

# World Premier International Research Center Initiative (WPI)

## Executive Summary (For Final Evaluation)

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

Instruction:

Based on the Center's Progress Report and Progress Plan, prepare this summary within 6 pages.

### A. Progress Report of the WPI Center

#### I. Summary

As a result of I<sup>2</sup>CNER's current accomplishments and our projected future achievements, approximately 0.43% of the total required CO<sub>2</sub> reductions, and approximately 5.26% of the total 70% required reductions, respectively, can be realized by I<sup>2</sup>CNER technologies and innovations when they are applied to appropriate energy systems in Japan. Many metrics, such as I<sup>2</sup>CNER's numerous scientific discoveries and breakthroughs, its active engagement with industrial partners and transfers of innovative technology to industry, and the multitude of international universities seeking partnerships with I<sup>2</sup>CNER, demonstrate and quantify the Institute's scientific impact and international acclaim. The high-impact transformational reforms being instituted by the Kyushu University Administration that I<sup>2</sup>CNER has driven, as well as I<sup>2</sup>CNER's strategy for furthering technology-driven research, is positioning Kyushu University as a world-wide leader. The continual evolution of I<sup>2</sup>CNER's research themes is forging new partnerships with additional 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. After nearly 10 years of unceasing effort, I<sup>2</sup>CNER is woven into the very fabric of Kyushu University and the overall international energy research landscape. Despite the advances made by I<sup>2</sup>CNER, many roadblocks remain, but through its partnerships with mathematics, political and social sciences, and economics, the Institute is prepared to address these complex challenges. I<sup>2</sup>CNER is already making vital contributions toward the development of a future carbon neutral society, and its plans for the future are calibrated precisely to ensure that Japan meets its energy needs while achieving its carbon reduction targets by 2050.

#### II. Items

##### 1. Overall Image of Your Center

I<sup>2</sup>CNER's vision is to contribute to the creation of a carbon-neutral society (CNS) through basic research underlying technology that will address the energy challenge for Japan and the world, and establish a model international academic environment for the 21st century. In executing this vision, I<sup>2</sup>CNER aims to develop energy materials and systems which, when deployed, lead to a large reduction of greenhouse gas (GHG) emissions (70-80% by 2050 from 1990 levels). As a whole, we consider 3E+S (Energy security, Economic efficiency, Environmental protection, and Safety) as basic view points for the vision.

In pursuing our mission, 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). By prioritizing different LCI and EI technologies, renewables, and CCS, and by considering the ongoing energy transition occurring in Japan, I<sup>2</sup>CNER's vision is built on a most likely future energy system which involves a combination of renewable energy deployment and carbon capture and storage technologies, with the addition of hydrogen into the energy system, predominantly imported from overseas. To carry out its mission, I<sup>2</sup>CNER's research is driven by well-defined milestones and targets that are identified in roadmaps of the underlying technologies. Our roadmaps are developed by our Energy Analysis Division (EAD) and continuously updated through a close collaboration between the technical research clusters (divisions) and the EAD. By necessity the research teams are composed of scientists and engineers from disparate disciplines including chemistry, physics, materials science, mechanics, geoscience, biomimetics, applied math, economics, and social sciences, and the research addresses phenomena that span many decades in spatial and temporal scales. I<sup>2</sup>CNER's roadmap and research portfolio updates are also informed by the Institute's scientific exchanges with a stellar list of distinguished scientists from 25 partnering institutions across the globe, including the University of California, Berkeley; the University of Wisconsin-Madison; MIT; the National Fuel Cell Research Center at the University of California, Irvine; the State of California Air Resources Board (CARB) in the US; Imperial College, London in the UK; and the University of Göttingen in Germany.

I<sup>2</sup>CNER'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.

In line with our energy system scenario and as a result of our current accomplishments and our projected future achievements, approximately 0.43% of the total required CO<sub>2</sub> reductions, and approximately 5.26% of the total 70% required reductions, respectively, can be realized by I<sup>2</sup>CNER technologies and innovations when they are applied to appropriate energy systems in Japan. Additionally, the relevance of the I<sup>2</sup>CNER research efforts and objectives to enabling the green innovation initiative of the government of Japan is demonstrated by the large number (122) of collaborative projects in which its researchers are involved with industry. A total of 53 projects resulted in technology transfer events. Since inception, I<sup>2</sup>CNER has filed for 239 patents and was granted 67 patents.

## 2. Advancing Research of the Highest Global Level

I<sup>2</sup>CNER's research activities are conducted within its technical divisions in partnership with the EAD, which ensures continuous assessment of the 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. Since inception, the Institute has realized 45 of the short-term and 7 of the mid-term milestones in our project roadmaps, reached 4 ultimate targets from our roadmaps, realized a NEDO Target in the Hydrogen Storage division, and established 14 international benchmarks. A selection of the Institute's breakthrough results/achievements are presented in terms of the milestones and targets of the respective project roadmaps.

Energy Analysis Division: In addition to developing division project roadmaps, the EAD carried out several technoeconomic studies on energy challenges for Japan and the impacts of I<sup>2</sup>CNER solution pathways for emission reductions. Collaborating with WPI Visiting Professor Hirose from Toyota Motor Corporation and using geographic information system analysis, the EAD investigated hydrogen station deployment, identifying optimal station locations to meet refueling demands from fuel cell vehicles. The analysis identified the optimal way to locate hydrogen stations so that the average distance between potential customers and stations is minimized. More hydrogen stations need to be located in internal city locations, especially in prefectural capitals. In addition, the EAD progressed the "people, technology and systems nexus" research for energy transitions. The link between Japan's relatively unambitious renewable energy deployment goals and progress toward a successful transition was identified. Building on these findings, an investigation of Japanese energy users identified three distinct tranches of consumer activeness toward energy system participation and reasoning to determine how a bottom-up approach might further Japan's progress. Finally, applying the participation preferences of "active" and "intermediate" households, it was found that this approach to transitions can have a marked impact on energy system transitions, security, and safety.

Molecular Photoconversion Devices: Photocatalytic hydrogen fuel production can support future transportation but is limited by the slow hydrogen evolution kinetics. To overcome this, by combining chemical synthesis, atomic resolution microscopy, and first-principles modeling, PI Ishihara's team demonstrated for the first time that dopant atoms embedded in titania can function as co-catalysts, yielding hydrogen production at rates up to ten times that of undoped systems. They also created the first direct comparison of measured activity across a spectrum of dopants to computational predictions, leading to the ability to engineer these catalysts. The most promising new photovoltaic energy generation technology is based on hybrid organic/inorganic perovskite semiconductors. PI Adachi was the first to realize that the increased number of hole traps lying above the valence band edge under solar illumination is responsible for the degradation in the devices when exposed to moisture. By controlling water and oxygen ingress, the perovskite devices exhibited reduced carrier recombination and suppressed formation of metallic lead, improving stability. The recently extrapolated 50%-lifetime is over 20,000 hrs and among the world's top reported values, thus making the device a strong contender for a successful product.

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<sub>2</sub> reduction via an O<sub>2</sub> adduct. This is the first example worldwide of a side-on iron (IV) peroxo complex of an O<sub>2</sub>-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. PI Yamauchi's group developed highly selective electrocatalysts and a flow-type electrolyzer to directly produce transportable and storable alcoholic fuels with high volumetric energy density. The group also succeeded in generating power from alcoholic fuels without CO<sub>2</sub> emission via selective oxidation of alcohols, which is the first demonstration of CO<sub>2</sub>-free power circulation using liquid fuels.

Thermal Science and Engineering: PI Takata's foundational studies on phase-change heat transfer in nano-confined systems, as well as surface wettability due to hydrocarbon adsorption from the atmosphere, have led to a globally-unmatched fundamental understanding of phase change heat transfer. These accomplishments are re-writing the foundational knowledge base in the field of surface science and phase change heat transfer by quantifying the environmental effects on sample wettability and degradation. 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) activated carbons with ultra-high ethanol uptake. The focus of Prof. Miljkovic's interdisciplinary research on novel micro/nanostructures for durable and scalable enhanced phase-change heat transfer 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 the fundamental degradation mechanisms of hydrophobic coatings as well as their design criteria for low surface tension fluids, set the global benchmark for performance, and has immense technological impact on renewable and non-renewable power generation, thermal management, building energy, distillation, and separation technologies.

Electrochemical Energy Conversion: The main shortcoming of polymer electrolyte fuel cells and Li-O<sub>2</sub> 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 team of Prof. Nakashima and PI Fujigaya, of covering the carbon catalyst support in polymer electrolyte fuel cells and Li-O<sub>2</sub> 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 team of PIs Kilner, Ishihara, and Staykov 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.

CO<sub>2</sub> Capture and Utilization: Industrial requirements for membranes for CO<sub>2</sub> separation over nitrogen require that the CO<sub>2</sub> permeance exceed 4,000 GPU. PI Fujikawa and his group succeeded in manufacturing high CO<sub>2</sub> solubility free-standing polysiloxane (PoliSil)-based nanomembranes with thickness less than 50nm and CO<sub>2</sub> permeance greater than 40,000, which is the world’s highest. When tested under atmospheric pressure conditions, modified versions of this membrane captured CO<sub>2</sub> from a CO<sub>2</sub>/N<sub>2</sub> mixture with a CO<sub>2</sub> concentration of 1000 ppm. This finding expands the relevance of our research goals beyond the capturing of CO<sub>2</sub> at fire-powered plants to the entirely new area of direct CO<sub>2</sub> capture from the air. For the separation of CO<sub>2</sub> from H<sub>2</sub> at integrated gasification combined cycle (IGCC) plants, I<sup>2</sup>CNER developed alkanolamine-containing polymeric membranes. Specifically, the 2-(2-aminoethylamino)ethanol-containing membranes developed by Prof. Taniguchi exhibited CO<sub>2</sub> permeance of 155 GPU with selectivity of 10 at CO<sub>2</sub> pressure of 1.0 MPa and 80 % relative humidity. This permeance is the best reported in the open literature, although the selectivity needs to be improved. For the electrochemical reduction of CO<sub>2</sub> to value-added chemicals, ~90% of the overall energy required is consumed at the anodic reaction. Prof. Kenis’ group successfully found that CO<sub>2</sub> reduction with glycerol oxidation as the anodic reaction is associated with lower cell potential than with conventional oxygen evolution reaction. Due to the low cell potential, I<sup>2</sup>CNER holds the benchmark for lowest overall energy requirement for CO<sub>2</sub> electrolysis.

Hydrogen Storage: In a collaborative effort, Prof. Akiba and PI 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, Prof. 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, Prof. Akiba achieved hydrogen storage capacity of 9wt% and on-set temperature of 90°C through amide/hydride composites, which satisfied a NEDO target for on-board hydrogen storage applications.

CO<sub>2</sub> Storage: The coupled pore-scale flow dynamics of CO<sub>2</sub> and brine in geologic media represents a critical component of accurately predicting large-scale migration of injected CO<sub>2</sub>. PI Christensen’s work in this area is the first quantitative study of liquid CO<sub>2</sub>-water flow in both homogeneous and heterogeneous porous micromodels (inspired by real rock) at reservoir-relevant conditions, providing a detailed picture of the flow physics during the migration of the CO<sub>2</sub> front, the evolution of individual menisci and the growth of the dendritic structures, so called fingers. 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<sub>2</sub> phase, validating the significance of inertial effects. Pore drainage events were shown to be cooperative, with a zone of influence that extends beyond tens of pores, confirming that Haines jumps are non-local phenomena. These advances imply that pore-scale models of liquid CO<sub>2</sub> migration must be modified to account for such dynamic flow processes, which can greatly alter macroscale migration of CO<sub>2</sub> in geologic reservoirs. The group of PI Tsuji developed a novel monitoring method to quantify CO<sub>2</sub> 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<sub>2</sub> saturation with monitoring-derived seismic velocity. This monitoring system is currently deployed in an ongoing CO<sub>2</sub> 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. For the first time, combining experiments and modeling, studies by the team of PIs Somerday, Kirchheim, Kubota, and Sofronis have revealed the physics governing inhibition of H<sub>2</sub>-accelerated fatigue crack growth by ppm-levels of O<sub>2</sub>. The significance of these development is in predicting the lifetime of metal components in a high-pressure hydrogen gas environment.

### 3. Feeding Research Outcomes Back into Society

The relevance of the I<sup>2</sup>CNER research efforts and objectives to enabling the green innovation initiative of the government of Japan is demonstrated by the large number (122) of collaborative projects in which its researchers are involved with industry. A total of 53 projects resulted in technology transfer. Since inception, I<sup>2</sup>CNER has filed for 239 patents and was granted 67 patents.

Representative examples of technology transfer include: 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 worked 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<sub>2</sub> monitoring system in collaboration with the Japan Oil, Gas and Metals National Corporation (JOGMEC) has been transferred and deployed in the ongoing CO<sub>2</sub> 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 have been submitted to the Ministry of Economy, Trade and Industry of Japan in the form of 73-page report in February 2017; x) PI Fujigaya received funding in FY18 from KU and the Fukuoka Bank for a **startup company** called FUJicat on novel electrocatalysts.

### 4. Generating Fused Disciplines

The Director has at his disposal "I<sup>2</sup>CNER Competitive Funding," which is intended to foster and advance interdisciplinary research. The Director has utilized the "Competitive Funding Initiative" to accelerate the Institute's strategic efforts and integrate applied math and economics into I<sup>2</sup>CNER's research portfolio. In FY15-FY17, a total of 13 applications were selected as "seed projects," and those projects are now a new interdisciplinary research direction of "Applied Math and Economics for Energy," which is and will be an important component of I<sup>2</sup>CNER. I<sup>2</sup>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 respective establishment of computational science and applied math as integral components of I<sup>2</sup>CNER's research portfolio.

I<sup>2</sup>CNER provides unique opportunities for bottom-up research, giving researchers opportunities to create and establish new research directions. In particular, young researchers have formed an important part of I<sup>2</sup>CNER. For example, Assistant Professor Perry and Associate Professor Ertekin (Illinois) were awarded internal seed funding so that they could focus on combined computational and experimental studies of oxygen exchange on electrode surfaces, which 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.

The disparate nature of the disciplines involved in the I<sup>2</sup>CNER research fields facilitates interdisciplinary work through collaborations across division boundaries. The work by PIs Kilner, Ishihara, and Staykov that led to the understanding of the oxygen surface exchange kinetics in solid oxide 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 (Sandia National Laboratories) with PI 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. Realizing an International Research Environment

The environment at I<sup>2</sup>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. Since inception, there have been a vast amount of international activities that enhanced I<sup>2</sup>CNER's global visibility. I<sup>2</sup>CNER has hosted 40 international symposia; held 143 seminars in the Institute Interest Seminar Series (IISS) with 256 speakers of which 158 were non-Japanese; 157 seminars in the I<sup>2</sup>CNER Seminar Series with 161 total speakers of which 105 were non-Japanese. The Institute's researchers were responsible for organizing, co-organizing, or serving on the scientific committees for 207 international conferences, 278 international conference sessions/symposia or workshops, and 68 I<sup>2</sup>CNER international workshops. Our researchers have given 565 keynote, plenary and invited presentations in international conferences and fora. In addition, our researchers have joint publications with researchers from 573 institutions around the world (38 new institutions in FY18) and hosted 343 internationally recognized researchers for scientific interactions and exchange. Lastly, since inception, of our 91 young researchers, 21 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.

As part of its commitment to fostering globally-aware researchers starting from the undergraduate level, I<sup>2</sup>CNER sends approximately 6 undergraduate students from KU to carry out research in the laboratories at the University of Illinois on an annual basis. The Institute also hosts 6 undergraduate students from the US (Illinois, Northwestern, and the University of California, Berkeley) who participate in summer research programs in I<sup>2</sup>CNER laboratories.

The I<sup>2</sup>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<sup>2</sup>CNER researchers 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. Making 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<sup>2</sup>CNER operations by President Kubo, iii) the cross-appointment employment system was institutionalized and applied throughout KU, iv) the Intra-university faculty transfer system was established, v) I<sup>2</sup>CNER faculty involvement with teaching is increasing, vi) KU introduced I<sup>2</sup>CNER's merit-based salary system across all units, vii) I<sup>2</sup>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) Adopting I<sup>2</sup>CNER as a model concept for the internationalization of research and education, KU established the Platform of Inter/Transdisciplinary Energy Research (Q-PIT), xii) EVP Wakayama led the efforts to expand I<sup>2</sup>CNER's collaborations with other units, e.g. IMI, xiii) faculty council regulations were changed dramatically, and xiv) KU switched to the Academic Quarter (4-term) System to enable faculty cross-appointments (from KU and overseas)

## **7. Others**

Evidence of I<sup>2</sup>CNER's international stature and relevance can be seen in its 2,022 journal publications since inception, of which, 142 were published in journals with an impact factor greater than 10. In fact, the Institute's rate of productivity continues to remain high (53, 150, 263, 318, 308, 316, 316 and 298 publications in CY2011, 12, 13, 14, 15, 16, 17, and 18 respectively). Since its inception, 386 of the Institute's publications have been cited between 10 and 19 times, 184 have been cited 20-29 times, 89 have been cited 30-39 times, 41 have been cited 40-49 times, and 128 have been cited 50 or more times.

Additionally, a delegation of 11 executives and faculty from various KU departments visited Illinois on May 8-10, 2019 to work on a joint vision statement for the future of the Kyushu-Illinois Strategic Partnership. The purpose of the KU delegation's visit is to build a strategic partnership between UIUC and KU that broadens the collaborations to other Colleges and departments. August 26, 2019 has been set as the date for the signing ceremony of the revised MOU between the two universities. KU's president, Prof. Kubo, will be visiting Illinois to sign the agreement alongside Illinois' Chancellor, Prof. Jones.

## **B. Progress Plan**

### **1. Mid- to Long-term Research Objectives and Strategies Based on the Center's Research Results to Date**

I<sup>2</sup>CNER has amassed a remarkable record of accomplishments over the past 10 years. It has defined and embraced the development of the science to dramatically reduce Japan's CO<sub>2</sub> emissions while strengthening Japan's energy security. I<sup>2</sup>CNER's many accomplishments have been built on the development and growth of extremely strong research teams at Kyushu University and at the Satellite Center at the University of Illinois at Urbana-Champaign. The capabilities of these research teams are further strengthened by a high level of engagement with other of the world's best scientists in I<sup>2</sup>CNER's areas of technical expertise. I<sup>2</sup>CNER's mission and accomplishments are directly in line with Japan's vision for a robust energy future which optimizes energy resources in concert with Japan's overarching energy vision: energy security, economic efficiency, and environmental protection without compromising safety (3E+S). I<sup>2</sup>CNER has moved its science accomplishments forward through large scale interactions with industry where I<sup>2</sup>CNER developments can be directly implanted for use in society.

From the very beginning, I<sup>2</sup>CNER recognized the need for the development of roadmaps with milestones and targets to guide its science initiatives toward the long-term 2050 CO<sub>2</sub> emissions reduction goal. Each division's progress is tracked by continuous assessment of research efforts toward their research milestones. This approach has guided the use of I<sup>2</sup>CNER's resource allocations which enabled a research portfolio that includes high-risk high-payoff science balanced with science with clearly identifiable directions and outcomes. *I<sup>2</sup>CNER sees that this approach, which has proven highly successful in the past, should direct the science and resource planning for the future.*

Our vision for the future will also ensure that Japan remains at the forefront of international science addressing the energy challenge and carbon emissions. Additionally, it ensures that Japan will lead

the technology transfer process to implement the best new developments to reduce carbon impact. Engaging the world's best scientists in this mission is critical to success. I<sup>2</sup>CNER has earned an international reputation for involvement of the best scientists to address an issue of major importance to all of humanity. The future I<sup>2</sup>CNER efforts will continue to develop and grow these relationships as a central, overarching element of all future activities.

To make best use of resources, I<sup>2</sup>CNER will streamline its research portfolio by reshaping its strongest research themes and phasing out those that are less impactful. Our focus continues to address basic science and engineering with the overall goal of reduced CO<sub>2</sub> emissions. Moving forward, the three streamlined thematic research clusters or **Thrusts** will be **Advanced Energy Materials, Advanced Energy Systems, and Energy Future and Environment**. This structure allows us to capture all of the most relevant existing capabilities and to organize them for the best future impact. It also provides an efficient mechanism for top international and Japanese researchers to work interactively to accomplish common goals which cut across disciplines. I<sup>2</sup>CNER will continue to rely on the central role of the current Energy Analysis Division that will be integrated in the Energy Future and Environment Thrust, in close cooperation with the other two Thrusts, to set near, medium, and long-term goals to meet I<sup>2</sup>CNER's mission. *This includes the continued use of Roadmaps to set research goals and assess progress.*

The Advanced Energy Materials Thrust combines the best features of the development of materials for hydrogen transport and storage, materials for selective CO<sub>2</sub> capture, and materials for efficient energy conversion, particularly for fuel cell and regenerative energy applications. The Advanced Energy Systems Thrust combines the efforts of multiple I<sup>2</sup>CNER researchers to develop systems approaches and capabilities for efficient energy conversion and applications. Progress in these areas requires systems-level approaches which can also make use of new materials developed in the Advanced Energy Materials Thrust. The Energy Future and Environment Thrust pulls together the range of challenges facing Japan's and the world's energy transition, namely the transition from largely fossil fueled energy technology to a carbon-neutral or a carbon-free energy supply. This Thrust enables the coordination of carbon reduction technologies, energy efficiency technologies, and guidance for social, political, and investment strategies to coordinate this transition.

