU), Universita Degli Studi di Torino (UNITO), Centre National de la Recherche Scientific (CNRS), the University of Birmingham (UoB), Université de Genève (UNIGE), Universität Stuttgart (USTUTT), National Centre for Scientific Research Demokritos (NCSRD), Zoz Gmbh (ZOZ), SAFT SAS (SAFT) and Rockwood Lithium GmbH (ROLI), Tohoku University and University of Southern Denmark (SDU)

Summary of an Agreement

The purpose of this consortium agreement is to specify with respect to the project the relationship among the parties, in particular concerning the organization of the work between the parties, the management of the project and the rights and obligations of the parties concerning inter alia liability, access rights, and dispute resolution relating to the project entitled "Novel Complex Metal Hydrides for Efficient and Compact Storage of Renewable Energy as Hydrogen and Electricity," in short "ECOSTORE."

3. Name of an Agreement

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

Dates of an Agreement

December 31, 2013

Counterpart of an Agreement

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

Summary of an Agreement

This agreement aims at bridging science to practical application, wherein I^2CNER focuses on the science and NFCRC focuses on the bridging of science to practical application. In this fashion, NFCRC will be able to complement/support the mission of I^2CNER by making the "connection" to practical application. The specific roles of NFCRC are to provide direct support to the Energy Analysis efforts of I^2CNER, to provide direct support through analyses of "Fuel Cell Systems" and "Energy Systems," and to provide direct support in planning methodologies associated with H_2 fueling infrastructure deployment. The general goal is to facilitate a sustained and enduring dialog, fundamental and practical research, and educational cooperation between the two parties.

4. Name of an Agreement

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

Dates of an Agreement

May 26, 2014

Counterpart of an Agreement

The University of Illinois at Urbana-Champaign, USA

Summary of an Agreement

The purpose of this university-wide agreement is to develop scientific, academic and educational cooperation on the basis of equality and reciprocity and to promote relations and mutual understanding including exchange of academic staff, administrative staff and students, joint research, exchange of academic information and publications, and other academic exchanges.

5. Name of an Agreement

Agreement for Research Collaboration and Engagement, University of New South Wales and Kyushu University

Dates of an Agreement

May 9, 2016

Counterpart of an Agreement

University of New South Wales, Australia

Summary of an Agreement

This is a university-wide agreement of which objective is to strengthen research collaboration and engagement between the two organizations in areas of common interest such as energy.

6. Name of an Agreement

Agreement on Academic Cooperation between International Institute for Carbon-Neutral Energy Research, Kyushu University (I^2CNER), Japan and the University of New South Wales, Australia

Dates of an Agreement

Pending

Counterpart of an Agreement

The University of New South Wales, Australia

Summary of an Agreement

The objective of the agreement is to facilitate further cooperation in research and education, including exchange of students and faculty, joint research activities and publications, participation in seminars and academic meetings, exchange of academic materials and academic publications, and graduate degree programs.

7. Name of an Agreement

Letter of Understanding

Dates of an Agreement

Pending

Counterpart of an Agreement

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

Summary of an Agreement

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

World Premier International Research Center Initiative (WPI)

Appendix 4-6 Holding International Research Meetings

* For each fiscal year, indicate the number of international research conferences or symposiums held and give up to two examples of the most representative ones using the table below.

FY 2010-2011: 5 meetings

Date	Meeting title and Place held	Number of participants
February 1, 2011	Kick-Off Symposium Kyushu University, Japan	From domestic institutions: 128 From overseas institutions: 26
March 6-7, 2012	I^{2}CNER Satellite Kick-Off Symposium University of Illinois at Urbana-Champaign, U.S.	From domestic institutions: 70 From overseas institutions: 30

FY 2012: 3 meetings

Date	Meeting title and Place held	Number of participants
December 7, 2012	I^{2}CNER Tokyo Symposium National Center of Sciences (Hitotsubashi Hall etc.), Japan	From domestic institutions: 130 From overseas institutions: 20
January 29, 2013	I^{2}CNER Annual Symposium Kyushu University, Japan	From domestic institutions: 159 From overseas institutions: 66

FY 2013: 4 meetings

Date	Meeting title and Place held	Number of participants
September 13, 2013	Catalytic Concepts for Energy University of Illinois at Urbana-Champaign, U.S.	From domestic institutions: 50 From overseas institutions: 10
January 30, 2014	I^{2}CNER & ACT-C Joint Symposium Kyushu University, Japan	From domestic institutions: 119 From overseas institutions: 58

FY 2014: 6 meetings

Date	Meeting title and Place held	Number of participants
December 12, 2014	I^{2}CNER Tokyo Symposium TKP Garden City Shinagawa, Tokyo, Japan	From domestic institutions: 98 From overseas institutions: 27
February 2, 2015	I^{2}CNER Annual Symposium 2015 Kyushu University, Japan	From domestic institutions: 79 From overseas institutions: 62