The three research Thrusts will be interwoven with the **Platform for International Collaborations and Partnerships**. This platform is intended to maintain and foster I<sup>2</sup>CNER's international identity. The members of this platform, who are world experts, will continue to collaborate with I<sup>2</sup>CNER's researchers from all three Thrusts. Since the Platform for International Collaborations and Partnerships and the three Thrusts are interwoven and the Thrusts' themes overlap, this will be an effective way to promote interdisciplinary collaborations across the institute and the world. I<sup>2</sup>CNER currently has 25 partnering institutes and these collaborations will continue to grow. More specifically, the aim is to expand on the substantive collaborations that already exist with institutes such as: Illinois, MIT, Paul Scherrer Institute at ETH, Imperial College, London, Goettingen, and the University of Edinburgh. Given I<sup>2</sup>CNER's portfolio on non-engineering aspects of energy, some of these partnerships may then grow into strategic partnerships with Kyushu University to involve various departments (e.g. Economics, Law, Humanities, and Mathematics).

The three major Research Thrusts will all contribute directly to the transition of future I<sup>2</sup>CNER science advances to applicable technology transfer through a large and growing network of I<sup>2</sup>CNER industrial interactions. The **Platform for Societal Implementation and Industrial Collaboration** will ensure this high level of tech transfer. This coordination with Japan's energy and transportation industries will also have an impact on Japan's international markets, where carbon-reduction technologies are lagging behind Japan's efforts. The future I<sup>2</sup>CNER Platform for Societal Implementation and Industrial Collaboration will also provide policy guidance for science and technology investments, as well as addressing possible social acceptance and social impact issues. With its strengths in both advanced energy science and energy analysis, I<sup>2</sup>CNER will provide critical direction and support to Japan's energy transition over the next 30 years to meet the 2050 carbon reduction goals with minimal social and economic disruptions.

I<sup>2</sup>CNER has built an effective, world-leading research and technology program that exemplifies the WPI vision. Additionally, I<sup>2</sup>CNER increased diversity, provided a new culture for young scientists to thrive independently and to foster collaborations for interdisciplinary research around the world. This altogether is directed toward solving Japan's energy and carbon challenge. This is the goal around which I<sup>2</sup>CNER coalesced from the very early stages, and the goal toward which I<sup>2</sup>CNER has taken great strides over the past 10 years. The drastic reduction of carbon emissions in concert with the 3E+S remains the Grand Challenge which will require a continued, concerted, focused effort to meet that goal. Japan's leadership in this area will open new international markets and have a positive impact on international societal evolution to a more carbon-free world. *The support for this effort through I<sup>2</sup>CNER's induction into the WPI Academy is critical to fulfilling this Grand Challenge.*

## **2. Management System of the Research Organization**

I<sup>2</sup>CNER will continue to operate under the strong leadership of Director Sofronis, who will be reporting to EVP Inoue on a monthly basis (see Section 6.1 of the Progress Report (for Final Evaluation)). Beginning in FY20, the organizational structure will be revised to the "*Three Thrust, Two Platform*" approach. I<sup>2</sup>CNER will maintain its international identity through the *Platform for International Collaborations and Partnerships*. This platform will involve the academic institutions of the international PIs, namely Illinois, MIT, Paul Scherrer Institute at ETH, Imperial College, London, Goettingen, Tsinghua, and institutions with which we developed research interactions and collaborations during the past 10 years of operation, e.g. the University of Edinburgh. *I<sup>2</sup>CNER's Platform for Societal and Industrial Implementation* will be tasked to accelerate impactful technology development and transfer to industry, and advance the engagement of I<sup>2</sup>CNER with the society at a broader institutional level.

A number of experts in applied math, social sciences, and economic systems from other units of KU will be invited to join I<sup>2</sup>CNER as WPI Professors in order to diversify the population and expertise of I<sup>2</sup>CNER, and expand its research portfolio.

### **3. Center's Position within the Host Institution, and Measures Taken by Host Institution to Provide Resources to the Center**

#### **I<sup>2</sup>CNER's Permanent Position within Kyushu University**

Effective April 1, 2013, with the revision of the "Regulations of Kyushu University," I<sup>2</sup>CNER's position is clearly defined as a permanent Research Institute of KU without regard to the length of the WPI Program.

#### **Kyushu University Platform for Inter/Transdisciplinary Energy Research (Q-PIT)**

The Q-PIT was inaugurated on October 1, 2016 to bring together green-energy engineers with unexpected partners such as mathematicians, political scientists, social scientists, and economists to "solve the global challenges necessary to achieve a balance between emissions caused by humans and the removal of greenhouse gasses in the second half of this century," as President Kubo announced. Drawing from its international research experiences and approaches, I<sup>2</sup>CNER will play a central role in this new organization by helping to promote and advance a wide range of collaborations on energy research with other KU units. This will allow the Institute to capitalize on opportunities to broaden and enrich its energy portfolio while also helping Q-PIT advance its mission to catalyze interactions between diverse and disparate disciplines and units. I<sup>2</sup>CNER's Director Sofronis is member of the strategic committee of Q-PIT.

#### **Securing and Filling I<sup>2</sup>CNER Tenured Faculty Positions**

KU implements the "University Reform Revitalization Program" to encourage its units to actively review and reform their structure to revitalize the University. The President's Vision for tenured PIs in I<sup>2</sup>CNER is that the units compete for tenured positions through annual proposal submissions. In line with this policy and the President's Vision for tenured PIs in I<sup>2</sup>CNER, I<sup>2</sup>CNER competes for tenured positions through this program through annual proposal submissions, and will make continued efforts to secure additional tenured positions. I<sup>2</sup>CNER has been successful at winning and filling positions. By the end of FY18, I<sup>2</sup>CNER filled a total of 6 Associate and 4 Full Professor positions, and 2 tenure-track assistant professors on applied math for energy jointly with IMI.

#### **I<sup>2</sup>CNER's Place in Kyushu University Infrastructure**

The university will grant I<sup>2</sup>CNER Building II (a total floor space of 5,014 m<sup>2</sup>) free of charge to provide the I<sup>2</sup>CNER researchers with the requisite environment to continue their cutting-edge research. The space provided by this support significantly exceeds the space allotment per researcher under the university's regular policy.

#### **Kyushu University Administration Support of I<sup>2</sup>CNER Administrative Office**

KU will support the salaries of the required staff members, thus securing the successful operation of the "*Three Thrust, Two Platform*" new I<sup>2</sup>CNER organization.

# World Premier International Research Center Initiative (WPI) Progress Report of the WPI Center (For Final Evaluation)

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

**Common Instructions:**

- \* Unless otherwise specified, prepare this report based on the current (31 March 2019) situation of your WPI center.
- \* As a rule, keep the length of your report within the specified number of pages. (The attached forms are not included to this page count.)
- \* Use yen (¥) when writing monetary amounts in the report. If an exchange rate is used to calculate the yen amount, give the rate.

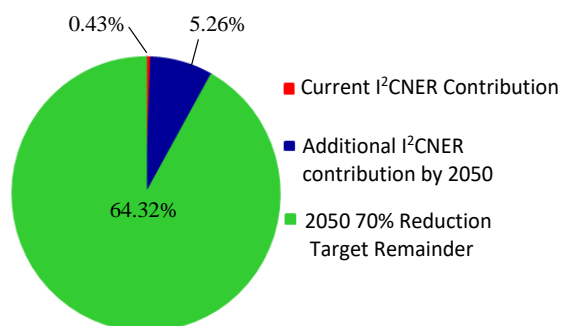
## 1. Overall Image of Your Center (write within 2 pages including this page)

Describe the Center's current identity and overall image.

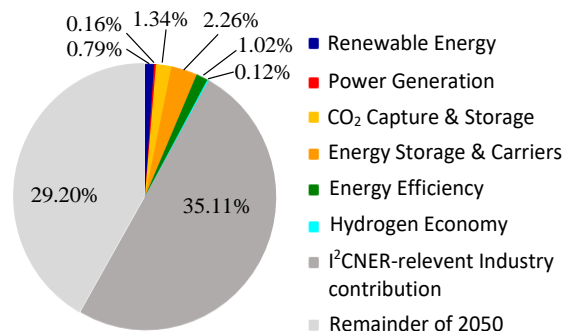
- List the Principal Investigators in Appendix 2, and enter the number of center personnel in Appendix 3-1, 3-2, diagram the center's management system in Appendix 3-3, draw a campus map in Appendix 3-4, and enter project funding in Appendix 3-5, 3-6.

I<sup>2</sup>CNER's vision is to contribute to the creation of a carbon-neutral society (CNS) through basic research underlying technology that will address the energy challenge for Japan and the world, and establish a model international academic environment for the 21st century. In executing this vision, I<sup>2</sup>CNER aims to develop energy materials and systems which, when deployed, lead 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 and takes into consideration the use of some GHG credits. As a whole, we consider 3E+S (Energy security, Economic efficiency, Environmental protection, and Safety) as basic view points for the vision.

(a) Current and Future Contributions



(b) Overall Contributions to 2050 CO<sub>2</sub> Reduction Target



**Figure 1.** I<sup>2</sup>CNER's current and future contributions toward the achievement of national GHG emission reductions, cognizant of our scenario and the likely transition pathway of Japan

Pursuing our mission, 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, and by considering the ongoing energy transition occurring in Japan, we explored and developed multiple scenarios. Currently I<sup>2</sup>CNER's vision is built on a **balanced scenario** involving a combination of renewable energy deployment and carbon capture and storage technologies, with the addition of hydrogen into the energy system, predominantly imported from overseas. I<sup>2</sup>CNER's research efforts are intimately tied to this scenario because the short-, mid-, and long-term milestones of each of our research project roadmaps were established in consideration for the removal of the roadblocks in the development and deployment timing of the various promising technology options within the scenario. Our roadmaps are developed and continuously updated through a close collaboration between the technical research clusters (divisions) and the Energy Analysis Division (EAD). The updating of the I<sup>2</sup>CNER roadmaps and research portfolio is also



informed by the Institute's scientific exchanges with a stellar list of distinguished scientists from 25 partnering institutions across the globe that includes the University of California, Berkeley; 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 US; Imperial College, London in the UK; and the University of Göttingen in Germany.

In line with our energy system scenario and as a result of our current accomplishments and our projected future achievements, approximately 0.43% of the total required CO<sub>2</sub> reductions, and approximately 5.26% of the total 70% required reductions, respectively, can be realized by I<sup>2</sup>CNER technologies and innovations when they are applied to appropriate energy systems in Japan (Fig. 1a). Significantly, in addition to I<sup>2</sup>CNER's direct contributions, development and implementation of technologies that are relevant to I<sup>2</sup>CNER's technology efforts by other agencies will account for a further 35.11% of the 2050 target (shown in dark grey in Fig. 1b), which demonstrates that I<sup>2</sup>CNER's research efforts underpin impactful energy technologies. As shown in Fig.1b, the leading contributors to I<sup>2</sup>CNER's 2050 CO<sub>2</sub> reduction efforts include energy storage and carriers, encompassing electrolysis and the reversible fuel cell; CO<sub>2</sub> capture and storage, through novel CO<sub>2</sub> separation membranes and monitoring technologies; and energy efficiency, utilizing energy saving loop heat pipe technologies and friction reducing coatings. Lastly, the positive impact of I<sup>2</sup>CNER's accomplishments, not only on science, engineering, and offsetting CO<sub>2</sub>, but also on employment, the active transfer of technology to industry, influence on social and academic impacts including education and cultural exchange, and international partnerships, is described in detail by a living and annually updated document titled "Powering the Future: Economic, Environmental, and Social Impacts of I<sup>2</sup>CNER."

A unique and important component of I<sup>2</sup>CNER 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 University (KU) and Illinois, and a specific agreement for undergraduate student exchange are in place.

Our researchers have joint publications with researchers from 573 institutions around the world, and 343 internationally recognized researchers visited I<sup>2</sup>CNER 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 207 international conferences, 278 international conference sessions/symposia or workshops, and 68 I<sup>2</sup>CNER international workshops. In addition, I<sup>2</sup>CNER researchers have received a total of 310 (including 33 in FY18) national and international awards (including best oral, poster, and encouragement presentation awards for young researchers) from various professional societies and institutions around the world.

The environment at I<sup>2</sup>CNER provides a rich platform for young researchers to pursue transformative research in a non-traditional and highly multi-disciplinary and international setting. Of the 91 young researchers, 21 went on to take faculty positions at universities in Japan (excluding KU) 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 three years is the fusion of applied math with energy engineering, based on the Institute's burgeoning relationship with KU's Institute of Mathematics for Industry (IMI) and various departments at the University of Illinois at Urbana-Champaign.

The relevance of the I<sup>2</sup>CNER research efforts and objectives to enabling the green innovation initiative of the government of Japan is demonstrated by the large number (122) 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 53 projects resulted in technology transfer events. Since inception, I<sup>2</sup>CNER has filed for 239 patents and was granted 67 patents.

I<sup>2</sup>CNER is spearheading KU's globalization efforts within the University Reform Revitalization Program, and I<sup>2</sup>CNER faculty are instructors in the international programs of KU. I<sup>2</sup>CNER'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, I<sup>2</sup>CNER is a highly successful research and education test bed. It is a national and global experiment that *tackles key scientific challenges along the path to providing Japan with carbon-neutral and sustainable energy supplies and the advancing of low-carbon energy transition despite limited energy resources* through internationalization of scientific research and education in Japan, the US, and the world at large.

## 2. Advancing Research of the Highest Global Level (within 15 pages)

### 2-1. Research results to date

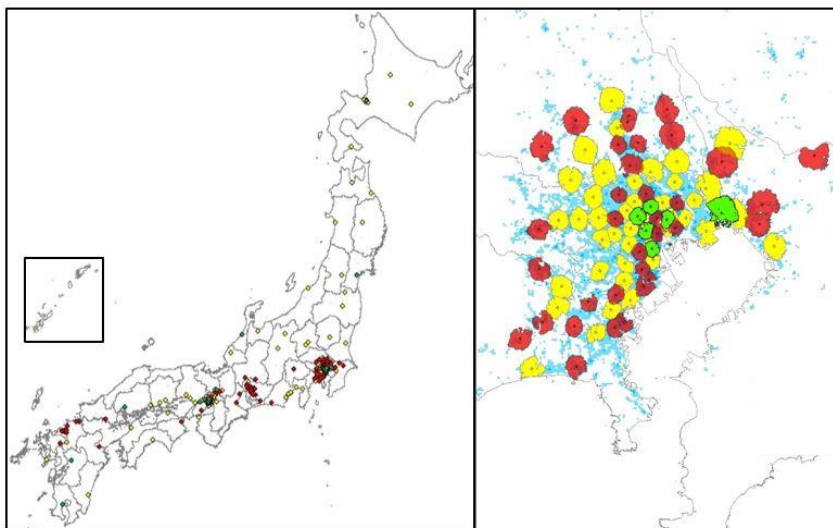
Describe issues of a global level that the Center has challenged, and give the results. Select 20 representative results achieved during the period from 2010 through March 2019. Number them [1] to [20] and provide a description of each. Place an asterisk (\*) in front of those results that could only have been achieved by a WPI center and explain the reason in the description.

- In Appendix 1-1, list the papers underscoring each research achievement (up to 40 papers) and provide a description of each of their significance. And in Appendix 1-4 list the center's research papers published in 2018.

Evidence of I<sup>2</sup>CNER's international stature and relevance can be seen in its 2,022 journal publications since inception of which 142 were published in journals with an impact factor greater than 10. In fact, the Institute's rate of productivity continues to remain high (53, 150, 263, 318, 308, 316, 316 and 298 publications in CY2011, 12, 13, 14, 15, 16, 17, and 18 respectively). Since its inception, 386 of the Institute's publications have been cited between 10 and 19 times, 184 have been cited 20-29 times, 89 have been cited 30-39 times, 41 have been cited 40-49 times, and 128 have been cited 50 or more times.

I<sup>2</sup>CNER's research activities are carried out within its technical divisions in collaboration/interaction with the 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. According to I<sup>2</sup>CNER's scenarios, the I<sup>2</sup>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. In the following, some of our best accomplishments are presented in relation to the advancement of the institute toward its roadmap milestones and targets. Since inception, the Institute has realized 45 of the short-term and 7 of the mid-term milestones in our project roadmaps, reached 4 ultimate roadmap targets, realized a NEDO Target in the Hydrogen Storage division, and established 14 international benchmarks.

**\*[1] Hydrogen station deployment for fuel cell vehicles:** The objective of this study was to develop an effective model for domestic hydrogen station deployment and identify prospective areas for hydrogen



**Figure 2.** 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.

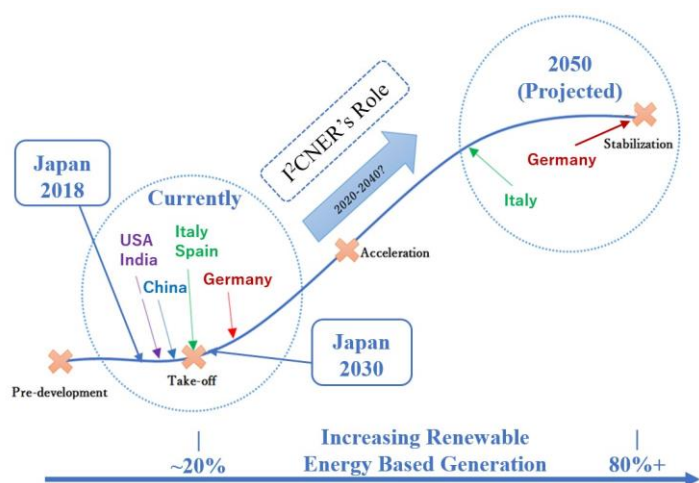
stations locations to meet future refueling demands of fuel cell vehicles (FCV). A deployment model employing location allocation theory using GIS (geographic information system) was used to consider user convenience and FCV penetration phases.

The model assumed that current high-priced luxury car (over 5 million yen) owners were the potential initial FCV customers and medium class car (over 3 million yen) owners were the potential FCV customers of the future. 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 (Fig. 2). 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 [1]. The results were directly reported to the Ministry of Economy, Trade and Industry and shared with hydrogen station stakeholders to support hydrogen deployment policy and planning in Japan. Also, the model results of follow-up analyses are currently used by JHyM (the Japan Hydrogen Station Network Joint Company), created by major car companies and energy companies to develop hydrogen refueling infrastructure.

**\*[2] Energy Transitions: The People, Technology, and Systems Nexus:** The Japanese energy system is undergoing an energy transition from a system traditionally highly reliant on nuclear and fossil fuel energy sources toward a low-carbon energy system which includes renewable energy and complementary technologies including hydrogen and battery storage, and carbon capture and storage. Our research focuses on a number of aspects including the influence of exogenous shocks and liberalization on the transition progress, and the role of the socio-technical regime on further influencing the nature of the market and technologies which will enable a successful low-carbon energy transition. In the 'people-technology-systems' nexus, we consider a broad range of issues underpinning the transition in a systemic manner, identifying policy implications and priority I<sup>2</sup>CNER technologies which may contribute to the transition in Japan and internationally.

The EAD carried out: i) a comparative review of Japan and transition leaders' progress and policies supporting the transition, drawing learnings to improve future progress, and, ii) a national survey to establish stakeholder activeness. As shown in Fig. 3, Japan's progress toward a successful transition lags



**Figure 3.** Leading countries' current position and projection toward a successful energy transition.

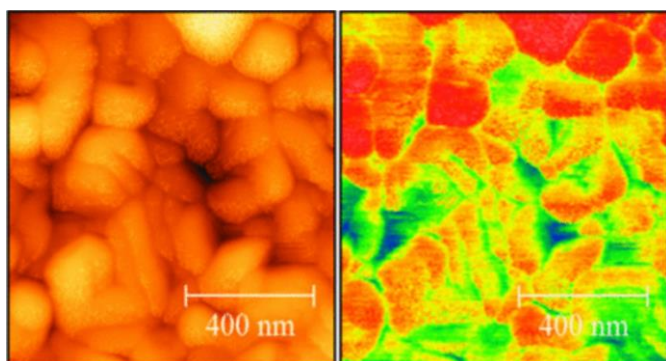
behind that of international leaders, however Japan may have a future competitive advantage in being a late enactor of energy market liberalization [2]. Further, through an investigation of householder knowledge, usage and preferences toward energy and energy policies, we were able to deduce three distinct tiers of stakeholder activeness and motivation. Approximately 14.6% of Japanese consumers are likely to actively seek economic and environmental benefits through market products and services, 41% of consumers act, depending on the level of perceived benefit, while a further 44.4% of people remain indifferent to new market products and services [3].