FY 2015: 5 meetings

Date	Meeting title and Place held	Number of participants
February 1-2, 2016	I^2CNER Annual Symposium 2016, Kyushu University, Japan	From domestic institutions: 127 From overseas institutions: 125
March 13-17, 2016	The First Pacific Rim Thermal Engineering Conference, Hawaii, U.S.	Total 500 - 600

FY 2016: 9 meetings

Date	Meeting title and Place held	Number of participants
September 11-14, 2016	2016 International Hydrogen Conference Jackson Lake Lodge, U.S.	From domestic institutions: 25-30 From overseas institutions: 100-125
February 1, 2017	I^2CNER Annual Symposium 2017 Kyushu University, Japan	From domestic institutions: 80 From overseas institutions: 86
February 2-3, 2017	University of New South Wales-I^2CNER 2nd Energy Workshop Kyushu University, Japan	From domestic institutions: 22 From overseas institutions: 8

World Premier International Research Center Initiative (WPI)

Appendix 5-1 Host Institution's Commitment

1. Contributions from host institution

(1) Fund, Personnel

* Regarding "Fund" entry, describe with reference to the items in the Progress Report (Jisseki-hokoku-sho) based on Article 12 of the Grant Guidelines (Kofu-yoko).
* Don't include competitive funding obtained by researchers (used as research project funding)
* Under "Personnel", enter the number of full-time administrative staff within the parenthesis.

(2010-2016)

<Fund> (million yen)

Fiscal Year	2010	2011	2012	2013	2014	2015	2016
Personnel	58	351	379	226	243	227	211
- Faculty members	44	299	330	187	199	180	158
Full-time	0	0	0	0	0	0	0
Concurrent	44	299	330	187	199	180	158
Postdocs	0	0	0	0	0	0	0
RA etc.	0	0	0	0	0	0	0
Research support staff	0	0	0	0	0	0	0
Administrative staff	14	52	49	39	44	47	53
Project activities	1	7	12	22	128	74	79
Travel	0	2	1	3	4	3	7
Equipment	0	0	819	10	1,957	34	8
Research projects	720	1,570	2,238	2,557	2,838	2,128	1,543
Total	779	1,930	3,449	2,818	5,170	2,466	1,848

<Personnel> (person)

Fiscal Year	2010	2011	2012	2013	2014	2015	2016
Personnel	49	62	65	48	49	47	45
- Faculty members	43	56	59	42	41	39	36
Full-time	0	0	0	0	0	0	0
Concurrent	43	56	59	42	41	39	36
Postdocs	0	0	0	0	0	0	0
RA etc.	0	0	0	0	0	0	0
Research support staff	0	0	0	0	0	0	0
Administrative staff	6	6	6	6	8	8	9

World Premier International Research Center Initiative (WPI)
Appendix 5-1　Host Institution's Commitment

1. Contributions from host institution
(2) Provision of land and/or building(s), lab space, etc.

I^{2}CNER Building 2
- Kyushu University offers space/land free for the I^{2}CNER building 2, which was built at the end of February 2015. The building has 4 stories and a total floor space of 5,000 m^2, and its floor plans include 8 large-scale labs, 2 open offices, and 1 administrative office, with the majority of rooms being designed as open, common experimental spaces in order to promote interdisciplinary research.

Tenured Positions
- So far, Kyushu University has allotted a total of 12 tenured faculty positions to I^{2}CNER, and 7 of them were awarded through the University Reform Revitalization Program (URRP). The breakdown of the allotted tenured positions each year is:

FY 2011 and 2012	5 Associate Professor
FY 2014	1 Professor (through URRP)
FY 2015	1 Professor and 2 Associate Professor (through URRP)
FY 2016	1 Professor and 1 Associate Professor (through URRP)
For FY 2017	1 Associate Professor (through URRP)

Additionally, as a result of a joint proposal that I^{2}CNER together with the Institute of Mathematics-for-Industry (IMI) submitted to the University, 2 tenure-track assistant professor positions were awarded and filled on December 16, 2016.

Intra-University Faculty Transfer System
- Under the initiative of President, Kyushu University introduced the "Intra-University Faculty Transfer System" on April 1, 2013. Since then, I^{2}CNER has been utilizing the system and had 9 senior-level faculty transferred from other units of the university in FY 2016. Their transfer is extended on an annual basis. For FY 2017, 7 of them will continue to serve as the core Kyushu-based PIs of I^{2}CNER for FY 2017 (*the other 2 will be retiring) and one additional faculty member will be transferred to I^{2}CNER from the Faculty of Engineering.

2. System under which the center's director is able to make substantive personnel and budget allocation decisions

I^{2}CNER's Permanent Position within Kyushu University
- Effective April 1, 2013, with the revision of the "Regulations of Kyushu University," I^{2}CNER's position is clearly defined as a permanent Research Institute of Kyushu University.

I^{2}CNER Director's Authority
- I^{2}CNER's governing documents have been developed to assure that the Institute Director is solely responsible for making decisions on research plans, research frameworks, budget implementation, and other issues related to Institute management. By way of example, the Director has the authority to recruit new faculty through open international calls and to make the final hiring decisions, in consideration of recommendations from the Faculty Recruiting Committee based on application screening and interviews.