Additional analysis was undertaken on potential impacts on the future transition, by incorporating householder preferences in

**\*[3] Photovoltaic conversion efficiency and stability in hybrid perovskite based devices:** Achievement of both high photovoltaic conversion efficiency and stability in hybrid perovskite based devices remains a key challenge to the technology. The Adachi group, working with international collaborators, has achieved globally-recognized successes in hybrid perovskite photovoltaics as well as demonstrated key mechanisms for degradation. Some of the most important contributions include the following:

- (i) The group was one of the first to identify degradation of the lead-iodide in lead-containing perovskites, resulting in formation of metallic lead. This was shown to be connected to moisture and oxygen in the device layers. The group showed that changing the processing conditions for the device to avoid exposure to these, they could dramatically improve lifetime (by a factor of 2.5). The formation of metallic lead was also connected directly to carrier recombination states in the materials, which is a primary cause of efficiency loss.
- (ii) The group has also demonstrated an entirely new method for stabilizing perovskite photovoltaics by including additives in the deposition precursor solutions [4]. As one example of this process they showed that addition of benzoquinone (BQ) to the precursors improved conversion efficiency and device stability by improving the crystal structure and morphology of the perovskite. In BQ-incorporated

perovskite solar cells, the power conversion efficiency was  $\sim 15\%$  and the 80%-lifetime (at which efficiency reduces to 80% of the initial under illumination) was 4,000 hrs. Our recently extrapolated 50%-lifetime is over 20,000 hrs and among the world's top reported values. This approach has been adopted world-wide for solution processed hybrid perovskite photovoltaics. We also demonstrated that our perovskite alloy solar cells fabricated by mixing several cations and anions were very thermally stable and that our lead-free tin iodide-based perovskite solar cells fabricated with a modified solvent bathing method had very high stability, with almost no degradation under continuous illumination over 1,000 hrs. More recently, our systematic optimization of hybrid perovskite materials and solar cell architectures led to an increase of power conversion efficiency to  $\sim 21.5\%$  and extrapolated 50%-lifetime to  $\sim 23,000$  hrs (manuscript under preparation). *These results exceed the milestone of  $>20\%$  in power conversion efficiency and  $>10,000$  hrs in 50%-lifetime for Project 1 in the Molecular Photoconversion Devices division's roadmap and are approaching the mid-term milestone.* (iii) In the past year the group has published results of a new approach to improving efficiency of the devices by addition of photochemically active additives which



**Figure 4.** Kelvin-probe force microscopy images of changes to hybrid perovskite materials when doped with benzoquinone [5]. Contact potential differences at grain boundaries decreased under illumination, leading to efficient carrier transport across grain boundaries.

populate grain boundaries in the hybrid perovskites. These reduce the contact potential at the boundaries, and were shown to promote carrier transport and collection. The mechanism for this improvement was demonstrated using scanning probe microscopy and provides a general understanding of a key method to improve device performances. (iv) Working with collaborators in Australia, the United States, and Lithuania, and other countries, our team has established a variety of fundamental understandings of the operation of these devices. We have developed a theory of carrier transport and carrier trapping in the devices, demonstrated the mechanisms for trap

formation, and simulated the behaviors with various numerical models including drift-diffusion and density functional theory methods. This fundamental understanding is improving optimization of devices world-wide. These and other results are widely cited by other groups as groundbreaking in the field of perovskite photovoltaics. *The research has direct connections to and is improving organic light emitting device performance and is opening new approaches to thin film transistor technologies.*

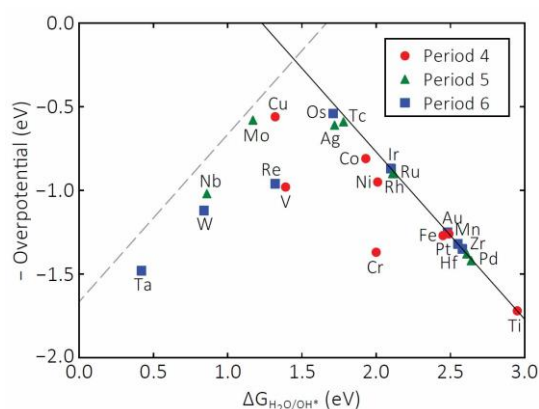
At the same time, the Adachi group has made world-recognized contributions to the technology of organic light emitting devices. Most notably, since the inception of I<sup>2</sup>CNER, the group has extended its prior work on triplet-to-singlet converter molecules, i.e., thermally activated delayed fluorescence (TADF), resulting in exceptionally high levels of luminosity in the devices. Using this approach, we achieved nearly 100% internal quantum efficiency converting injected current into light emission [5] and clarified the TADF mechanism. More recently we have focused on developing new light emitting molecules to enhance the performance and lifetime of blue light emitters. These are particularly difficult because the higher the energy of emitted photons (as in blue light) the lower the typical lifetime of molecules providing the emission. Furthermore, current injection into these molecules becomes increasingly difficult when high energy photons are to be produced. Finally, it is critical to develop efficient blue light emitters as these can be used to drive emission at longer wavelengths, yielding a white light source.

**\*[4] Novel Photocatalysts:** Photocatalytic splitting of water to form hydrogen and release oxygen is one of the approaches being explored for inexpensive transportation fuel production and is a key component of Project 2-2 in the Molecular Photoconversion Division. A successful approach requires an improved photocatalyst that will directly absorb sunlight and transfer the energy into breaking a H-O bond in water molecules. Typically, this can be limited by slow reaction kinetics for hydrogen evolution. PI Ishihara and his collaborators at Kyushu University, Imperial College, London, the University of Illinois at Urbana-Champaign, and elsewhere have been working to understand the fundamental properties of electrode materials and to improve these through theory-guided molecular and inorganic solid design. The result is an integrated multiscale modeling approach combined with experiments to demonstrate intelligent design of advanced photocatalysts. The approach has already resulted in dramatic improvements in materials performance.

Combining first-principles electronic structure calculations with experimental data and intelligent materials design, the team in collaboration with the Ertekin theory group at the University of Illinois have demonstrated a model for co-catalyst activity in which rhodium (Rh) atoms are incorporated into titania (TiO<sub>2</sub>) nanosheets [6]. Atomistic first-principles methods were used to reveal the process by which photo-generated charges are transferred to the Rh reaction center. The Rh atom was shown to capture free photoelectrons from the TiO<sub>2</sub> and transfer them to adsorbed H<sub>2</sub>O molecules, resulting in catalytic release of H<sub>2</sub> at increased rates relative to TiO<sub>2</sub> without the Rh dopant. Having demonstrated the basic mechanism, the team then assessed the potential for other transition metal atoms to function in similar ways and to determine which would produce the optimal catalysis of the reaction (Fig. 5) [7]. Experiments with pure TiO<sub>2</sub> and with doping of both Rh and Pd showed the predictive capability of the model. Design rules were developed for identifying rate-limiting steps in the reaction. This provided the first direct comparison between experiment and computation and the first reliable method for design of advanced co-catalyst dopants for photocatalysis.

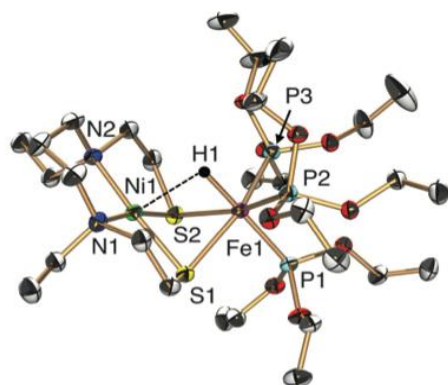
Taking the next step, the model was integrated with a drift-diffusion simulation tool to understand charge transfer at a macroscopic scale. This approach couples the atomic scale first-principles method with the full device scale behavior. Using this method an improved two-layer photocatalyst involving TiO<sub>2</sub> coating of CaFe<sub>2</sub>O<sub>4</sub> was designed and demonstrated. The CaFe<sub>2</sub>O<sub>4</sub> acts as the solar absorber material while the TiO<sub>2</sub> protects the absorber from corrosion during operation. The combination also reduces recombination of photogenerated carriers. This was combined with the Ru co-doping to produce efficient water splitting under visible (470 nm) light. The model correctly explained why illumination under 300 nm light produced inferior results due to photogeneration in the TiO<sub>2</sub>, demonstrating the importance of the multiscale modeling approach.

The design of advanced photocatalysts has also been extended by the team through their development of new processing methods to create the catalysts that theory predicts should work well. The team showed, for the first time worldwide, that high pressure torsion could stabilize unique new crystal structures of ZnO and TiO<sub>2</sub> and their mixtures with other compounds[8]. The resulting materials are characteristic of high pressure phases of the mixtures. These were shown to have novel engineered optical properties and to function as photocatalysts with enhanced catalytic activity. Improvements were found in GaN-ZnO oxynitride mixtures and tantalite perovskites by a factor of three due to nitrogen and oxygen vacancies. The findings were explained using theoretical calculations and further optimization and intelligent design of new materials was demonstrated using this method. In summary, some of the unique contributions of PI Ishihara's team include: i) Demonstration that single atoms incorporated into TiO<sub>2</sub> nanosheets can catalyze water reduction to produce H<sub>2</sub>, ii) Development and demonstration of the capabilities of a multiscale approach to simulating photocatalysis and allow intelligent design of novel photocatalysts with superior properties. The resulting model is unique on a global scale for understanding photocatalysis, iii) Visualization of the mechanism for such a process and testing of alternate dopants without the need for experiments a-priori, iv) Development of novel processing methods based on high-pressure torsion resulting in metastable mixtures of compounds with enhanced photocatalytic performances. *These advances address the short-term milestone for project 2 of the Molecular Photoconversion Devices Division.*



**Figure 5.** Calculated activity profiles for a broad spectrum of transition and rare earth metals as cocatalyst dopants

**\*[5] A functional [NiFe] hydrogenase mimic that catalyzes electron and hydride transfer from H<sub>2</sub>:** The search for biomimetic hydrogen activation by the Ogo team was crowned with our report of a functional [NiFe]-based catalyst (Fig. 6) [9], the first synthetic analog for H<sub>2</sub> activation in the world. The

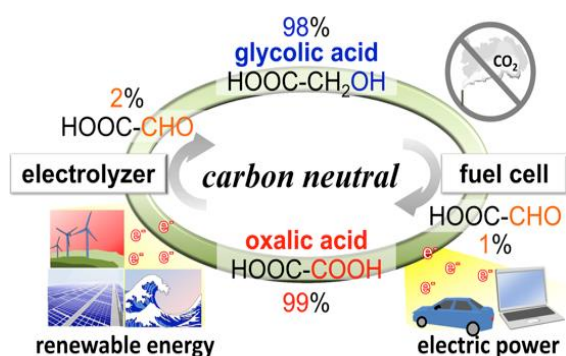


**Figure 6.** Bio-inspired catalyst for hydrogen activation.

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<sub>2</sub> 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. *This accomplishment along with the development of the model complex of O<sub>2</sub>-tolerant [NiFe]hydrogenase that functions as a non-Pt cathode catalyst for the reductions of O<sub>2</sub> and H<sub>2</sub>O<sub>2</sub> [10] meets the short-term milestone for*

*Project 1 in the Catalytic Materials Transformations Division's roadmap.*

**\*[6] One model, two enzymes: activation of hydrogen and carbon monoxide:** A second major advance, also coming from the Ogo group, targets bio-mimetic (or bio-inspired) catalysis. The focus remains on transformations of small molecule substrates including H<sub>2</sub>, N<sub>2</sub>, CO<sub>2</sub>, and H<sub>2</sub>O, since these are central to the I<sup>2</sup>CNER mission of producing clean fuels for carbon neutral power generation cycles. Following the division roadmap, research efforts of the Ogo group have made particular progress on single catalysts for transformations of multiple energy-relevant substrates. The ability to catalyze the oxidation of both H<sub>2</sub> and CO in one pot is highly relevant to our future hydrogen economy since CO is a persistent contaminant of H<sub>2</sub> supplies. The newly reported catalyst is based on a NiIr core, comparable in design to the active site of the iconic [NiFe]-hydrogenases and the CO-dehydrogenases (CODH), two of the most important enzymes in this area. The CO and H<sub>2</sub> bind to the Ir center, as verified by X-ray crystallography. An additional advantage of this design is its compatibility with aqueous media, which allows the operator to control product distribution by manipulating pH. The catalyst has been demonstrated in an actual fuel cell using H<sub>2</sub>, CO, and H<sub>2</sub>/CO as fuels for oxidation at the anode [11]. *This effort satisfies the short-term milestone for project 1 of the Catalytic Materials Transformation Division.*



**Figure 7.** Schematic of a carbon-neutral energy circulation by highly selective electrocatalyses using the glycolic acid/oxalic acid redox couple. Numbers indicate product selectivity.

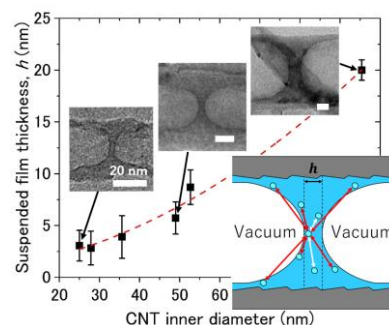
**\*[7] CO<sub>2</sub>-free electric power circulation via direct charge and discharge using the glycolic acid/oxalic acid redox couple:** This discovery by PI Yamauchi involves a CO<sub>2</sub>-free way to distribute electric power by exploiting an incredibly simple, bio-derived redox couple. The components 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). 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. This is the first ever demonstration of direct storage/generation of electric power using solution type carriers without CO<sub>2</sub> emission. Aiming at technology development, we first constructed a liquid flow-type electrolyzer as an electric power storage device, namely a polymer electrolyte alcohol electrosynthesis cell (PEAEC) [12] which is applicable for glycolic acid/oxalic acid redox reaction. The aqueous solution of glycolic acid ensures high energy density, up to 528 Ah<sup>-1</sup>, by a consideration of its maximum solubility (~4.93 M at 60 °C), which is almost ten times higher than that of the reported redox

flow battery. The energy conversion efficiency of this newly fabricated PEAC is 59.4% [13] (recently 65%) and it is the best ever reported on storing electric power into an easily transportable alcoholic solution. Using an alkaline fuel cell (Fig. 7), we also achieved CO<sub>2</sub>-free power generation via electro-oxidation of glycolic acid into oxalic acid for the first time [14]. This coupling of power storage and generation based on the alcohol/acid couple holds great promise toward addressing the intermittency problem of renewable electricity. *This achievement is directly relevant to the Catalytic Materials Transformation division's long-term target for Project 2.*

**\*[8] Fundamental understanding of phase change heat transfer:**

Condensation and boiling on smooth and engineered surfaces has received much attention in the past century due to its inherently high heat transfer efficiency. Although widely used in a plethora of industries, the fundamental mechanisms governing the physics of phase change heat transfer are poorly understood. The team of Takata and Miljkovic, working with international collaborators, have challenged this by answering century old questions in the fields of condensation [15] and evaporation (Fig. 8) [16] and developing the most comprehensive fundamental understanding of phase change heat transfer anywhere in the world. The knowledge gained from our work is being applied to the development of more compact energy systems, including condensers for Heating, Ventilation, Air Conditioning, Refrigeration (HVAC&R), and power generation industries, anti-icing surfaces, and highly efficient electronics thermal management devices. *This work has achieved the short and mid-term milestones of projects HMT-1 and HMT-2, and it currently targeting the long term milestone of projects HMT-1 and HMT-2.*

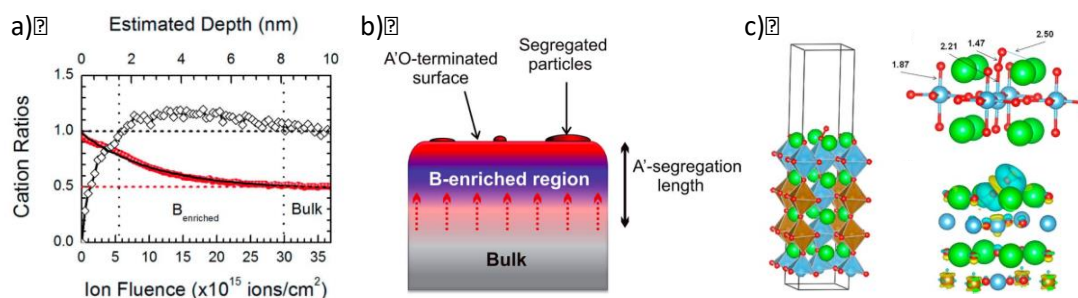


**Figure 8.** TEM images of suspended water film in CNT under high vacuum conditions.

**\*[9] Fundamental understanding of hydrophobic coating degradation:** Dropwise condensation of steam on metallic surfaces coated with hydrophobic films has the potential to achieve remarkable heat transfer coefficients resulting in 2% efficiency enhancement on 85% of the baseload power generating infrastructure globally. However, the main challenge of using these coatings for the past 8 decades is their lack of long-term durability. The senior and junior members of the Takata and Miljkovic teams have developed the world's first fundamental understanding of degradation of hydrophobic coatings during condensation [17]. We elucidated failure mechanisms linked to mechanics of thin-films along with heterogeneous nucleation physics. We used our unique understanding to develop, for the first time, scalable and durable hydrophobic coating approaches, in collaboration with the biggest coatings and paints company in the world (PPG), that can be applied to a variety of industrial energy systems [18]. *This work has achieved the short and mid-term milestones of projects HMT-1, and it currently targeting the long term milestone of projects HMT-1.*

**\*[10] Achieving dropwise condensation of low surface tension fluids:** A major challenge in the thermal science field is the inability to develop engineered surfaces that can enhance the condensation heat transfer with low surface tension working fluids (refrigerants). The Miljkovic team has overcome this challenge for the first time ever through utilizing liquid infused surfaces (LIS). They rigorously investigated lubricant-condensate pairs to develop rational design guidelines for LIS with low surface tension fluids and to develop, for the first time in the world, an engineered surface coating that can achieve dropwise condensation of an alkane [19, 20]. They demonstrate for the first time, stable dropwise condensation of ethanol and hexane on LISs impregnated with Krytox 1525, attaining a 200% enhancement in condensation heat transfer coefficient for both fluids compared to filmwise condensation on hydrophobic surfaces. *This work has achieved the short term milestones of projects HMT-1 and TES-2, and it currently targeting the mid-term milestone of projects HMT-1 and TES-2.*

**\*[11] Air electrodes in high temperature electrochemical devices: An atomistic study of composition and mechanisms:** This interdisciplinary international effort directed by PI Kilner lies at the intersection of surface science, materials science, electrochemistry and theoretical and molecular chemistry

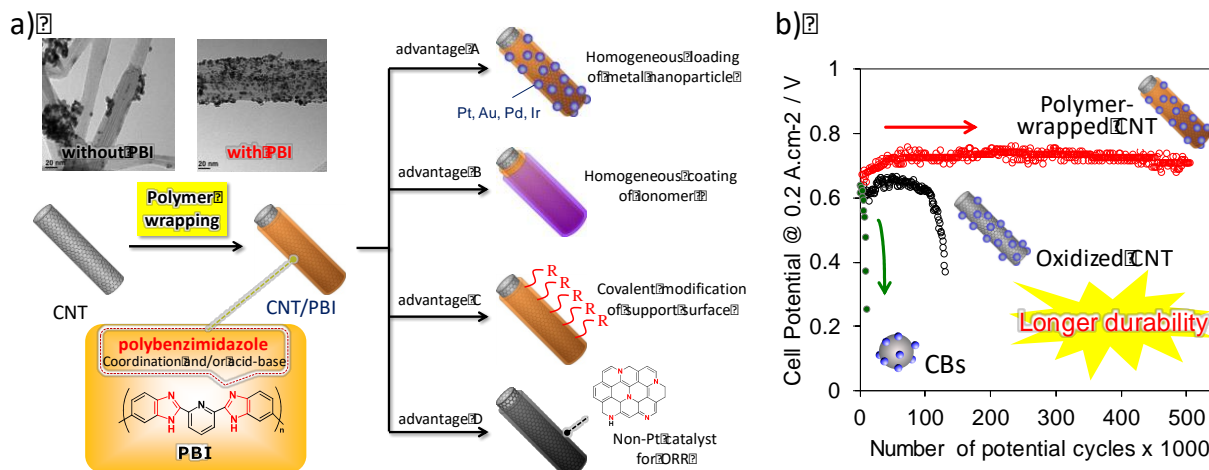


**Figure 9.** a) Measured compositional profile shows segregation of cations to the surface, b) Schematic of measured composition profile. The segregation is closely linked to performance degradation, c) Atomistic modelling has unveiled a vacancy-assisted mechanism for surface oxygen exchange involved in the ORR.

and was enabled by the formation of cross divisional team at I<sup>2</sup>CNER. This team tackled the very difficult problem of understanding the surface properties of multicomponent oxide air electrodes at high temperatures in the complex gaseous environment of ambient air. Air electrodes can typically experience degradation under operation consequently limiting the commercialization of high temperature electrochemical devices for efficient energy conversion. The role of the air electrode is to either incorporate oxygen, by the oxygen reduction reaction (ORR), or evolve oxygen by the oxygen evolution reaction (OER), during operation in either fuel cell or electrolysis mode. The evolution of surface composition, surface reactions, and the degradation mechanism are longstanding puzzles that must be addressed for wide-scale technology adoption. Using a combination of advanced surface analysis techniques and first principles theoretical studies, we have unravelled the significant phenomena that control the performance of the ORR and OER in these multicomponent materials in the complex gaseous environment of ambient air. The most common materials used as air electrodes are the mixed ionic electronic conducting perovskite oxides with a general formula of  $A_{1-x}A'_xBO_3$ , where the transition metal B cations such as Co or Fe are thought to be essential to the ORR/OER process and the large A and A' atoms, most usually La and Sr respectively, were both thought to be inert. The first part of this investigation showed two previously unknown characteristics, that are universal to a large class of air electrodes and closely linked to their degradation [21]. First, under the conditions of operation the surface quickly reorganizes to a termination consisting entirely of A type cations and O ions, covering the catalytically active B cations. Second, there is a rapid segregation of substituted A' cations to produce a majority A'O (e.g. SrO) rich near-surface region (Fig. 9 a, b). Using this knowledge of the surface composition, we computationally modelled the adsorption and incorporation of molecular oxygen onto these segregated electrode surfaces. Our analysis shows that pristine segregated SrO surfaces are inactive for oxygen adsorption, and that systems must rely on active site mediated mechanisms for adsorption to occur [22]. These active sites are the surface oxygen vacancies that provide a window to access the active B site transition metals (Fig. 9c). We have extended this analysis, and again by a combination of experiment and theory we have shown the importance of understanding the role of the other oxygen bearing molecules in the air environment to optimise the ORR reaction. Finally we have shown that in related A' free materials, e.g.  $La_2NiO_4$ , the surfaces are again AO dominated and that, in this case, and contrary to conventional thought, the surface La cations are an active participant in the ORR reaction. This is due to the electronic configuration of these rare earth elements which shows a marked degree of covalency in their interaction with oxygen. These new insights highlight the critical need for rational design of surfaces to enhance performance; a finding that was previously not recognised points the way to the optimisation of high performance low degradation air electrodes. *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.*



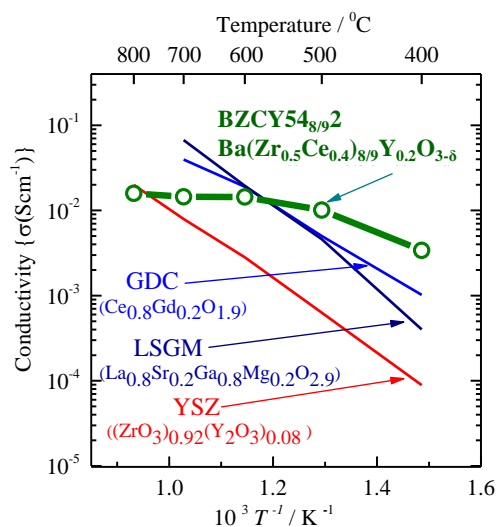
**\*[12] Novel electrocatalyst design based on polymer-wrapping of carbon nanotubes:** To overcome the critical limiting feature of low durability of electrocatalysts, Prof. Nakashima and PI Fujigaya have developed the use of polymer-wrapped carbon supports. This unique approach has now been applied 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 (Fig. 10a). Notably, the team has demonstrated extremely high durability, with lifetimes of the polymer electrolyte fuel



**Figure 10.** 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.

cell (PEFC) for single cell tests exceeding 500,000 cycles at 80 °C under humidified conditions (Fig. 10b) [23] and > 400,000 cycles at 120 °C under non-humidified condition [24], which to the best of our knowledge is the world-top durable fuel cell catalyst. 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'.*

**\*[13] Highly-Conductive Proton-Conducting Oxide for Intermediate temperature steam electrolysis:** The group of PI Matsumoto made significant advancements on steam electrolysis, currently the most energy-efficient process of water splitting for hydrogen production using renewable energy. We developed BZCY54<sub>8/9</sub>2, a proton conducting electrolyte exhibiting high performance at intermediate temperatures (400-600 °C) [25, 26]. Conductivities at 500 and 400 °C are higher than those of LSGM and GDC which are the most frequently used benchmark for oxide ion conducting solid electrolytes (Fig. 11).



**Figure 11.** Ionic conductivity of (BZCY54<sub>8/9</sub>2) compared with existing oxide-ion-conducting electrolyte materials.

We determined the composition to be the best in the series of perovskite-type BaZr<sub>x</sub>Ce<sub>1-x-y</sub>Y<sub>y</sub>O<sub>3-δ</sub> (BZCY) electrolyte materials with protonic conductivity of 10<sup>-2</sup> S/cm or higher at 500 °C [25] as well as for thermodynamic stability. The reported BaZr<sub>0.1</sub>Ce<sub>0.7</sub>Y<sub>0.2</sub>O<sub>3-δ</sub> (9 × 10<sup>-3</sup> S/cm at 500 °C) as holding the benchmark conductivity is disadvantageous due to its low stability in CO<sub>2</sub> and H<sub>2</sub>O environments. We discovered the cerium/zirconium ratio of 5/4 at the B-site of the perovskite exhibits both a higher conductivity and stability than the benchmark. A steam electrolysis voltage as low as 1.45 V was obtained at current densities of 0.2 and 0.5 A cm<sup>-2</sup> at 550 °C and 600 °C, respectively, with current efficiency >82% using our developed BaZr<sub>0.44</sub>Ce<sub>0.36</sub>Y<sub>0.2</sub>O<sub>3-δ</sub> electrolyte. From this performance, the calculated amount of electricity required to produce 1 N·m<sup>3</sup> of hydrogen is 4.2 kWh, which is lower than the 5 kWh required for the same amount of hydrogen using ordinary water electrolysis. Regarding the air electrode, we clarified the availability of protons in double perovskite oxide BaGd<sub>0.8</sub>La<sub>0.2</sub>Co<sub>2</sub>O<sub>6-δ</sub> at 300 °C from which new air

electrode materials tailored for use with protonic electrolytes could be designed. We have established a standard protocol for highly efficient intermediate temperature steam electrolysis, which has been shared with Nippon Shoukubai Co. Ltd through collaborative research initiated in 2013 toward commercialization. *The conductivity of this new material meets the short-term milestone in the Electrochemical Energy Conversion division's roadmap for Project 2.*

**\*[14] Membrane materials for CO<sub>2</sub> separation in power generation and industrial processes**

**CO<sub>2</sub>/N<sub>2</sub> separation:** Industrial requirements for membranes for CO<sub>2</sub> separation over nitrogen require that the CO<sub>2</sub> permeance exceed 4,000 GPU which is the target of the CO<sub>2</sub> Capture and Utilization division's roadmap. PI Fujikawa and his group demonstrated that membrane thinning markedly improves the gas flux performance, and hence our efforts have been directed to preparing ultimately-thinned membranes at the nanometer scale (nanomembrane) without gas leaks [27]. We succeeded in manufacturing free-standing polysiloxane(PoliSil)-based nanomembranes with high CO<sub>2</sub> solubility and thickness less than 50nm. The associated CO<sub>2</sub> permeance of more than 40,000 is the world's highest, better than the current benchmark of 2,000 GPU held by MTR Inc., USA, ten times larger than our division's roadmap target (4000 GPU), and with moderate 10 to 11 CO<sub>2</sub>/N<sub>2</sub> selectivity. Based on this achievement, we are now focusing our efforts on improving the selectivity of these ultrafast CO<sub>2</sub> permeable membranes by introducing a CO<sub>2</sub> selective layer, whereby the PoliSil nanomembrane is functioning as a gutter layer [28, 29]. Preliminary results show that the modified membranes exhibit selectivity that exceeds our project's target value of 40, though the CO<sub>2</sub> permeance falls well below the target value [28]. Additionally, when tested under atmospheric pressure conditions, the membranes captured CO<sub>2</sub> from CO<sub>2</sub>/N<sub>2</sub> mixture with a CO<sub>2</sub> concentration of 1000 ppm. This finding expands the relevance of our research goals beyond the capturing of CO<sub>2</sub> at fire-powered plants to the entirely new area of direct CO<sub>2</sub> capture from the air.

**\*[15] Membrane materials for CO<sub>2</sub>/H<sub>2</sub> separation:** Separation of CO<sub>2</sub> over H<sub>2</sub> at integrated gasification combined cycle (IGCC) plants (pre-combustion CO<sub>2</sub> capture) requires membranes with CO<sub>2</sub> permeance and selectivity respectively equal to 100 GPU (1 GPU=7.5×10<sup>-12</sup> m<sup>3</sup>(STP)/(m<sup>2</sup>·s·Pa)) and 30, under CO<sub>2</sub> partial pressure <1.0 MPa and temperature up to 60°C. The I<sup>2</sup>CNER developed alkanolamine-containing polymeric membranes, and especially, the 2-(2-aminoethylamino)ethanol-containing membranes developed by Prof. Taniguchi exhibited CO<sub>2</sub> permeance of 155 GPU with selectivity of 10 at CO<sub>2</sub> pressure of 1.0 MPa and 80 % relative humidity [30]. Investigating the mechanism of preferential CO<sub>2</sub> permeation at the molecular level, we found that the CO<sub>2</sub> permeance is significantly enhanced under humidified conditions. The amine-containing membrane turns into a hydrogel and the CO<sub>2</sub> migrates through the membrane in a bicarbonate ion form. The measured CO<sub>2</sub> permeance exceeds the division's roadmap target of 100GPU, while the selectivity of 10 should be further improved to 30. This performance is better than that of the membranes developed at RITE (permeance of 2.6 GPU and selectivity of 17) and which are being tested at pilot-scale. It should be noted that CO<sub>2</sub> permeance of 206 GPU with CO<sub>2</sub> selectivity of 103 at 107C were reported by researchers of Ohio State University at a RITE symposium last January; however these results have not appeared in a refereed journal publication. Currently, our efforts are focused on the development of a hollow fiber membrane module to explore the scaling-up of our membrane project to a demonstration level for technology transfer. I<sup>2</sup>CNER established a facile and scalable technique to prepare hollow-fiber membrane modules by circulating membrane materials inside the hollow-fibers. The resulting membrane modules not only show high CO<sub>2</sub> separation properties but they also exhibit good durability at 50°C and Δ*p* (CO<sub>2</sub>) of 40 kPa for about 300 h.

**\*[16] Glycerol Oxidation as Alternative Anode Reaction for Energy Efficient Electrochemical CO<sub>2</sub> Reduction:**

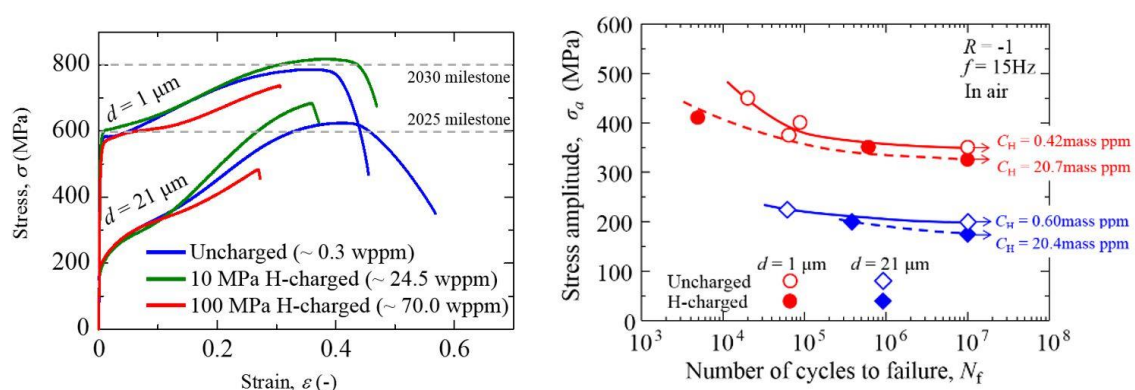
Since the seminal work of Hori et al. on transition-group metal cathode catalysts for the electrochemical reduction of CO<sub>2</sub> to value-added chemicals, much research has focused on engineering catalysts to improve the selectivity and activity of the CO<sub>2</sub> reduction reaction on the cathode. However, the oxygen evolution reaction (OER) which occurs at the anode consumes ~90% of the overall energy required for CO<sub>2</sub> reduction. Prof. Paul Kenis' group successfully investigated the effect of using glycerol oxidation as the anodic reaction rather than conventional OER [31]. Using a mixture of 2 M Glycerol and 2 M KOH as the anolyte, an onset potential of -0.85 V (a 53% reduction in overall energy requirement for CO<sub>2</sub> electrolysis) is possible, compared to an onset potential of -1.60 V using OER. Furthermore, we showed that current densities of 90 mA cm<sup>-2</sup> can be achieved at -1.50 V using glycerol oxidation vs. -2.20 V using conventional OER. *This achievement directly addresses the short-term milestone under Project 2 for low-efficient and low energy requiring anode catalysts.* In fact, due to the low cell potential when using anodic glycerol oxidation, I<sup>2</sup>CNER holds the benchmark for lowest overall energy requirement for CO<sub>2</sub> electrolysis.

**\*[17] Inertial effects in liquid CO<sub>2</sub>-water flow behavior for CO<sub>2</sub> storage:** The coupled pore-scale

flow dynamics of CO<sub>2</sub> and brine in geologic media represents a critical component of accurately predicting large-scale migration of injected CO<sub>2</sub>. PI Christensen's 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<sub>2</sub> front, the evolution of individual menisci and the growth of the dendritic structures, so called fingers [32, 33]. 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<sub>2</sub> 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<sub>2</sub> Storage Division.*

**\*[18] Continuous and accurate monitoring system for injected CO<sub>2</sub>:** In Carbon Capture and Storage, the monitoring of injected CO<sub>2</sub> is crucial for (a) predicting the risk of CO<sub>2</sub> leakage from reservoirs, (b) increasing the efficiency of CO<sub>2</sub> injection and reducing the cost, and (c) reducing the risk of injection-induced seismicity. To date time-lapse seismic surveys have been used to monitor injected CO<sub>2</sub> distribution. However, the interval of the time-lapse monitoring surveys is long due to their high cost and it is difficult to continuously monitor the injected CO<sub>2</sub>. In addition, continuous monitoring of the dynamic CO<sub>2</sub> behavior is crucial for detecting accidental incidents, such as CO<sub>2</sub> leakage. To address these issues, the group of PI Tsuji first developed a continuous monitoring approach to estimate spatio-temporal variation of seismic velocity using ambient noise [34, 35]. Since this method constructs virtual seismic data from noise, we can extract subsurface information using only passive seismometer data. However, the disadvantage also of this monitoring system that relies on ambient noise is that the temporal variation of ambient noise would decrease the monitoring accuracy. To overcome this problem, we have developed a new novel monitoring method for injected CO<sub>2</sub> using a continuous and controlled seismic source. This new monitoring system generating controlled seismic signal is cost-effective, with high temporal resolution and accuracy. By deploying this system to the ongoing CCS project in Canada, we successfully identified spatial and temporal variation in the shallow subsurface [36]. High spatial resolution of our approach makes it possible to identify leaked CO<sub>2</sub>. Also, the system's low cost and high temporal resolution are particularly attractive for long-term monitoring of sequestered CO<sub>2</sub>. Lastly, a smaller scale system of this monitoring device was used to monitor geothermal fields of the Kyushu Island. *This effort directly addresses the short-term milestone of Project 3 of the CO<sub>2</sub> Storage Division (Field-scale CO<sub>2</sub> investigation), specifically the milestone: Develop effective monitoring system.*

**\*[19] Next-generation high-strength, low-cost alloy for hydrogen service:**



**Figure 12.** Data for Fe-16Cr-10Ni with ultra-fine grain size ( $d = 1 \mu\text{m}$ ) and conventional grain size ( $d = 21 \mu\text{m}$ ). (a) Tensile stress vs. strain data after exposure to hydrogen gas up to 100 MPa, (b) Stress amplitude vs. cycles to failure relationships with hydrogen concentration indicated for each data set.

Research teams supervised by PI Takaki have 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. 12a). As for hydrogen compatibility, two metrics were met: tensile ductility and fatigue life. As shown in Fig. 12a, the strain to failure of ultra-fine grain (UFG) Fe-16Cr-10Ni remains above 30% after exposure to 100 MPa

hydrogen [37]. Regarding fatigue life, the fatigue limit (stress amplitude at  $10^7$  cycles) for UFG Fe-16Cr-10Ni is not degraded by hydrogen ( $\sim 20$  wppm), as shown in Fig 12b [38]. To date, no other austenitic stainless steel can rival this experimental alloy's combined attributes: cost-competitive, high strength, and hydrogen compatible. *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 Nippon Steel & Sumitomo Metals Corporation.

**\*[20] Mitigation of Hydrogen Embrittlement:** For the first time, a study By PIs Somerday, Kirchheim, and Sofronis combining experiments and modeling has revealed the physics governing inhibition of H<sub>2</sub>-accelerated fatigue crack growth by ppm-levels of O<sub>2</sub>. A predictive analytical model was formulated that accurately quantifies how key variables (e.g. O<sub>2</sub> concentration and load) affect the onset of accelerated crack growth in H<sub>2</sub> gas containing trace O<sub>2</sub> concentrations [39]. In parallel, first-principles density functional theory (DFT) modeling by PI Staykov revealed the characteristics of hydrogen-oxygen competitive co-adsorption on iron surfaces that impede hydrogen uptake into steel. This study not only set the benchmark for understanding the inhibiting effect of trace impurities on hydrogen gas-accelerated crack growth but also spurred further I<sup>2</sup>CNER research activities on this topic supported by Air Liquide [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.

I<sup>2</sup>CNER provides a rich platform for its researchers to pursue transformative research in non-traditional and highly multi-disciplinary environments. Specific details of the I<sup>2</sup>CNER environment are:

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

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

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

A second I<sup>2</sup>CNER building, which has 4 stories and a total floor space of 5,014 m<sup>2</sup>, 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 cross-team and cross-division research interactions. This building was funded by the FY12 supplementary budget from the Japanese government. Construction of I<sup>2</sup>CNER building 2 was completed at the end of February 2015.

### Six main apparatus in I<sup>2</sup>CNER

- i) *Field Emission Scanning Electron Microscope (SEM): JSM-7900F FIELD EMISSION SEM*  
The JSM-7900F Field Emission SEM is a uniquely flexible platform that combines the best high-resolution imaging with unparalleled nanoscale microanalysis. This tool excels in lightning fast data acquisition through simple and automated operation. The JSM-7900F is equipped with a large specimen chamber that accommodates a wide variety of detectors simultaneously, including: multiple EDS, EBSD, WDS, STEM, BSE, and CL. A new Soft X-ray Emission Spectrometer (SXES) allows efficient and parallel collection of very low-energy rays with chemical state analysis. The system can also be equipped with a variety of sub stages including tensile, heating, and cooling stages for in situ experimentation. For analysis of non-conducting specimens, the JSM-7900F/LV is available with variable pressure. Applications include imaging and analysis of metals, magnetic materials, semiconductors, ceramics, medical devices, and biological specimens.
- ii) *Automated multipurpose X-ray diffractometer (XRD) with Guidance software: SmartLab 9kW AMK*  
Rigaku SmartLab is the newest and most novel high-resolution X-ray diffractometer (XRD) available today. This system incorporates a new X-ray diffraction system featuring the high-flux 9 kW rotating

anode X-ray source coupled with a high-energy-resolution 2D multidimensional semiconductor detector. Its unique feature is the new SmartLab Studio II software, which provides the user with an intelligent User Guidance expert system functionality. This equipment accepts powder, liquid, films, and even textile samples and allows mapping measurements within suitable samples.

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 3-6, describe the transition in acquiring research project funding.

### **Strategy and action plan for acquiring external funding**

The Director's vision is that I<sup>2</sup>CNER can remain strong and agile by developing cores of embedded centers funded by external agencies (both industrial and governmental) and securing industrial projects that will last beyond the WPI funding period.

Drawing from the experience gained from the establishment of the NEXT-RP Center, I<sup>2</sup>CNER will intensify its efforts to establish similar internal research centers in response to national initiatives by government agencies such as NEDO, METI, Riken, JSPS, and JST. Riken, for example, currently does not have a location in the Western part of Japan, making KU a strong option for a potential future center. With regard to establishing internal research centers, I<sup>2</sup>CNER will i) be active on implanting future research themes in government agencies for new national agency research initiatives, ii) rely on the input from the Industrial Advisory Board to create new ideas that will attract funding from industry, government, and national and international foundations (e.g. Gates Foundation, Simons Foundation), and iii) utilize the new Industrial Research Unit to attract industrial projects for collaborative efforts in the form of open innovation.

An example of attracting industrial funding is the workshops that were organized jointly with Toshiba Corporation to explore the possibilities of joint research on topics of mutual interest. The first workshop targeting chemistry applications was held at I<sup>2</sup>CNER on October 31, 2017 and the second workshop targeting materials for adverse environments was held at Toshiba on March 6, 2018. Following the workshops, two executives from Toshiba's Power and Industrial Systems R&D Center visited I<sup>2</sup>CNER on December 4, 2018: Dr. Toru Kuriyama and Dr. Nagayoshi Ichikawa, Chief Fellow and Senior Fellow (respectively). Dr. Ichikawa visited I<sup>2</sup>CNER again on April 23, 2019. As a result of these workshops, there is an ongoing discussion between I<sup>2</sup>CNER and Toshiba on the funding of these initiatives. Specifically, Toshiba is interested in I<sup>2</sup>CNER's research in reversible fuel cells and thermal management of fuel cells.

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).

### **Ongoing Funded Research Programs**

I<sup>2</sup>CNER researchers leverage the established infrastructure, research culture, and international visibility of the Institute to aggressively pursue funding. By way of example, some major I<sup>2</sup>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) a large-scale research grant awarded by NEDO to Prof. Higashi's research team in the Next Generation Refrigerant Properties (NEXT-RP) at a level of 159 million JPY from FY18-FY20; iv) the joint PIRE program awarded by the US NSF and JSPS to researchers at Illinois and KU at a level of ~ 495 million JPY from FY15 to FY19 (4.5 million USD at an exchange rate of 110 JPY); v) the Kakenhi Grant-in-Aids awarded to Profs. Ishihara and Sakai at a level of ~385 million JPY from FY15 to FY19; vi) 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; vii) The Center for Small Molecule Energy (CSME) awarded to Prof. Ogo at a level of 99 million JPY from FY14 to FY18; viii) 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; ix) the JSPS Grant-in-Aids for Specially Promoted Research awarded to Prof. Ogo from FY14 to FY18 at a level of ~440 million JPY; and x) a large-scale JSPS KAKENHI Grant-in-Aids awarded to Prof. Miho Yamauchi at a level of 175 million JPY from FY18 to FY22.

### **I<sup>2</sup>CNER's International Research Programs and Activities**

I<sup>2</sup>CNER's success has enabled the acquisition of large additional research grants and the establishment of prestigious international partnerships/programs. These expanded I<sup>2</sup>CNER's research portfolio and advanced I<sup>2</sup>CNER's global visibility. Notable examples are:

#### *JSPS Core-to-Core Program*

This is an international joint research project led by PI Matsumoto. The project, funded at a level of 90 million JPY (13.5 million JPY in FY18), is a collaboration between I<sup>2</sup>CNER, Imperial College, London, Paul Scherrer Institut (PSI, Switzerland), and the Massachusetts Institute of Technology on "Solid Oxide Interfaces for Faster Ion Transport (SOIFIT)." Three of I<sup>2</sup>CNER postdocs visited the counterpart research institutions for more than 1 month: Dr. V. Thoréton in Imperial College, London for 5 weeks; Dr. D. Klotz in MIT for 1.5 months; Dr. K. Ghuman Kaur in PSI for 2 months.