3. Support for the center director in coordinating with other departments at host institution when recruiting researchers, while giving reasonable regard to the

educational and research activities of those departments

Support for KU Dual-Appointment Researchers

- Kyushu University provides active support for the researchers who hold dual appointments at I²CNER and another unit of Kyushu University to facilitate their engagement in I²CNER's activities in coordination with their home departments, such as making request for cooperation and arrangements with the head of his/her home department.

4. Revamping host institution's internal systems to allow introducing of new management methods

(e.g., English-language environment, merit-based pay, cross appointment, top-down decision making unfettered by conventional modes of operation)

Merit-based Salary System

- I²CNER follows a special salary system which deviates from the established salary ranges. Individual faculty and researcher salaries are determined based on their accomplishments and contributions to the interests of the Institute, as decided by the Director, in consultation with the two Associate Directors.

Cross Appointment of Director Sofronis

- In consultation with the administration of the University of Illinois, it was decided that Prof. Sofronis be employed by Kyushu University as of June 1, 2012. This is KU's first case of cross appointment.

5. Utilities and other infrastructure support provided by host institution.

(*In addition to listed in the item 1. Contributions from host institution)

I²CNER Building 1 (Space Sharing with NEXT-FC)

- I²CNER building 1 (approximately 4,873 m^2) was completed at the end of November, 2012. A spacious lounge with a high ceiling and electronic black boards was designed in the lobby on the first floor in order to encourage impromptu meetings among I²CNER members. Also, an additional 7 labs, 15 researcher's offices, and a server room have been secured for I²CNER's researchers out of the space allocated to the Next-Generation Fuel Cell Research Center (NEXT-FC) of Kyushu University. The rooms secured for us out of the NEXT-FC include the labs for our collaborators from MIT and Imperial College London.

6. Support for other types of assistance

Associate Directors

- The two Associate Directors, Professors Ishihara and Takata, are "transferred faculty" from the Faculty of Engineering through the Intra-University Faculty Transfer System. They work in tandem with and on behalf of the Director to meet the objectives of the Institute, as well as coordinating with related departments of Kyushu University. When the Director is in Illinois or traveling, Professors Ishihara and Takata maintain daily communication with him in order to relay and implement the Director's plans.

Kyushu University Platform of Inter/Transdisciplinary Energy Research (Q-PIT)

- Kyushu University established the "Kyushu University Platform of Inter/Transdisciplinary Energy Research (Q-PIT)" in October 2016. The Q-PIT sets its vision to establish new energy systems for 2100 by "All Kyushu University" and aims to organize an innovative and all-encompassing international center for future energy research and education. I²CNER is expected to become a central pillar within this new organization.

World Premier International Research Center Initiative (WPI)

Appendix 5-2 The Host Institution's Mid-term Plan

[Mid-term Objective and Mid-term Plan of Kyushu University (excerpt)]

The Second Term (April 1, 2010 - March 31, 2016)

○ **Objectives on Research (Research Activities and Accomplishments)**

- Undertake exceptional research activity at the world's highest level as a global research and education center.

○ **Measures to Achieve the Objectives on Research**

- Promote leading-edge research related to the carbon-neutral energy research domain, upon which Kyushu University possesses its strength and unique characteristics. In collaboration with the University of Illinois, the International Institute for Carbon-Neutral Energy Research (I^2CNER) will contribute to this effort.
- Invite foreign researchers from the top universities in the world, such as the Massachusetts Institute of Technology, and conduct international joint research of the world's highest level.

The Third Term (April 1, 2016 - March 31, 2022)

○ **Objectives on Research (Research Activities and Accomplishments)**

- Further develop the University's strength—such as a wide diversity of academic fields, growing potentials of global expansion (based on the East-Asia-Strategy), and the profoundness of research and education—and undertake exceptional research activity at the world's highest level.

○ **Measures to Achieve the Objectives on Research**

- Promote leading-edge research related to the carbon-neutral energy research domain, which is primarily conducted at the International Institute for Carbon-Neutral Energy Research (I^2CNER) in collaboration with the University of Illinois, and strengthen the systems for conducting such research.
- Invite foreign researchers from top universities and institutes in the world, and conduct the international joint research of the world's highest level.
- Proactively advance collaboration and cooperation between I^2CNER and other diverse fields/domains, such as natural science (especially theory), mathematics, humanities, and social sciences, etc.

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Appendix5-3 Transition in the Number of Female Researchers

* Enter the number and percentage of female researchers in the top of each space from 2013 to 2016 and the total number of all the researchers in the bottom.

		FY2013	FY2014	FY2015	FY2016	Final goal FY 2020
Researchers		18, 12%	18, 11%	18, 11%	23, 13%	29, 17%
		156	166	166	174	172
	Principal investigators	1, 4%	1, 4%	1, 4%	1, 4%	1, 4%
		26	24	26	27	25
	Other researchers	17, 13%	17, 12%	17, 12%	22, 15%	28, 19%
		130	142	140	147	147