#### *Partnership with the University of Göttingen*

PI Reiner Kirchheim, an elected member of the US National Academy of Engineering, and I<sup>2</sup>CNER's Director, lead the collaboration between KU and the University of Göttingen to establish an International Research Training Group that is to be co-funded by the DFG and JSPS. On January 6, 2018, two professors from the University of Göttingen visited I<sup>2</sup>CNER. In April 2018, a two-day KU/Göttingen workshop was also organized in Göttingen and the KU and Göttingen teams identified and constructed the research themes of the joint proposal. In the proposed joint Ph.D. program, Ph.D. students will visit the counterpart institute for 1 year to participate in research/educational activities. The concept paper is currently being finalized for submission to DFG this Summer, with the full proposal to be submitted in Spring 2020. Similarly, the full proposal for JSPS will be submitted this Fall.

#### *Partnership for International Research and Education (PIRE)*

Please see section 5-1-3 below for more information about PIRE.

### **Industrial Research Unit**

Additional resources are being secured through projects sponsored by industrial partners within the newly established "Industrial Research Unit." This Unit was established in FY17 with its purpose being to advance technology transfer with corporations and pursue stronger relationships with industry and government programs. This new "Unit" comprises of several industry-sponsored research projects, wherein a team of I<sup>2</sup>CNER researchers and embedded-industry-affiliates work on a particular research area of mutual interest. Through this new unit, I<sup>2</sup>CNER will expand its outreach to promote the deployment of its technology to industries that will fund I<sup>2</sup>CNER projects in the future. The first such project is "Mobile Energy Storage for Low-Carbon Society" sponsored by Mazda Motor Corporation for 71 million JPY with a duration of three years beginning in FY17. Additionally, the IHI Corporation has sponsored 5 million JPY on the "Study of High-temperature Co-electrolysis of CO<sub>2</sub> and H<sub>2</sub>O."

## **2-4. State of joint research**

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

I<sup>2</sup>CNER has 25 partnering institutes, some of which are listed below with the corresponding research interactions.

### **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<sup>2</sup>CNER and the NFCRC at the University of California, Irvine exchanged visits and participated in respective center events.

### **California Air Resources Board (CARB)**

To reinforce the idea of Green Innovation, CARB reviewed all of I<sup>2</sup>CNER's division roadmaps and evaluated I<sup>2</sup>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<sup>2</sup>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<sup>2</sup>CNER, NTNU, and SINTEF, a joint workshop was held November 15-16, 2012. After over 1 year of mutual effort, an MOU was signed on March 17, 2014 and was renewed on March 17, 2019. As part of I<sup>2</sup>CNER's collaborative research with NTNU, a joint research proposal on understanding the fundamentals of materials degradation in hydrogen-containing environments has been awarded. The project is funded by the Norway Research Council.

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

From inception through March 2016, I<sup>2</sup>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 is the Division Lead PI of I<sup>2</sup>CNER's Hydrogen Materials Compatibility Division. In FY16, 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 has continued to lead the Hydrogen Materials Compatibility Division from his new post. These interactions have allowed I<sup>2</sup>CNER to stay informed about hydrogen-related technologies in the US and development of codes and standards for hydrogen materials compatibility.

### **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 I<sup>2</sup>CNER 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.
- To substantiate the above evaluation, list the main awards received and invitational/Keynote lectures given by the Center's researchers in Appendix 1-3.

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

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

### **Interactions with 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 US. Other former and current US DOE Energy employees who worked and interacted with I<sup>2</sup>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 Technology Program.

## **Connections with Government Agencies**

### *Prof. 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" (FY07-FY11), R&D for on-board hydrogen storage systems for fuel cell vehicles, and Hydrogen Utilization Technology Development (FY13-FY17). 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" (FY12).

### *PI Tsuji*

PI Takeshi Tsuji worked with the Ministry of Economy, Trade, and Industry (METI) on the interactions with CO<sub>2</sub> storage and earthquakes as well as with the Ministry of the Environment on the regulations for CO<sub>2</sub> geological storage in offshore areas. Additionally, Prof. Tsuji was a member of the committee on the "International Ocean Discovery Program" (US NSF; 2014-2016).

### *PI Takahara and PI Sakai*

PI Atsushi Takahara is a member and PI Ken Sakai is an Associate Member of the Science Council of Japan.

### *PI Saha*

PI Bidyut Baran Saha works with the Government of India's Department of Science and Technology on the development of India's roadmap for advanced solar thermal energy technologies and is a Foreign Expert for their Ministry of Human Resource Development.

### *PI Matsumoto*

PI Hiroshige Matsumoto advises the Japan Aerospace Agency (JAXA) on ceramic-based water electrolysis that can operate in "zero gravity".

### *Prof. Higashi*

Prof. Yukihiro Higashi collaborates with the Ozone Layer Protection Policy Office of METI on the development of next generation low-GWP refrigerants.

### *PI Watanabe*

PI Hiroaki Watanabe advised the Subcommittee on Energy and Resources of the House of Councilors of Japan on energy transitions. February 27, 2019.

### *Prof. Itaoka*

Prof. Kenshi Itaoka advises: METI on Hydrogen fueling station deployment, the Ministry of the Environment MOE on the development of the roadmap for Japan's CCS project, and the Japan Society of Energy and Resources on Energy Policy.

## **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 Ian Robertson and Petros Sofronis won the US Department of Energy Hydrogen and Fuel Cells Program Research and Development Award. In 2014, PI Brian Somerday also won the same award.

### *The 2012 Somiya Award (awarded biennially to scientists who collaborated across two continents)*

PIs John Kilner, Harry Tuller, and Tatsumi Ishihara were part of a group of scientists who earned this prestigious award.

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

Students from KU, including team members from I<sup>2</sup>CNER, won the 2012-2013 Hydrogen Student Design Contest, which was sponsored by the US DOE, the National Renewable Energy Laboratory, Mercedes-Benz, and Toyota.

### *The Commendation for Science and Technology by MEXT, 2013*

PI Seiji Ogo

### *JST Breakthrough Report 2013*

PI Seiji Ogo's research was featured in this important publication of JST.

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

PI Harry Tuller served as the President of the society and PI Tatsumi Ishihara served as Treasurer.



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

*Medal with Purple Ribbon, 2015*  
PI. Zenji Horita

*Commendation for Science and Technology by MEXT, 2015*  
PI Takeshi Tsuji and Prof. Shintaro Ida

*Daiwa Adrian Prize 2016*  
PIs Tatsumi Ishihara and John Kilner, and Profs. Aleksander Staykov, John Druce, and Helena Téllez

*Commendation for Science and Technology by MEXT, 2016; The Society of Polymer Science, Japan, 2016 for outstanding achievements*  
Prof. Naotoshi Nakashima

*Foreign Affiliate of the US National Academy of Engineering, 2017*  
PI Reiner Kirchheim

*Incentive Award by the Japan Society of Analytical Chemistry, 2018*  
Prof. Yukina Takahashi

*Early Career Award by the US Department of Energy, 2018*  
Prof. Nicola Perry

### **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.

Please refer to Section 1 "Overall Image of Your Center" for the center's vision and scenario of transition to a low-carbon society.

The relevance of the I<sup>2</sup>CNER research efforts and objectives toward enabling the green innovation initiative of the government of Japan is demonstrated by the large number (122) of collaborative projects in which its researchers are involved with industry. A total of 53 projects resulted in technology transfer events. A detailed list of all the I<sup>2</sup>CNER Technology Transfer Events is outlined in the report "**Technology Transfer Summary: I<sup>2</sup>CNER's Interaction with and Impact on Industry**". In FY18, I<sup>2</sup>CNER filed for 16 patents, and was granted 8, bringing the total of patent applications since inception to 239 and patents awarded since inception to 67.

Representative examples of technology transfer include: 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 has 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 worked 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<sub>2</sub> monitoring system in collaboration with the Japan Oil, Gas and Metals National Corporation (JOGMEC) has been transferred and deployed in the ongoing CO<sub>2</sub> 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 have been submitted to the Ministry of Economy, Trade and Industry of Japan in the form of 73-page report in February 2017; x) PI Fujigaya received funding in FY18 from KU and the Fukuoka Bank for a **startup company** called FUJicat on novel electrocatalysts.

### **Industrial Research Unit**

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<sup>2</sup>CNER established the Industrial Research Unit in FY17, wherein industry liaisons are embedded in I<sup>2</sup>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. See "Industrial Research Unit" under section 2-3 for more details.

### **Industrial Advisory Board**

On April 1, 2017, I<sup>2</sup>CNER established the "Industrial Advisory Board (IAB)," whose members are prominent executives from industry, government agencies, and national laboratories that advise I<sup>2</sup>CNER on opportunities for interactions with industry and technology transfer. The first IAB meeting was held on February 1, 2018 and attended by 9 out of 10 IAB members. The meeting provided invaluable inputs to I<sup>2</sup>CNER researchers in regards to research areas that industries would have interest for promoting the development of new technologies.

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

\* Describe what was accomplished in the center's outreach activities during the period from 2010 through March 2019 and how the activities have contributed to enhancing the center's "globally visibility." In Appendix 5, describe the concrete contents of these outreach activities and media reports or coverage of the activities.

I<sup>2</sup>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<sup>2</sup>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<sup>2</sup>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, US Department of Energy. A total of 30 researchers from KU travelled to Illinois to participate in this event.

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

Since the Institute's inception, the I<sup>2</sup>CNER 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 I<sup>2</sup>CNER'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 I<sup>2</sup>CNER'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 I<sup>2</sup>CNER 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 more details about individual symposia, please see Section 5-2.

#### **I<sup>2</sup>CNER Symposia in Tokyo Sponsored by the US Embassy**

The hosting of the Tokyo Symposia, which is sponsored by the US Embassy in order to bring I<sup>2</sup>CNER research activities to the attention of the energy stakeholders in the capital of Japan and the international community, is another growing I<sup>2</sup>CNER 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. A celebratory symposium for I<sup>2</sup>CNER's accomplishments over the last 10 years will also be held in Tokyo on December 16, 2019.

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

The Institute publishes two outreach publications, "Hello! I<sup>2</sup>CNER" (for high school students) and "Energy Outlook" (for industrial stakeholders), three times per year. We regularly receive requests from local high schools who are familiar with "Hello! I<sup>2</sup>CNER" 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, policy experts, and industry CEOs, e.g. Nobel Laureate Prof. Mike Celia from Princeton University, Shin-ichi Nakao from the Research Institute of Innovative Technology (RITE), Hajime Okazaki, the Senior Vice President of JX Nippon Oil and Energy Corporation.

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

In FY15, I<sup>2</sup>CNER partnered with WebsEdge, the company in charge of all the video programming of the Materials Research Society (MRS), 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 FY16 in order to increase our international visibility.

([https://www.youtube.com/watch?v=xkM6rys\\_SYM&feature=youtu.be&list=PL](https://www.youtube.com/watch?v=xkM6rys_SYM&feature=youtu.be&list=PL))

## **4. Generating Fused Disciplines (within 3 pages)**

### **4-1. State of strategic (or "top-down") undertakings toward creating new interdisciplinary domains**

The Director has at his disposal the "I<sup>2</sup>CNER Competitive Funding," which is intended to foster and advance interdisciplinary research. Competitive funding is allocated to those faculty members who are productive, and whose achievements (including papers, awards, winning external research funds, etc.) are relevant to I<sup>2</sup>CNER'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.

Since FY15, the Director has utilized the "Competitive Funding Initiative" to accelerate the Institute's strategic efforts to integrate mathematics (applied math) and economics into I<sup>2</sup>CNER's research portfolio. In FY15-FY17, a total of 13 applications were selected as "seed projects," and those projects are now a new interdisciplinary research direction of "Applied Math and Economics for Energy," which is and will be an important component of I<sup>2</sup>CNER. The projects in I<sup>2</sup>CNER "Applied Math and Economics for Energy" program are:

#### *Topology and Materials*

- i) Prof. D. Triadis, "Anomalous diffusion in realistic pore-scale simulations of two-phase flow for geologic CO<sub>2</sub> sequestration," Institute of Mathematics for Industry (IMI), Australia Branch, Trobe University.
- ii) Prof. T. Tsuji, "Characterization of heterogeneous rock pore structure using persistent homology: Insight into scale dependence of hydrological and elastic properties," I<sup>2</sup>CNER (in collaboration with Prof. T. Shirai, IMI).

#### *Smart Grid and Renewables*

- iii) Prof. N. Hoa, "Distributed Grid Optimization with Renewable Generation," IMI and I<sup>2</sup>CNER (in collaboration with Prof. S. Bose, UIUC).
- iv) Prof. S. Bose, "Scalable grid optimization," UIUC (in collaboration with Prof. N. D. Hoa, IMI and I<sup>2</sup>CNER).
- v) Prof. S. Bose, "Strategic interactions in electricity markets," UIUC (in collaboration with Prof. N. D. Hoa, IMI and I<sup>2</sup>CNER).

#### *Social Aspects of Power Systems*

- vi) Prof. K. Hirose, "Statistical analysis of energy consumption," IMI.
- vii) Prof. J. Murata, "Design of Demand Response Programs Using Inverse Optimization," KU Department of Electrical Engineering (in collaboration with Prof. K. Itaoka, I<sup>2</sup>CNER).
- viii) Prof. S. Managi, "Energy innovation and human behavior," KU Department of Urban and Environmental Engineering.

#### *New Power Concepts*

- ix) Prof. K. Matsue, "Characterization of dynamic events in flame fronts in turbulent combustion," IMI and I<sup>2</sup>CNER (in collaboration with Prof. M. Matalon, UIUC).
- x) Prof. M. Matalon, "Outwardly expanding premixed flames," UIUC (in collaboration with Prof. K. Matsue, IMI and I<sup>2</sup>CNER).

- xi) Prof. H. Watanabe, "Solar Power Assisted Hydrogen Production and Carbon-Free High Efficiently Thermal Power Generation," I<sup>2</sup>CNER.
- xii) Prof. N. Nakashima, "Carbon Nanotube-based Non-precious Metal Electrocatalysts for Fuel Cell, Water Electrolyzer and Metal-air Battery Devices," I<sup>2</sup>CNER.

*Biofuels*

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

In January 2019, Prof. Andrew Chapman of the EAD, who specializes in socio-environmental energy science, was promoted to Associate Professor with tenure at KU. The tenured faculty status allows for Prof. Chapman to teach courses and supervise students in the School of Economics (as I<sup>2</sup>CNER faculty) beginning in FY19. This development will accelerate our efforts to augment I<sup>2</sup>CNER's interdisciplinary research in the areas of energy socio-economics and national policy on energy engineering through the introduction of the "Energy Economics" specialty to the School of Economics curriculum.

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

#### **4-2. State of "bottom-up" undertakings from the center's researchers toward creating new interdisciplinary domains**

Describe the content of measures taken by the Center to advance research by fusing disciplines. For example, measures that facilitate doing joint research by researchers in differing fields.

##### **Coffee and Collaboration (CO<sup>2</sup>)**

The I<sup>2</sup>CNER buildings brought our researchers under the same roof and this instigated collaborations across the disciplines. In particular, informal social events, such as the I<sup>2</sup>CNER-sponsored "Coffee and Collaboration (CO<sup>2</sup>)," has led to a number of collaborations among I<sup>2</sup>CNER 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<sup>2</sup>, 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. iii) PIs Somerday and Staykov "On hydrogen and oxygen adsorption on metallic surfaces." This work fused materials science with computational chemistry.

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

Since its inception, young researchers have been giving presentations at the IISS with the goal of initiating cross-division collaborations. Since the inception of the Institute, a total of 257 speakers (including 45 speakers in FY18) presented at 159 Institute Interest Seminars (including 24 seminars in FY18). 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, an Illinois graduate student from Satellite faculty Prof. Paul Kenis' group at Illinois, presented her research before the groups of PIs Nakashima and Sasaki. I<sup>2</sup>CNER Prof. Lyth approached Ms. Jhong after the presentation to suggest that she try some of his N-doped carbon materials for CO<sub>2</sub> conversion. A joint collaboration on materials synthesis and electrochemistry was produced and the results were published in ChemSusChem (2017),

### **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 workshop between I<sup>2</sup>CNER and AIMR (Advanced Institute for Materials Research) was organized by Prof. Staykov at I<sup>2</sup>CNER 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 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 I<sup>2</sup>CNER and KU, led to active and robust discussions and novel projects, among which were the successful KAKENHI grant application of Dr. Han (AIMR) and Dr. Watanabe (I<sup>2</sup>CNER) and the long-term theoretical collaboration between Dr. Packwood (formerly AIMR, presently iCeMS) and Dr. Staykov (I<sup>2</sup>CNER). Collaborations between I<sup>2</sup>CNER researchers and Dr. Packwood are ongoing. In fact, Dr. Packwood gave a presentation at the 2019 I<sup>2</sup>CNER International Workshop for the Molecular Photoconversion Devices division.

### **4-3. Results of research in fused research fields**

Describe the Center's record and results by interdisciplinary research activities yielded by the measures described in 4-1 and 4-2.

- In Appendix 1-2, list up to 20 of the Center's main papers on interdisciplinary research that substantiate the above record of results, and describe their content.

Using **bioinspiration**, Prof. Miljkovic of the Thermal Science and Engineering division is exploring the boundaries of wetting through the fusion of mechanical engineering, material science, entomology, chemistry, and biotechnology. The team was the first to show that wettability in nature is correlated with taxonomy, life cycle, and reproductive strategies, rather than habitat [1]. Using the discovered knowledge, the team selected insect species to analyze their functional molecular makeup which govern wettability in order to create artificial bioinspired scalable metal-based anti-bacterial superhydrophobic surfaces. This work enables the development of artificial surfaces for energy and water applications such as anti-icing, self-cleaning, anti-bacterial, anti-fogging, water harvesting, and enhanced phase change heat transfer.

**Mining Biology for New Hydrogen Processing Catalysts**, the group of Prof. Ogo have characterized an extraordinary H<sub>2</sub> oxidation catalyst by bioprospecting. The catalyst is a hydrogenase found in the bacterium *Citrobacter* sp. S-77. This new catalyst tolerates air and carbon monoxide but is more active than platinum [2]. The new catalyst, which features nickel and iron (not platinum), operates by first splitting hydrogen gas (H<sub>2</sub>) into hydride (H<sup>-</sup>) and proton (H<sup>+</sup>). This initial step is followed by the splitting hydride into electrons (2 e<sup>-</sup>) and another proton (H<sup>+</sup>). These results further demonstrate the dramatic progress and design attributes made possible through this interdisciplinary bioorganometallic program [3].

PIs Horita and Associate Professor Edalati fusing the disciplines of **materials engineering** with i) **surface science and crystallography** and in collaboration with Prof. Akiba discovered the defect activation mechanism [4] for hydrogen adsorption of TiFe intermetallics by High Pressure Torsion (HPT), a promising system for renewable stationary energy storage; ii) **mechanochemistry** and in collaboration with the groups of PIs Ishihara, Yamauchi, and Staykov introduced a new research direction [5] to the development of new visible-light-active photocatalysts by stabilizing high-pressure phases through using the high-pressure torsion (HPT) approach. It was shown that unlike thermodynamically stable phases of TiO<sub>2</sub> and ZnO which are photocatalytically-active only under UV light, the high-pressure TiO<sub>2</sub>-II and rocksalt-ZnO are active under visible light due to their low bandgap in good agreement with the first-principles calculations.

Applied mathematics area was mostly split between *computational gas and combustion dynamics* and

*smart grid* research, with two additional groups dealing with models of *porous geomaterials*, and *statistical models of pheno-to-genotype* function (biomathematics).

Two groups addressed the area of **Computational Gas and Combustion Dynamics**. The goal is to develop predictive tools that incorporate the relevant combustion physics and chemistry to model, design, and optimize the next generation of low-emission automotive engines and gas turbines for power generation. The models of Profs. Matalon (Illinois) and Matsue (I<sup>2</sup>CNER and IMI) addressing centrally-ignited outgrowing flames in laminar and turbulent media are based on the hydrodynamic theory of premixed flames systematically derived from the general governing equations using a multi-scale approach [6, 7]. The results clarify the physical mechanisms responsible for the onset of instabilities and their nonlinear consequences [7]. The group of PI Watanabe developed highly accurate gas-particle two-phase large-eddy simulations [8] for phenomena taking place in a solar assisted biomass gasifier, and in which the turbulent eddies are resolved within the grid scale through experiments (University of Adelaide). Efficiently energy conversion of solid material to syngas in a turbulent flow within the gasifier is essential to realize the carbon negative hydrogen production system. Their results showed that the particle distribution was significantly affected by the interaction between the turbulent boundary layer formed on the inner wall of the injector nozzle and the particles, and this behavior could be classified by the particle Stokes number.

Four research groups work in the area of **Mathematics for Smart Grid**: i) Prof. Bose's group (Illinois) focused on algorithm design and game-theoretic analysis of power systems and their associated markets. Their first project deals with security-constrained economic dispatch (SCED) problems that seek to minimize dispatch costs within engineering constraints of the grid [9]. They formulated a novel risk-sensitive SCED problem that explores the tradeoffs between power procurement costs and reliability of power delivery and, designed a scalable distributed algorithm to solve it. Their second project deals with strategic behavior of generators in electricity markets and the potential role of system operators in mitigating their market power [10]. Precisely, they characterized equilibria in Cournot/Stackelberg market models and analyzed how system operators can choose 'good' equilibria through market design. These projects provide new techniques to tackle risks associated with uncertain engineering components and strategic market participants. Such risks will only grow as the grid becomes more complex. ii) The group of Prof. Hirose (IMI) addressed statistical modeling for energy data analysis. Using electricity demand data of Chikushi campus in KU, they developed a regression model that is robust against outliers to forecast the electricity consumption, based on the current weather readings and historic observations [11]. iii) Research of Prof. Nguyen Dinh Hoa deals with distributed grid optimization with renewable generation. To this end he developed a distributed optimization approach called distributed consensus-based Jacobian alternating direction method of multipliers (DCJ-ADMM) to assist a potential mediating agent (operator) in setting prices, with generator and consumer agents adjusting power in parallel [12]. Prof. Hoa's work (in collaboration with Prof. Bose) is the first to prove the convergence of the objective function arguments to their optima, for both centralized and distributed agent-based Mirror Descent methods [13]. iv) Prof. Murata's (IMI) group dealt with consumer modeling in energy markets in which the consumer is treated as a decision maker. They developed a modeling technique aimed at designing demand response programs (DRPs), based on an inverse-reinforcement-learning-based technique that estimates consumer unhappiness from observed energy consumption data [14, 15]. They tested DRP designs on thousands of consumer models. The developed consumer model is the first ever proposed in which the incentive payment design method for DRPs is mathematically grounded.

Increasing fundamental understanding of **flow processes relevant to CO<sub>2</sub> storage**, the team of Prof. Triadis (IMI), Prof. Jiang (I<sup>2</sup>CNER/Yamaguchi University), and Prof. Bolster (University of Notre Dame) observed surprisingly persistent anomalous dispersion in numerical investigations for non-wetting fluid flow (CO<sub>2</sub>) in the presence of trapped wetting phase fluid (brine) [16, 17]. Anomalous dispersion was insensitive to the applied fluid-fluid slip boundary conditions, highlighting the primary importance of the induced complex flow network, rather than the inherent multiphase nature of the flow. We are aware of no other studies that systematically demonstrate the degree and persistence of anomalous dispersion in two phase flow resulting from varying molecular diffusivities and initial tracer distributions, highlighting strong dependencies on both factors.

**Geomorphology using persistent homology**: PI Tsuji and Prof. Shirai (IMI) used the apparatus of applied topology to characterize pore geometry of rock structures, in particular to estimate their permeability [18]. As pores are notoriously heterogeneous, they deployed persistent homology, created exactly to understand the geometry where the relevant scales are a priori unknown. They were the first in

developing novel comparison metrics and predictors based on persistent homology in structural geology studies [19]. By linking such parameters derived from persistence diagrams to hydrologic and elastic properties, this approach has significant potential to facilitate the development of new models to predict physical/elastic/hydraulic properties directly from pore geometry.

In the area of **biomathematics** Prof. Nishii (IMI) in collaboration with Mochida (RIKEN) used network models for gene-expression system to understand the gene transcription system, a key regulatory apparatus in cells [20]. Their goal is to understand which systems induce heterosis, a genetically driven difference in growth rates. The results could lead to better understanding of the intricate interconnection of the expression in plants, which has a potential to impact the development of promising biofuels (*Jatropha curcas*) and revolutionize agriculture.

## **5. Realizing an International Research Environment (within 4 pages)**

### **Globalization by the numbers**

In FY18 there was a vast amount of international activities that enhanced I<sup>2</sup>CNER's global visibility. I<sup>2</sup>CNER hosted 3 (40 in total since inception) international symposia; held 23 seminars in the Institute Interest Seminar Series (IISS) (143 in total since inception) with 44 speakers (256 in total since inception) of which 31 were non-Japanese (158 in total since inception); 10 seminars in the I<sup>2</sup>CNER Seminar Series (157 in total since inception) with 10 speakers (161 in total since inception) of which 7 were non-Japanese (105 in total since inception). The Institute's researchers were responsible for organizing, co-organizing, or serving on the scientific committees for 21 (207 in total since inception) international conferences, 44 international conference sessions/symposia or workshops (278 in total since inception), and 10 I<sup>2</sup>CNER international workshops (68 in total since inception). Our researchers have given 107 keynote, plenary and invited presentations in international conferences and fora (565 in total since inception). In addition, our researchers have joint publications with researchers from 38 new institutions (573 in total since inception) around the world and hosted 83 (343 in total since inception) internationally recognized researchers for scientific interaction and exchange. Our researchers also hosted 100 (389 in total since inception) distinguished visitors, of which 83 were distinguished researchers (343 in total since inception) at KU from across the world. Additionally, we maintain interactions with 4 internationally recognized research centers/universities, namely, the Paul Scherrer Institut, and Laboratory of Inorganic Chemistry, ETH Zurich, Switzerland, the Helmholtz Institute Forschungszentrum Juelich, the Southwest Research Institute, and the University of Göttingen. Lastly, we hold agreements with 4 internationally recognized research centers/universities: the University of Illinois at Urbana-Champaign, the National Fuel Cells Research Center (NFCRC) of the University of Irvine, SINTEF/NTNU of Norway, and the California Air Resources Board (CARB). As of March 31, 2018, I<sup>2</sup>CNER has a total of 25 partner institutions in the US, Europe, and Asia. Lastly, in FY18, I<sup>2</sup>CNER placed 7 (44 in total since inception) of our researchers at various Japanese (excluding KU) and international institutions.

### **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 their stays as joint researchers at the Center.

- In Appendix 3-2, give the number of overseas researchers among all the Center's researchers, and the yearly transition in their numbers. In Appendix 4-2 give the achievements of overseas researchers staying at the center to substantiate this fact.

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

All 9 of our overseas Principal Investigators are top-world researchers who are actively involved in I<sup>2</sup>CNER's research operations. They spend between one to seven weeks at KU and participate in events and exchange opinions on collaborative research projects with their KU counterparts. By way of example, Prof. Kilner, an international authority in the field of ionic and mixed conducting ceramics, spent 5 weeks in I<sup>2</sup>CNER during FY18. Jointly with KU faculty, he won international awards and research program grants, e.g. core-to-Core, and hosted one postdoc from I<sup>2</sup>CNER at Imperial College London for 5 weeks. 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<sup>2</sup>CNER and hosts postdocs from I<sup>2</sup>CNER at MIT for multiple months every year. PI Lippert invited a group of researchers from I<sup>2</sup>CNER to the I<sup>2</sup>CNER-PSI Joint Workshop at the Paul Scherrer Institut (PSI), Switzerland twice and accepted two I<sup>2</sup>CNER postdocs at PSI for two months in FY18. He visits I<sup>2</sup>CNER for 2 weeks a year on average to accelerate joint research projects. Dr. Somerday is a leading scientist in the area of mechanical metallurgy. He visited I<sup>2</sup>CNER for 2 weeks and hosted a group of researchers from I<sup>2</sup>CNER at the Southwest Research Institute for the

Hydrogen Materials Compatibility Division retreat. Aside from PIs, I<sup>2</sup>CNER hosted world top-level researchers 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.

- Enter the following to substantiate the facts provided above:
  - In Appendix 4-3, describe the Center's state of international recruitment of postdoctoral researchers, the applications received, and selections made.
  - In Appendix 3-2, give the percentage of postdoctoral researchers employed from abroad
  - In Appendix 4-4, describe the positions that postdoctoral researchers acquire upon leaving the Center.

### **I<sup>2</sup>CNER Young Researchers' Job Placement after Leaving the Center**

The environment at I<sup>2</sup>CNER provides a rich platform for young researchers to pursue technology impacting research in a highly international setting. To date, a large number of I<sup>2</sup>CNER young researchers have leveraged their appointments at the Institute to advance their professional careers. By way of example, Dr. Masaaki Sadakiyo, who was at I<sup>2</sup>CNER for 7 years (since April 1, 2012), accepted a position as a Lecturer at Tokyo University of Science; Dr. Nicola Perry, who was at I<sup>2</sup>CNER for over 5 years (since September 1, 2012), was promoted to Assistant Professor in our Electrochemical Energy Conversion division in FY14, then was recruited as an Assistant Professor at the University of Illinois at Urbana-Champaign beginning January 1, 2018; Dr. Seiichiro Kumura, who was at I<sup>2</sup>CNER for 1 year (since April 1, 2013), moved to the Matsushita Institute of Government and Management, then accepted a position as a Senior Researcher at the Renewable Energy Institute; Dr. Daniel Orejon, who was at I<sup>2</sup>CNER for 5 years (since October 1, 2013), was promoted to Assistant Professor in our Thermal Science and Engineering division in FY16, then was recruited as a Lecturer at the University of Edinburgh beginning December 1, 2018. Even after leaving I<sup>2</sup>CNER, Dr. Kimura and Profs. Perry and Orejon continue to be involved in our projects as Visiting Faculty from their new institutions.

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

- In Appendix 4-1, describe the state of cooperation with overseas satellites and other cooperative organizations. In Appendix 4-5, describe the state of the Center's agreements concluded with these organizations.

### **Illinois Satellite**

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<sup>2</sup>CNER's overall research culture. The efforts undertaken at the Satellite to promote the mission of I<sup>2</sup>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<sup>2</sup>CNER research activities at KU, and they are continually re-assessed based upon their relevance to the overall I<sup>2</sup>CNER vision and roadmap. As of March 31, 2019, there are 7 WPI Faculty and 3 WPI Principal Investigators participating at the Satellite. One member of I<sup>2</sup>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<sup>2</sup>CNER: Prof. Ian Robertson, Dean of the College of Engineering at the University of Wisconsin-Madison (WPI Principal Investigator); Prof. Ken Christensen, Aerospace and Mechanical Engineering Department Chair at the University of Notre Dame (WPI Principal Investigator), and Prof. Angus Rockett, Metallurgical and Materials Engineering Department Head, Colorado School of Mines (WPI Professor, member of I<sup>2</sup>CNER's IPRC).

#### *Revised Satellite Agreement*

The Kyushu-Illinois Satellite Agreement was renewed and went into effect on 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 KU, including mutual exchange, writing of joint papers, use of the I<sup>2</sup>CNER affiliation in publications, etc. Indeed, the signing of the MRA can serve as a model for the entire WPI Program.

#### *Kyushu-Illinois I<sup>2</sup>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. This agreement came into effect on May 26, 2014 and is currently in the process of being revised and renewed for the Kyushu-Illinois Strategic Partnership (see section 7 "Others"). A "Student Exchange Program Agreement" between KU and Illinois was also signed on October 24, 2014. The numbers of KU undergraduate students who visited Illinois are 5 (FY13), 6 (FY14), 6 (FY15), 6 (FY16), 6 (FY17), and 6 (FY18). During their month long 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 Illinois' 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. In FY16, two of the students were involved in research that *resulted in a paper publication: LANGMUIR, DOI: 10.1021/acs.langmuir.7b03948*. An exchange student from the FY18 program, will also be a co-author in a future publication.

#### *Partnership for International Research and Education (PIRE)*

The joint PIRE award to Illinois and KU, "Integrated Computational Materials Engineering for Active Materials and Interfaces in Chemical Fuel Production," is a result of I<sup>2</sup>CNER's successful fusion of computational science with experiment, and was awarded beginning in FY15 for a total of 5 years. The PIRE project brings together researchers from I<sup>2</sup>CNER (both Illinois and KU), Northwestern University (NU), Imperial College, London, and the University of California, Berkeley (UCB). Every year since FY16, PIRE has funded the x-FU(s)ION (eXchange: FUKuoka, Illinois, califOrnia, Northwestern) exchange program for undergraduates from the US to spend 2 months at I<sup>2</sup>CNER in KU conducting research. The number of exchange students who visited I<sup>2</sup>CNER under this program are 6 in FY16 (all from UIUC), 5 in FY17 (3 from UIUC, 1 from NU, and 1 from UCB), and 6 in FY18 (5 from UIUC and 1 from UCB). In FY19, 7 students will be participate in the PIRE/x-FU(s)ION program, 6 from UIUC and 1 from UCB. Out of the total 24 students, 15 are female.

#### *Student Exchange Workshops Sponsored by the US Consulate*

Every year since 2016, there has been a workshop where each of the PIRE/x-FU(s)ION Exchange students that visit Kyushu and the I<sup>2</sup>CNER Exchange students that visit the Illinois Satellite, give a presentation in Fukuoka. The presentations cover both their research conducted and cultural experiences. In 2018, this workshop was sponsored by the US Consulate and was publically held at the Fukuoka American Center. A similar workshop will be hosted by the US Consulate and will be held on July 31, 2019.

### **Total Graduate/Undergraduate Students Visits to KU**

As of March 31, 2019, the Institute has hosted a total of 73 graduate/undergraduate students from various institutions around the world, including Illinois, since its inception. The numbers of visiting students are 1(FY10), 9 (FY11), 6 (FY12), 7 (FY13), 7 (FY14), 6 (FY15), 10 (FY16), and 17 (FY17), 10 (FY18) of which, 1, 6, 1, 3, 1, 3, 8, 14, and 10 respectively, stayed for more than a month at KU. Of the total 73, 38 students were from Illinois and 23 of these students stayed for more than a month.

### **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.

#### **Kyushu University Energy Week in Support of Q-PIT**

"KU Energy Week" is a week-long sequence of international workshops and symposia hosted by various energy research centers of KU. KU has held Energy Week during the last week of January since 2016 in order to support Q-PIT (see section 6-4-2 for more about Q-PIT) becoming an international hub for "future energy" research and education. Energy week is centered around I<sup>2</sup>CNER's Annual Symposium and International Workshops organized by I<sup>2</sup>CNER's divisions. The 2019 KU Energy Week was held from January 28 through February 1 with a theme of "Energy Intelligence beyond Borders: Cultivating Creativity

in Future Generations.” The 5-day event welcomed a total of over 1,900 participants from academia, industry, and government, both locally and overseas.

### **2019 Annual Symposium**

The 2019 I<sup>2</sup>CNER Annual Symposium, titled “Energy Transitions and the Role of CCS toward a Carbon-Neutral Energy Society”, was held on January 31, 2019 and was attended by 150 participants (26 from overseas). This symposium brought together top level researchers both from Japan and abroad to discuss the issues surrounding the transition to a low-carbon energy future, considering both the deployment of renewable energy and the role of CCS. Through discussion and exchange of ideas in the symposium, participants explored ideal technological combinations, policy approaches, as well as emerging opportunities, and assessed where I<sup>2</sup>CNER’s research activities should be focused on a moving-forward basis. The symposium included 6 invited lectures such as a lecture titled “Clean Energy Technologies for Economic Transitions” by Dr. Jill Engel-Cox, Director of Joint Institute for Strategic Energy Analysis at National Renewable Energy Laboratory, and a lecture titled “CCS and its Role in the Low-Carbon Energy Transition” by Prof. Michael Celia, a Nobel Laureate from Princeton University’s Department of Civil and Environmental Engineering.

### **2018 Annual Symposium**

The 2018 I<sup>2</sup>CNER Annual Symposium, titled “Challenges in Thermal Science and Engineering towards a Sustainable Society”, was held on January 31, 2018 and was attended by 166 participants (86 from overseas). The vision of the symposium provided a platform for discussion and debate on the science and engineering for efficiency increase in power generation, smart utilization of waste heat, nanomaterials and metal-organic frameworks for efficient heat pump cycles, next generation working fluids, and nanoscale transport and heat transfer mechanisms. The Symposium included 2 keynote lectures (i) titled “Thermal Waste Heat Utilization for Achieving Super Smart Community” by Prof. Takao Kashiwagi (Tokyo Institute of Technology) and (ii) titled “Different Regimes of Pool Boiling” by Prof. Gautam Biswas (Indian Institute of Technology, Guwahati).

### **2017 Annual Symposium**

The 2017 I<sup>2</sup>CNER 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 than 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 titled “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 titled “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, a Nobel Laureate from Princeton University’s Department of Civil and Environmental Engineering.

### **2016 Annual Symposium**

The 2016 I<sup>2</sup>CNER 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 I<sup>2</sup>CNER. 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 I<sup>2</sup>CNER, 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 titled “Trends in Scientific Computing and Data” was given by Prof. Edward Seidel, the Director of National Center for Supercomputing Applications (NCSA) at UIUC.

### **2015 Annual Symposium**

The I<sup>2</sup>CNER Annual Symposium 2015: "Fuel Generation and Use for the 21<sup>st</sup> 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 I<sup>2</sup>CNER'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.

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

On January 30, 2014, co-organized the "I<sup>2</sup>CNER & ACT-C Joint Symposium 2014" with the Advanced Catalytic Transformation program for Carbon utilization (ACT-C) of the Japan Science and Technology Agency (JST). The symposium was attended by 177 people, including many international guests.

### **Japan-France Workshops on Nanomaterials**

From May 17-19, 2017, The 12<sup>th</sup> Japan-France Workshop on Nanomaterials (3<sup>rd</sup> WPI Workshop on Materials Science) was held at I<sup>2</sup>CNER Hall, with 69 people (40 from overseas), including the Directors of 4 WPI institutes (AIMR, MANA, iCeMS and I<sup>2</sup>CNER) and top-level researchers from 10 French Centers of Competence in Nanoscience (C'Nano) in attendance. The workshop allowed I<sup>2</sup>CNER researchers to strengthen existing partnerships and explore potential opportunities for future collaborations with their French colleagues.

### **International Hydrogen Conference**

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 approximately every four years, is the premier topical meeting worldwide on hydrogen effects on materials.

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

One of the most important goals of the I<sup>2</sup>CNER Seminar Series is to engage key members of the international community from academia, national laboratories, industry, and government agencies (policy makers). In FY18, the Institute hosted a total of 10 speakers (7 non-Japanese) in 10 I<sup>2</sup>CNER Seminars. Cumulatively, 161 speakers have presented at 157 I<sup>2</sup>CNER Seminars.

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

Describe the Center's preparations to provide an environment conducive for overseas researchers 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 I<sup>2</sup>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<sup>2</sup>CNER researcher 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 KU. "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<sup>2</sup>CNER 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<sup>2</sup>CNER established the "Collaborative Foreign Exchange Program" in order to encourage young researchers to visit our overseas collaborating institutions. So far, 21 young researchers had their proposals approved, and 14 of them visited the Illinois Satellite for the extended period between one and nine months. Through this program, in FY17, Prof. S. Harish stayed at the University of Edinburgh for 5 months and Prof. N. D. Hoa stayed at the Illinois Satellite, each for 5 months. In FY18, Prof. D. Orejon also spent 4 months at the Illinois Satellite.

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

### **6-1. Decision-making system in the center**

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

- In Appendix 3-3, draw a concrete diagram of the Center's management system.

### **Director's Authority**

KU regulations and rules give the authority for the I<sup>2</sup>CNER 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 Finance, Prof. Kazuhide Inoue. Regular meetings are held between the Director and the EVP in charge of Research and Finance. 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.

### **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 Office**

As of March 31, 2019, the administrative office consists of 19 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 (2 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.

### **Administrative Director**

Since April 1, 2015, Mr. Shunichi Masuda has been the I<sup>2</sup>CNER Administrative Director, which includes responsibility for the oversight of the Administrative Office and other duties as assigned by the Director, e.g. interactions with other KU units, government agencies, and corporations. Mr. Masuda has extensive experience working in industry, both in the US and Japan.

### **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. (If any describe the ripple effects on other institutions.)

In order to ensure smooth management of the Institute, the I<sup>2</sup>CNER Director has requested that the KU 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<sup>2</sup>CNER to leverage the existing "Kyushu University Joint Research Department System."

### **Switching to Academic Quarter (4-term) System**

In FY17, KU made a noteworthy academic change by implementing the Academic Quarter (4-term) System in order to facilitate student exchange programs from universities in the US, such as Illinois. The system also enables cross-appointed faculty from overseas to teach courses more easily at KU and makes it possible for KU faculty to participate in research/teaching activities at overseas partner institutions, and vice versa.

### **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, Prof. Y. Baryshnikov of the University of Illinois will be employed by IMI during the summers of 2019 and 2020.

### **Intra-University Faculty Transfer System**

KU'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<sup>2</sup>CNER has been utilizing this system since FY13, and in FY18, 7 senior-level faculty were transferred to I<sup>2</sup>CNER and served as the core KU-based PIs of I<sup>2</sup>CNER.

### **I<sup>2</sup>CNER Faculty Involvement with Teaching**

I<sup>2</sup>CNER continues its tradition of collaborating with KU's School of Engineering, Graduate School of Engineering, and Graduate School of Integrated Frontier Sciences because it brings faculty into the classroom who have international experiences with cutting-edge research.

I<sup>2</sup>CNER will be involved in KU's new School of Interdisciplinary Science and Innovation, which opened in April 2018. A new international energy course will be developed, in which I<sup>2</sup>CNER faculty are expected to be involved with teaching, with the purpose being to contribute to the international education of Japanese students.

I<sup>2</sup>CNER will play a crucial role in the KU "Excellent" Graduate School initiative that will establish an "Excellent" Graduate School in KU with Q-PIT at its core. A number of the admitted students to this "Excellent" Graduate School will be advised/supervised by I<sup>2</sup>CNER faculty. KU envisions that I<sup>2</sup>CNER's faculty involvement in this innovative and attractive graduate education program will advance the research/educational capabilities of KU and foster the international graduate education culture throughout KU.

### **I<sup>2</sup>CNER's Merit-based Salary System/ KU's New Merit-based Annual Salary System**

In view of the effectiveness of the I<sup>2</sup>CNER's Merit-based Salary System, KU adopted and introduced this system across all units. As of March 1, 2019, 17.0% of KU faculty are paid within this system. KU'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, I<sup>2</sup>CNER 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 KU.

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

The following two items concern the support that the host institution provides the Center. Describe the functional measures that the host institution has taken to sustain and advance the Center's project. That include 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.

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

- In Appendix 6-1, describe the concrete measures being taken by the host institution.

### **I<sup>2</sup>CNER's Permanent Position within Kyushu University**

Effective April 1, 2013, with the revision of the "Regulations of Kyushu University," I<sup>2</sup>CNER's position is clearly defined as a permanent Research Institute of KU without regard to the length of the WPI Program.

## **President Kubo's Vision Regarding Tenured Faculty and PIs**

President Kubo envisioned that by 2020, I<sup>2</sup>CNER will employ 20-25 PIs, including 10 tenured PIs organically in the Institute (3 to 4 of which will be non-Japanese PIs). Following this vision, KU has allotted a total of 11 tenured faculty positions to I<sup>2</sup>CNER (Professor and Associate Professors; 10 are organically at I<sup>2</sup>CNER and 1 transferred from I<sup>2</sup>CNER to KU's ERE department). Of the 10 tenured I<sup>2</sup>CNER faculty, 6 are PIs. The remaining PI positions are filled either through faculty transfer, KU faculty, or from international partnering institutions. The total number of PIs as of March 31, 2019 is 26. Future PI positions can also be filled through either: i) the Intra-University Transfer System (i.e., faculty transfer from other units of KU), ii) cross-appointments between I<sup>2</sup>CNER and other units of KU (e.g. economics, sciences, mathematics, life sciences, etc.), or iii) cross-appointments between I<sup>2</sup>CNER and its international partner institutes and industry.

## **Tenure-Track Positions**

I<sup>2</sup>CNER and the Institute of Mathematics-for-Industry (IMI) jointly hired 2 tenure-track assistant professors, Drs. K. Matsue and H. Nguyen-Dinh, in Fall 2016 after submitting a joint proposal to KU's newly initiated tenure-track faculty program. These two faculty work to foster the research intersection between energy and mathematics and strengthen the ties and interactions between I<sup>2</sup>CNER and IMI. Profs. Matsue and Nguyen-Dinh did their sabbatical at Illinois from Sept. 23, 2018 to Mar. 29, 2019 and Oct. 30, 2017 to Mar. 30, 2018, respectively.

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

- To Appendix 6-2, excerpt the places, in the host institution's "Mid-term objectives" and/or "Mid-term plan" that clearly show the positioning of the WPI center within its organization.

## **Kyushu University's Mid-term Plan**

I<sup>2</sup>CNER is at the center of KU'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<sup>2</sup>CNER)."

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

In order to promote the concept of I<sup>2</sup>CNER 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)". I<sup>2</sup>CNER plays a key role in this organization by helping to cross-pollinate a wide range of collaborations on energy research between KU research units of diverse disciplines including social sciences, economics, law, and political sciences. This will allow I<sup>2</sup>CNER to capitalize on opportunities to broaden and enrich its energy portfolio while also helping Q-PIT advance its mission to catalyze interactions between disparate disciplines and units.

As of March 31, 2019, KU has allotted 5 tenured faculty positions to Q-PIT. To date, 3 tenured Professor positions have been filled, and a total of 14 faculty members are engaged in energy research as Q-PIT Faculty. Director Sofronis is a member of the Q-PIT Strategic Committee.

## **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 3-1, 3-2, give the transition in the number and ratio of female researchers.

## **Evaluation of Young Investigators**

The research progress of all young faculty members is reviewed by the Director, Associate Directors, and the corresponding Division Lead PI on 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 from the Director. In FY18, following their interviews, all young researchers were asked by the Director to present in the Institute Interest Seminar Series (IISS) to further foster interdisciplinary research in I<sup>2</sup>CNER.

## **Director's Discretionary Funding**

The "I<sup>2</sup>CNER Competitive Funding" initiative has mainly been used by young faculty and postdocs. In addition, the Director's discretionary 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<sup>2</sup>CNER full-time researchers to develop their research environment are, 22 (FY11), 56 (FY12), 52 (FY13), 26 (FY14), 27 (FY15), 29 (FY16), 23 (FY17), and 16 (FY18) million JPY.

### **I<sup>2</sup>CNER Graduate Students and Super Research Assistants (SRA) Program**

I<sup>2</sup>CNER provides a rich platform for both young researchers and students to pursue technology impacting research in a highly international setting. Since the inception of I<sup>2</sup>CNER, a total of 142 (including 73 non-Japanese) KU graduate students have been carrying out their Ph.D. thesis work under the supervision of I<sup>2</sup>CNER faculty. Of the total 142, 29 excellent students were recruited as "Super Research Assistants (SRA)" and supported by the WPI fund. In FY18, I<sup>2</sup>CNER employed 3 SRAs. These SRAs are carefully selected from a large pool of graduate students and are supervised by our young faculty. This helps I<sup>2</sup>CNER young faculty develop educational and research supervision skills. The ascending careers of the former I<sup>2</sup>CNER SRAs are another strong demonstration that the environment at I<sup>2</sup>CNER fosters excellence for young graduate students. By way of example, Dr. Arnaud Macadre (a former I<sup>2</sup>CNER SRA) joined I<sup>2</sup>CNER as a Postdoc after graduation, and then accepted a position as an Associate Professor at Yamaguchi University beginning April 1, 2018; Dr. Yutaku Kita (a former I<sup>2</sup>CNER SRA) was selected to receive the JSPS Research Fellowship (DC2 then PD) after his SRA appointment, and then accepted a position as an Assistant Professor at KU beginning January 1, 2019.

### **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. From FY15, such skill-building was administered on an individual basis. It is an established tradition in the Institute that I<sup>2</sup>CNER's full-time researchers with a proven record of winning KAKENHI grants provide advice/consultation to young researchers.

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

It is a priority within the Institute to hire and retain excellent female researchers. The Director specifically reviews applications by every woman applicant for any postdoc or faculty position. As a result, the number of female researchers in I<sup>2</sup>CNER has been 4 (FY10), 7 (FY11), 9 (FY12), 12 (FY13), 11 (FY14), 11 (FY15), 10 (FY16), and 14 (FY17) and 13 (FY18). The number of female researchers in I<sup>2</sup>CNER are, although not at the desired level, certainly larger than corresponding totals in the other sciences, math, and engineering units of KU. The fact that there are now 7 full-time female researchers in I<sup>2</sup>CNER is a direct result of the Director's concentrated efforts to make the I<sup>2</sup>CNER environment more attractive to women applicants. Among the 6 newly hired faculty and postdocs in FY18, one was a woman (postdoc). As of March 31, 2019, I<sup>2</sup>CNER has a total of 26 women researchers: 13 at KU, 9 at Illinois, and 4 at other international/domestic institutions.

### **Plans for Graduate Student Exchange**

The I<sup>2</sup>CNER Undergraduate Exchange Program has become such a success that a similar program is being explored for graduate students between KU and Illinois. This effort was initiated by the former Dean of the KU School of Engineering, Prof. Takamatsu, who visited the Illinois College of Engineering in November, 2017. The establishment of this institutionalized exchange program is currently part of the discussions held for the Kyushu-Illinois Strategic Partnership.

## **7. Others**

In addition to the above 1.-6. evaluation items, note any of the Center's leading activities, distinctive features or other important points that denote its status as an "internationally visible research center."

### **Kyushu-Illinois Strategic Partnership**

A delegation of 11 executives and faculty from various KU departments, led by KU's Executive Vice President for International Affairs, Prof. Masato Wakayama, visited Illinois on May 8-10, 2019 to work on a joint vision statement for the future of the Kyushu-Illinois Strategic Partnership. So far, the relationship between the two universities has primarily been held up by I<sup>2</sup>CNER. The purpose of KU's delegation visit is to build a strategic partnership between UIUC and KU that broadens the collaborations to other colleges and departments (such as engineering, social sciences, humanities, economics, law, agriculture etc.). The vision

of this strategic partnership and the corresponding agreements are currently being discussed. This partnership could include several exchanges (of students, postdocs, and sabbaticals of young faculty) and dual degree programs. August 26, 2019 has been set as the date for the signing ceremony of the revised MOU between the two universities. KU's president, Prof. Chiharu Kubo, will be visiting Illinois to sign the agreement alongside Illinois' Chancellor, Prof. Robert Jones.

### **Argonne National Laboratory**

I<sup>2</sup>CNER's research and impact has initiated discussions between UIUC and Argonne National Laboratory on a future partnership on Fuel Cells, Electrolyzers, Hydrogen, and Grid Management. A successful workshop was held at Argonne on December 17, 2018. A concept paper is being written that will constitute the basis for the creation of a Midwest Energy Hub. This will strengthen the future collaboration of the Satellite with I<sup>2</sup>CNER at KU.

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

The membership of I<sup>2</sup>CNER's External Advisory Committee was further expanded and diversified in FY15 to better align with all aspects of the Institute's research. In April 2015, Prof. Michael Celia, Princeton University, expert on CO<sub>2</sub> storage and 2007 Nobel Laureate, specifically on pore scale behavior and upscaling to reservoir behavior, officially accepted our invitation to serve on the EAC. Prof. Celia made his first visit to I<sup>2</sup>CNER on January 29, 2016 and spent the day taking lab tours, attending presentations and engaging in discussion with members of the CO<sub>2</sub> Storage Division, and giving a seminar in the I<sup>2</sup>CNER Seminar Series, which was filmed and presented again on February 2 as part of the pore scale flow processes subtheme session of the 2016 I<sup>2</sup>CNER Annual Symposium. He was also an invited speaker at the 2019 I<sup>2</sup>CNER Annual Symposium where he gave a presentation titled "CCS and its Role in the Low - Carbon Energy Transition".

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

The Institute's 4<sup>th</sup> EAC Retreat was held at UIUC on March 9-10, 2016, and involved 8 of the 10 members of the EAC (Prof. Adrian and Prof. Armstrong were unavailable to attend). The purpose of the retreat was to assess the current status and progress of I<sup>2</sup>CNER projects, and actions we can take to position ourselves strategically for a third term beyond 2020. In the form of a report submitted to the Director, the EAC offered constructive feedback on all aspects of the Institute, including the Institute's structure, technical issues, and administrative matters.

The full list of members as of April 1, 2019 is as follows:

- Dr. Deborah Myers (Chair), Argonne National Laboratory, USA
- Dr. Kevin Ott, (Vice-Chair), Los Alamos National Laboratory, USA
- Prof. Ronald J. Adrian, Arizona State University, USA, *National Academy of Engineering (NAE)*
- Dr. Robert J. Finley, Illinois State Geological Survey, USA
- Prof. Reiner Kirchheim, University of Göttingen, Germany
- Prof. Robert McMeeking, University of California, USA, *National Academy of Engineering (NAE)*
- Prof. Tetsuo Shoji, Tohoku University, Japan
- Prof. Fraser Armstrong, University of Oxford, UK, *Fellow of the Royal Society (FRS)*
- Prof. Michael Celia, Princeton University, USA, *Nobel Laureate*
- Dr. Monterey Gardiner, BMW Japan (formerly with DOE), Japan

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

The Internal Programs Review Committee (IPRC) is an important standing committee of the Institute which is called by the Director whenever necessary to review individual programs within the Institute. The members of the IPRC and the Chair of the Committee are appointed by the Director. Once the review(s) are complete, the IPRC provides the Director with a written advisory report. The final decision about what action to take regarding any individual research program is the responsibility of the Director. In FY16, 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 FY16, 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. Since then, the Director has consulted with the IPRC on several individual research projects, with regard to its progress as it relates to the respective roadmap.

### **Director as a Fukuoka City Ambassador**

On February 1, 2018, Director Sofronis was reappointed by the Mayor of the City of Fukuoka as a city Ambassador for two additional years. His duties include the advancement of the international image of Fukuoka and the organization of international conferences in the city. On December 5, 2018, Director Sofronis participated in the 6<sup>th</sup> Fukuoka City Ambassador Seminar and shared with the audience some of the major accomplishments that I<sup>2</sup>CNER has made to the advancement of Fukuoka City’s international image. Additionally, Director Sofronis is assisting the City of Fukuoka, along with KU, to bring the 2024 World Hydrogen Energy Conference (WHEC) to Fukuoka. This would be a joint proposal from the city of Fukuoka and KU and if successful, it would attract approximately 1,800 attendees.

## **8. Center’s Response to Results of FY 2018 Follow-up (including Site Visit Results)**

\* Describe the Center’s response to results of FY 2018 follow-up. Note: If you have already provided this information, please indicate where in the report.

### **Actions required and recommendations from the Site Visit Report**

I<sup>2</sup>CNER has at present about 10 faculty members, which number the president of Kyushu University promised to maintain. The Institute has been positioned as a permanent organization for energy research within Kyushu University due to the efforts of I<sup>2</sup>CNER itself and the University’s administration. However, this is the time to make a clear and detail plan for sustaining the Institute after WPI support ends. The plan should include among other things the number of PI’s and researchers, the budget and space for I<sup>2</sup>CNER, and the Institute’s relationship with the UIUC satellite. Kyushu University’s administration also should make clear how it will support the sustainability of I<sup>2</sup>CNER. In addition, the position of I<sup>2</sup>CNER in Q-PIT should be clearly defined, which will facilitate the fusion of research in a wide range of fields, including mathematics, sociology, and political science.

Kyushu University will fully support employment expenses for 20 of I<sup>2</sup>CNER's core faculty (10 are organically tenured at I<sup>2</sup>CNER, 6 transferred PIs (Ishihara, Ogo, Takata, Sasaki, Sugimura, Takata) and 4 additional PIs (Fujigaya Tsuji, Sakai, and Watanabe). With regard to the remaining PI positions which are not “tenured and organic in I<sup>2</sup>CNER,” they will be filled through either: i) the Intra-University Transfer System, ii) cross-appointments between I<sup>2</sup>CNER and other units of KU (e.g. economics, sciences, mathematics, life sciences, etc.), or iii) cross-appointments between I<sup>2</sup>CNER and its international partner institutes and industry. The list of the tenured faculty in I<sup>2</sup>CNER will be augmented by the addition of two tenure-track faculty hired jointly with the Institute of Mathematics for Industry. Additionally, I<sup>2</sup>CNER has a remaining point balance of 0.791 that will be used to hire another tenured Associate Professor in FY19. KU will grant I<sup>2</sup>CNER Building II (a total floor space of 5,014m<sup>2</sup>) free of charge. The space provided by this support significantly exceeds the space allotment per researcher under the university's regular policy. The Institute’s relationship with the UIUC satellite will continue through a new strategic partnership agreement that will be signed by the UIUC Chancellor and President Kubo on August 26, 2019. I<sup>2</sup>CNER plays a key role in Q-PIT by helping to cross-pollinate a wide range of collaborations on energy research between KU research units of diverse disciplines including social sciences, economics, law, and political sciences. This allows I<sup>2</sup>CNER to capitalize on opportunities to broaden and enrich its energy portfolio while also helping Q-PIT advance its mission to catalyze interactions between disparate disciplines and units. The strengthening of collaborations with the Institute of Mathematics for Industry (IMI) through the joint hiring of two tenure-track assistant professors allowed I<sup>2</sup>CNER to make significant inroads in the Applied Mathematics for Energy research field. The cross-appointment of Prof. Chapman with the Department of Economics (60% at I<sup>2</sup>CNER and 40% at the Department of Economics) as of April 1, 2019 will further advance interdisciplinary research between I<sup>2</sup>CNER and Economics.

Another significant issue is that large-scale funding needs to be continuously and aggressively pursued by

the efforts of I<sup>2</sup>CNER itself as well as by individual researchers.

The Director's vision is that I<sup>2</sup>CNER can remain strong and agile by developing cores of embedded centers funded by external agencies (both industrial and governmental) and securing industrial projects that will last beyond the WPI funding period. Drawing from the experience gained from the establishment of the NEXT-RP Center, I<sup>2</sup>CNER will intensify its efforts to establish similar internal research centers in response to national initiatives by government agencies such as NEDO, METI, Riken, JSPS, and JST. Riken, for example, currently does not have a location in the Western part of Japan, making Kyushu University a strong option for a potential future center. With regard to establishing internal research centers, I<sup>2</sup>CNER will i) be active on implanting future research themes in government agencies for new national agency research initiatives, ii) rely on the input from the Industrial Advisory Board to create new ideas that will attract funding from industry, government, and national and international foundations (e.g. Gates Foundation), and iii) utilize the Industrial Research Division (Project with Mazda Motor Corporation), and (after April 1, 2020) the planned Platform for Societal Implementation and Industrial Collaboration to attract industrial projects for collaborative efforts in the form of open innovation. An example of attracting industrial funding are the workshops that were organized jointly with Toshiba Corporation to explore the possibilities of joint research on topics of mutual interest.

### **Actions required and recommendations from the Follow-up Report**

It is necessary to have a detailed plan of budget, space, size and scope of I<sup>2</sup>CNER after the end of the WPI grant. One of the biggest concerns is how to maintain the excellent balance and other strengths of the program as I<sup>2</sup>CNER adapts to new sources of funding. It is the most important issue and would like to receive this plan by next year.

Please see above answers to "Actions required and recommendations from the Site Visit Report."

I<sup>2</sup>CNER has been able to attract international postdocs and enable them to launch and build their career to become tenured faculty of Kyusyu U or to be attracted to overseas universities in similar positions, including UIUC. This is one of the most difficult aims of WPI and I<sup>2</sup>CNER should be commended for making this happen.

I<sup>2</sup>CNER continues to be an exemplar of the WPI mission on helping young postdocs and faculty launch their careers. By way of example, as of April 2, 2018, Postdoc A. Macadre joined the Yamaguchi University as Associate Professor; and as of April 1, 2019, Assistant Professor M. Sadakiyo joined the Tokyo University of Science as Associate Professor.

Interaction with other institutes outside of Kyushu U is highly recommended as the subject of energy research is so vast. This is needed for the brain circulation of young scientists as their careers grow.

I<sup>2</sup>CNER continuously seeks to advance its international interactions with institutes, industries, government agencies, and laboratories outside KU and this is demonstrated by the large number of 25 institutions with which I<sup>2</sup>CNER interacts, collaborates, and publishes jointly. Highlights of I<sup>2</sup>CNER's globalization efforts, apart from those with the Satellite at the University of Illinois, include a new partnership with the University of Göttingen, led by Prof. Reiner Kirchheim and I<sup>2</sup>CNER's Director, to establish an International Research Training Group that will be co-funded by the German Research Foundation (DFG) and JSPS, as well as the JSPS Core-to-Core program which provides funding for joint research and postdoc exchanges carried out between I<sup>2</sup>CNER, Imperial College, London, Paul Scherrer Institut, and the Massachusetts Institute of Technology.

## Appendix 1-1 List of Papers Underscoring Each Research Achievement

- \* List papers underscoring each research achievement [1] ~ [20] listed in the item 2-1 "Research results to date" of 2. "Advancing Research of the Highest Global Level" (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] Hydrogen station deployment for fuel cell vehicles

- \*1. K. Itaoka, S. Kimura, K. Hirose (2019) Methodology Development to Locate Hydrogen Stations for the Initial Deployment Stage, *E3S Web of Conferences*, 83(01014), 18.  
(DOI: 10.1051/e3sconf/20198301014)

This work presented comprehensive methodologies to deploy hydrogen station including a demand estimation methodology for the initial deployment stage of fuel cell vehicles (FCVs) and an optimum location allocation methodology, while considering applications of the methodology to the real world. This paper suggested efficient location sites not only in major metropolitan areas but also in prefectural capital cities and regional principal cities. The methodologies and results were submitted to the government to help guide companies and local governments that wish to identify location for new hydrogen stations (K. Itaoka, K. Hirose, S. Kimura, Y. Kikuchi, Y. Higuma, K. Honda and K. Shimokawa (2017) Basic Research on Hydrogen Supply Infrastructure Development (Research on Locating New Hydrogen Station) submitted to Ministry of Economy Trade and Industry, entrusted by Next Generation Vehicle Promotion Center, contract file number 28-0366)

### \*[2] Energy Transitions: The People, Technology, and Systems Nexus

- \*2. A. J. Chapman, K. Itaoka (2018) Energy transition to a future low-carbon energy society in Japan's liberalizing electricity market: Precedents, policies and factors of successful transition, *Renewable and Sustainable Energy Reviews*, 81(2), 2019-2027.

This paper identifies world leaders' progress in achieving their energy transitions, and draws lessons for Japan, a late liberalizer, toward achieving a successful, policy driven energy transition. Key policy and technological lessons are identified to contribute to this goal. It was found that Japan lacks ambitious future renewable energy deployment goals, and requires a long term (2050) vision to ensure that a 'successful' transition can be achieved.

- \*3. A. J. Chapman, K. Itaoka (2018) Curiosity, economic and environmental reasoning: Public perceptions of liberalization and renewable energy transition in Japan, *Energy Research & Social Science*, 37, 102-110.

This research uncovers Japanese householder's opinions toward the use, knowledge, and purchasing choice for energy. For the first time, we were able to define householders into three discrete active, intermediate, and passive groups, identifying motivations for participation in the energy market.

### \*[3] Photovoltaic conversion efficiency and stability in hybrid perovskite based devices

- \*4. 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 of perovskite solar cells by fabricating them in nitrogen, these perovskite solar cells still contained a small amount of metallic lead. Therefore, we introduced benzoquinone (BQ) into a precursor solution used for the fabrication of the perovskite films. This further suppresses the formation of metallic lead and improves device stability. The extrapolated device 80%- and 50%-lifetimes reached 4,000 and 10,000 hrs, respectively, one of the longest ever reported.

5. H. Uoyama, K. Goushi, K. Shizu, H. Nomura, C. Adachi (2012) Highly efficient organic light-emitting diodes from delayed fluorescence, *Nature*, 492, 234-238.

The inherent flexibility afforded by molecular design has accelerated the development of a wide variety of organic semiconductors over the past two decades. In particular, great advances have been made in the development of materials for organic light-emitting diodes (OLEDs), from early devices based on fluorescent molecules to those using phosphorescent molecules. In OLEDs, electrically injected charge carriers recombine to form singlet and triplet excitons in a 1:3 ratio; the

use of phosphorescent metal–organic complexes exploits the normally non-radiative triplet excitons and so enhances the overall electroluminescence efficiency. Here we report a class of metal-free organic electroluminescent molecules in which the energy gap between the singlet and triplet excited states is minimized by design, thereby promoting highly efficient spin up-conversion from non-radiative triplet states to radiative singlet states while maintaining high radiative decay rates, of more than  $10^6$  decays per second. In other words, these molecules harness both singlet and triplet excitons for light emission through fluorescence decay channels, leading to an intrinsic fluorescence efficiency in excess of 90 percent and a very high external electroluminescence efficiency, of more than 19 percent, which is comparable to that achieved in high-efficiency phosphorescence-based OLEDs.

#### **\*[4] Novel Photocatalysts**

\*6. S. Ida, K. Sato, T. Nagata, H. Hagiwara, M. Watanabe, N. Kim, Y. Shiota, M. Koinuma, S. Takenaka, T. Sakai, E. Ertekin, T. Ishihara (2018) A Cocatalyst that Stabilizes a Hydride Intermediate during Photocatalytic Hydrogen Evolution over a Rhodium-Doped TiO<sub>2</sub> Nanosheet, *Angewandte Chemie*, 57(29), 9073-9077.

This combined computational and experimental study establishes the detailed mechanism by which isolated Rh atom co-catalysts facilitate the hydrogen evolution reaction on doped 2D titania nanosheets. The original observation was first reported by Ertekin, Ishihara, et al. in *J. Am. Chem. Soc.* 137 239-244 (2015), showing that Rh-doped sheets may show an activity ten times higher than that of the undoped sheet. However, the precise role of the single atom co-catalyst remained unclear. Through combined first principles modeling, FTIR and NMR spectroscopy, and EXAFS measurements, the present analysis provides unprecedented insights into the mechanism by which Rh dopant atoms enhance activity. The results show that the the Rh cocatalyst facilitates the formation of oxygen vacancies in the titania nano sheet, which then stabilizes the formation of a hydride on the atomic Rh site, which serves as an intermediate species for hydrogen evolution. These insights are expected to contribute to the design of cocatalysts for photocatalytic hydrogen evolution and the field of artificial photosynthesis using semiconducting materials.

\*7. N. Kim, E. M. Turner, Y. Kim, S. Ida, H. Hagiwara, T. Ishihara, E. Ertekin (2017) Two-Dimensional TiO<sub>2</sub>Nanosheets for Photo and Electro-Chemical Oxidation of Water: Predictions of Optimal Dopant Species from First-Principles, *Journal of Physical Chemistry C*, 121(35), 19201-19208.

This work establishes a set of design rules, determined with quantum mechanical simulations, for the selection of optimal transition metal dopants, to increase the catalytic activity of doped 2D titania nanosheets. First-principles density functional theory simulations were used to simulate the energy landscape of the oxygen evolution reaction on both pristine and transition metal doped TiO<sub>2</sub> systems. The results show that selected dopants modify the binding strength of the reaction intermediates and can most effectively reduce rate limiting thermodynamic barriers and theoretical required over potentials for oxygen evolution. Subsequent photocatalytic measurements of OER activity with selected dopants were carried out - the first such demonstration of a direct link between theoretical predictive capability and experimental validation.

\*8. H. Razavi-Khosroshahi, K. Edalati, M. Hirayama, H. Emami, M. Arita, M. Yamauchi, H. Hagiwara, S. Ida, T. Ishihara, E. Akiba, Z. Horita, M. Fuji (2016) Visible-light-driven photocatalytic hydrogen generation on Nanosized TiO<sub>2</sub>-II stabilized by high-pressure torsion, *ACS Catalysis*, 6(8), 5103-5107.

This study reports the first application of high-pressure phases for photocatalysis. A simple mechanical treatment using the high-pressure torsion method was employed to stabilize the high-pressure TiO<sub>2</sub>-II phase. It was shown that unlike stable phases of TiO<sub>2</sub> such as anatase or rutile, which are photocatalytically active only under UV light, the high-pressure TiO<sub>2</sub>-II phase was active under visible light due to its low bandgap. This study introduces a new research direction to produce visible-light-active photocatalysts from high-pressure phases

#### **\*[5] A functional [NiFe] hydrogenase mimic that catalyzes electron and hydride transfer from H<sub>2</sub>**

\*9. 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<sub>2</sub>, *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 division's research theme of "H<sub>2</sub>-catalyst for low cost and highly efficient practical application."

\*10. Y. Mori, T. Ando, T. Matsumoto, T. Yatabe, M. Kikkawa, K.S. Yoon, S. Ogo (2018) Multifunctional Catalysts for H<sub>2</sub>O<sub>2</sub>-resistant Hydrogen Fuel Cells, *Angewandte Chemie International Edition*, 57(48), 15792-15796.

The development of hydrogen fuel cells is greatly hindered by the unwanted generation of H<sub>2</sub>O<sub>2</sub> at the cathode. This paper reports the simultaneous reductions of O<sub>2</sub> and H<sub>2</sub>O<sub>2</sub> by the model complex of O<sub>2</sub>-tolerant [NiFe]hydrogenase, thus rendering H<sub>2</sub>O<sub>2</sub> a useful part of the feed stream. The applicability of this unique catalyst is demonstrated by employing it in a fuel cell running on H<sub>2</sub>/CO and O<sub>2</sub>/H<sub>2</sub>O<sub>2</sub>. This is the first observation in a non-Pt material.

**\*[6] One model, two enzymes: activation of hydrogen and carbon monoxide**

\*11. S. Ogo, Y. Mori, T. Ando, T. Matsumoto, T. Yatabe, K.S. Yoon, H. Hayashi, M. Asano (2017) One Model, Two Enzymes: Activation of Hydrogen and Carbon Monoxide, *Angewandte Chemie International Edition*, 56(33), 9723-9726.

This paper reports the first evidence of activation of hydrogen and carbon monoxide by using one model complex that has two functional activities of natural [NiFe]-hydrogenase and [NiFe]-carbon monoxide dehydrogenase. The results, together with the previous short-term milestone of a functional [NiFe] hydrogenase mimic (*Science* 2013), will help accelerate hydrogen fuel cell technology and emphasize the dramatic progress of hydrogen activation using a non-precious metal catalyst. This breakthrough study supports the short-term target/benchmark of the specific milestone for the H<sub>2</sub>-activation: synthetic hydrogenase model complex that can activate either or both H<sub>2</sub> and CO molecules.

**\*[7] CO<sub>2</sub>-free electric power circulation via direct charge and discharge using the glycolic acid/oxalic acid redox couple**

\*12. M. Sadakiyo, S. Hata, X. Cui, M. Yamauchi (2017) Electrochemical Production of Glycolic Acid from Oxalic Acid Using a Polymer Electrolyte Alcohol Electrosynthesis Cell Containing a Porous TiO<sub>2</sub> Catalyst, *Scientific Reports*, 7,17032.

A liquid flow-type electrolyser that continuously produces an alcohol from a carboxylic acid was constructed by employing a polymer electrolyte, named a polymer electrolyte alcohol electrosynthesis cell (PEAEC). Glycolic acid (GC, an alcoholic compound) is generated on anatase TiO<sub>2</sub> catalysts via a four-electron reduction of oxalic acid (OX, a divalent carboxylic acid), accompanied with water oxidation, which achieves continuous electric power storage in easily stored GC. Porous anatase TiO<sub>2</sub> directly grown on Ti mesh (TiO<sub>2</sub>/Ti-M) or Ti felt (TiO<sub>2</sub>/Ti-F) was newly fabricated as a cathode having favourable substrate diffusivity. A membrane-electrode assembly composed of the TiO<sub>2</sub>/Ti-M, Nafion 117, and an IrO<sub>2</sub> supported on a gas-diffusion carbon electrode (IrO<sub>2</sub>/C) was applied to the PEAEC. We achieved a maximum energy conversion efficiency of 49.6% and a continuous 99.8% conversion of 1 M OX, which is an almost saturated aqueous solution at room temperature.

\*13. T. Fukushima, M. Higashi, S. Kitano, T. Sugiyama, M. Yamauchi (2019) Multiscale Design for High-Performance Glycolic Acid Electro- Synthesis Cell: Preparation of Nanoscale-IrO<sub>2</sub>-Applied Ti Anode and Optimization of Cell Assembling, *Catalysis Today*, 21, in press (invited paper).

Performance of a polymer electrolyte alcohol electrosynthesis cell (PEAEC) using a glycolic acid (GC)/oxalic acid (OX) redox couple was enhanced via a multiscale approach, i.e., increase of reaction rate on an anode by employing nanometer-scale (nanoscale) IrO<sub>2</sub> catalysts and increase of selectivity for GC production via optimization of cell structures. We prepared nanoscale IrO<sub>2</sub> anode catalyst, which is mixture of IrO<sub>2</sub> nanoparticles (d = 3.7 ± 1.8 nm) and their agglomerates (d < 200 nm). The linear sweep voltammetry measurement for water oxidation revealed that the nanoscale IrO<sub>2</sub> catalyst deposited on a porous carbon paper reduces overpotential for water oxidation by 196 mV from that obtained with an anode composed of commercial microscale IrO<sub>2</sub> grains. Furthermore, application of the nanoscale IrO<sub>2</sub> catalyst on porous titanium paper not only improved durability but also doubly enhanced water oxidation performance. We examined various PEAEC architectures composed of the nanoscale IrO<sub>2</sub> applied Ti anode. Both nanometer- and millimeter-scale approaches realized the best PEAEC performance for GC production, i.e., 59.4% of energy conversion efficiency with 97.1% of Faradaic efficiency for the GC production at 1.8 V and 98.9% of conversion for 3M OX, which is an almost saturated aqueous solution at operating temperature of the PEAEC (60 °C).

\*14. R. Watanabe, M. Yamauchi, M. Sadakiyo, R. Abe, T. Takeguchi (2015) CO<sub>2</sub>-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 electric power circulation method that does not emit CO<sub>2</sub> and is based on the glycolic acid (GC)/oxalic acid (OX) redox couple.

### **\*[8] Fundamental understanding of phase change heat transfer**

\*15. 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.

\*16. Y. Tomo, A. Askounis, T. Ikuta, Y. Takata, K. Sefiane, and K. Takahashi (2016) Superstable Ultrathin Water Film Confined in a Hydrophilized Carbon Nanotube, *Nano Lett.*, 18(3), 1869-1874.

This paper observes water confined in the open hydrophilized CNTs, with diameter of tens of nanometers, using TEM. A 1–7 nm water film adhering to most of the inner wall surface was observed and remained stable in the high vacuum. Suspended ultrathin water films with thickness of 3–20 nm were also found inside the nanotubes. The stability of these water phases cannot be explained by the existing thermodynamics-based theories but these results should advance our understanding of water behavior at the nanoscale and open the door for new applications of phase-change heat transfer, for example, lowering the superheat of boiling initiation by controlling the surface wettability.

### **[9] Fundamental understanding of hydrophobic coating degradation**

\*17. H. Cha, A. Wu, M.-K. Kim, K. Saigusa, A. Liu, N. Miljkovic (2017) Nanoscale-Agglomerate-Mediated Heterogeneous Nucleation, *Nano Letters*, 17(12), 7544-7551.

This paper was the first study to discover a novel nucleation-mediated degradation mechanism caused by deposition of atmospheric contaminants and agglomerates. Our experimental results revealed that the agglomeration mechanism is universally present on functional surfaces and stems from volatile organic compounds. Our findings have important implications toward the potential development of durable coatings, as well as past and future nucleation and heat transfer studies on functional surfaces.

\*18. X. Yan, Z. Huang, S. Sett, J. Oh, H. Cha, L. Li, L. Feng, Y. Wu, C. Zhao, D. Orejon, F. Chen, N. Miljkovic (2019) Atmosphere-Mediated Superhydrophobicity of Rationally Designed Micro/Nanostructured Surfaces, *ACS NANO*, 13(4), 4160–4173.

(DOI: 10.1021/acsnano.8b09106)

This paper develops a radically different approach to achieve durable superhydrophobicity. By utilizing laser processing and thermal oxidation of copper (Cu) to create a high surface energy hierarchical copper oxide (CuO), followed by repeatable and passive atmospheric adsorption of hydrophobic volatile organic compounds (VOCs), we show that stable superhydrophobicity with apparent advancing contact angles  $\approx 160^\circ$  and contact angle hysteresis as low as  $\approx 20^\circ$  can be achieved. We exploit the structure length scale and structure geometry-dependent VOC adsorption dynamics to rationally design CuO nanowires with enhanced superhydrophobicity. To gain an understanding of the VOC adsorption physics, we utilized X-ray photoelectron and ion mass spectroscopy to identify the chemical species deposited on our surfaces in two distinct locations: Urbana, IL, United States and Beijing, China. Our work not only provides rational design guidelines for developing passively durable superhydrophobic surfaces with excellent flooding-resistance and self-healing capability but also sheds light on the key role played by the atmosphere in governing wetting.

### \*[10] Achieving dropwise condensation of low surface tension fluids

\*19. S. Sett, P. Sokalski, K. Boyina, L. Li, K.F. Rabbi, H. Auby, T. Foulkes, A. Mahvi, G. Barac, L.W. Bolton, N. Miljkovic (2019) Stable Dropwise Condensation of Ethanol and Hexane on Rationally-Designed Ultra-Scalable Nanostructured Lubricant-Infused Surfaces, *Nano Letters*, in press.

This paper is the first to develop an engineered surface coating that can enhance the condensation heat transfer with low surface tension working fluids. We demonstrate stable dropwise condensation of ethanol and hexane on LISs impregnated with Krytox 1525, attaining about 200% enhancement in condensation heat transfer coefficient for both fluids compared to filmwise condensation on hydrophobic surfaces. This work not only demonstrates the first stable dropwise condensation of ethanol and hexane, it develops the fundamental design principles for creating durable LISs for enhanced condensation heat transfer of low-surface-tension fluids.

\*20. S. Sett, X. Yan, G. Barac, L.W. Bolton, N. Miljkovic (2017) Lubricant-Infused Surfaces for Low Surface Tension Fluids: Promise vs Reality, *ACS Applied Materials & Interfaces*, 9(41), 36400–36408.

This paper rigorously investigated lubricant-condensate pairs to develop rational design guidelines for LIS surfaces with low surface tension fluids. Through miscibility and cloaking experiments coupled with interfacial tension theory, we developed lubricant selection design guidelines for stable LIS for enhanced condensation.

### \*[11] Air electrodes in high temperature electrochemical devices: An atomistic study of composition and mechanisms

\*21. 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.

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 B-site 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.

\*22. 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 principles 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 as they provide a window to the B-site transition metal atoms in the layer below, and thereby provided insight suitable for further optimization of performance.

### \*[12] Novel electrocatalyst based on polymer-wrapping of carbon nanotubes

\*23. M. R. Berber, I. H. Hafez, T. Fujiyaya, N. Nakashima (2015) A highly durable fuel cell electrocatalyst based on double-polymer-coated carbon nanotubes, *Scientific Reports*, 5, 16711.

This research demonstrated the remarkable durability of the polymer-wrapped CNT-based electrocatalyst at current operation condition (80°C under humidified conditions) compared to the state-of-the-art electrocatalysts. The results proved how I<sup>2</sup>CNER technology can contribute to the current polymer electrolyte fuel cell PEFC technology.

\*24. 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 PEFC above 100 °C is one of the targets of the fuel cell industry. This paper reported the most durable PEFC at 120 °C 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.

### **\*[13] Highly-Conductive Proton-Conducting Oxide for Intermediate temperature steam electrolysis**

\*25. 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.

\*26 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.

### **\*[16] Membrane materials for CO<sub>2</sub> separation in power generation and industrial processes CO<sub>2</sub>/N<sub>2</sub> separation**

\*27. R. Selyanchyn, S. Fujikawa (2017) Membrane Thinning for efficient CO<sub>2</sub> Capture, *Science and Technology of Advanced Materials*, 18(1), 816-827.

Enhancing the fluxes in gas separation membranes is required to utilize the membranes on a mass scale for CO<sub>2</sub> capture. Membrane thinning is one of the most promising approaches to achieving high fluxes. In addition, sophisticated molecular transport across membranes can boost gas separation performance. Based on our current results of CO<sub>2</sub> capture nanomembranes and related works, this review attempts to summarize the current state of CO<sub>2</sub> separation membranes, especially from the viewpoint of thinning the selective layers and the membrane itself. The gas permeation behavior of membranes with various ultimate thicknesses and their future directions are discussed.

\*28. R. Selyanchyn, M. Ariyoshi, S. Fujikawa (2018) Thickness Effect on CO<sub>2</sub>/N<sub>2</sub> Separation in Double Layer Pebax-1657®/PDMS Membranes, *Membranes*, 8(4), 121-133.

We have developed the double-layered membrane of polyamide-polyethyleneoxide copolymer (Pebax®-MH1657) and poly(dimethylsiloxane)(PDMS) as a selective and gutter layer, respectively. Pebax®-MH1657 has high CO<sub>2</sub> selectivity of 50 to 70 over nitrogen and it is one of the most investigated for the selective layer in double-layered membranes for CO<sub>2</sub> capture. We have succeeded to prepare the series of double-layered membranes and some of the membranes exceeded our target value (the CO<sub>2</sub>/N<sub>2</sub> selectivity: 40), though CO<sub>2</sub> permeance is suppressed. The thickness ratio of the selective and gutter layer was systematically investigated to understand the effect of the selective layer on the CO<sub>2</sub> permeance and selectivity. In addition, the influence of porous support on gas permeance were discussed to establish the rational design of membrane composition.

\*29. R. Selyanchyn, S. Fujikawa (2019) Molecular hybridization of polydimethylsiloxane with zirconia for highly gas permeable membranes, *ACS Applied Polymer Materials*, 1(5), 1165-1174.

Inorganic-organic nanocomposite hybrids containing zirconium dioxide (ZrO<sub>2</sub>) as inorganic



crosslinker/filler and polydimethylsiloxane (PDMS) as a polymeric matrix have been synthesized using the in-situ sol-gel reaction. Small gases (He, H<sub>2</sub>, O<sub>2</sub>, N<sub>2</sub>, and CO<sub>2</sub>) permeability experiments were carried out to study the effect of the inorganic component amount on the properties of the ZrO<sub>2</sub>@PDMS hybrids. The permeability of the developed hybrids considerably exceeded the permeability of conventional PDMS which is known as “gold standard” highly gas-permeable rubbery polymer. Depending on the ZrO<sub>2</sub> content, fabricated hybrids demonstrated increased permeability for all gases with improvement inversely proportional to the kinetic diameter of gas molecules. Such behavior suggests the formation of the size-sieving amorphous zirconia domains within PDMS. As a result, gas separation membranes prepared using the developed materials demonstrated better separation performance for CO<sub>2</sub>/N<sub>2</sub>, H<sub>2</sub>/N<sub>2</sub>, and O<sub>2</sub>/N<sub>2</sub> pairs compared to the conventional PDMS.

### \*[15] Membrane materials for CO<sub>2</sub>/H<sub>2</sub> separation

\*30. I. Taniguchi, K. Kinugasa, M. Toyoda, K. Minezaki (2017) Effect of amine structure on CO<sub>2</sub> capture by polymeric membranes, *Science and Technology of Advanced Materials*, 18(1), 950-958.

This paper demonstrated that monoethanol amine, one of the alkanolamines, exhibited better performance than PAMAM, which was used for pre-combustion CO<sub>2</sub> capture in RITE. The importance is the finding of a better amine, which transports CO<sub>2</sub> in the membranes. Gas separation properties under pressure were not introduced in this paper because the properties under humidity with mixed gas (CO<sub>2</sub> and H<sub>2</sub>) have not been studied. With a different alkanolamine, 2-(2-aminoethylamino)ethanol, single gas permeances under pressure were measured at UT Austin.

### \*[16] Glycerol Oxidation as Alternative Anode Reaction for Energy Efficient Electrochemical CO<sub>2</sub> Reduction

\*31. S. Verma, S. Lu, P.J.A. Kenis (2019) Co-electrolysis of CO<sub>2</sub> and glycerol as a pathway to carbon chemicals with improved techno-economics due to low electricity consumption, *Nature Energy*. (DOI: 10.1038/s41560-019-0374-6)

This paper presents a novel approach to lowering energy requirements for the CO<sub>2</sub> reduction process by replacing on the anode side the energy-intensive oxygen evolution reaction (OER) with the low-energy glycerol oxidation. By using oxidation of waste chemicals like glycerol (byproduct of biofuel production), operating at a much lower cell potential is possible, which translates in significant energy savings: ~53% less overall energy requirement. In addition, this paper provides techno-economic and cradle-to-gate insights for possibly carbon-neutral CO<sub>2</sub> reduction even when using grid electricity that is generated from a mix of fossil and renewable fuels.

### \*[17] Inertial effects in liquid CO<sub>2</sub>-water flow behavior for CO<sub>2</sub> storage

\*32. Y. Li, F. Kazemifar, G. Blois, K.T. Christensen (2017) Micro-PIV measurements of multiphase flow of water and liquid CO<sub>2</sub> in 2-D heterogeneous porous micromodels, *Water Resources Research*, 53(7), 6178-6196.

This paper used a state-of-the-art experimental technique that surpasses previous studies. The wider context of this work is the conceptual upscaling of multiphase flow from the pore scale to the Darcy scale, which is a long-standing problem. This work moves the lower boundary upwards by providing direct experimental evidence that pore scale phenomena extend into what is believed to be Darcy scale. New findings on inertial effects and the zone-of-influence of pore-scale phenomena challenge previous assumptions on the range of validity of Darcy's law, and the criteria for selecting a representative element volume for modeling and lab experiments. These experiments are the first of their kind.

\*33. Y. Li, F. Kazemifar, G. Blois, K.T. Christensen (2019) High-speed quantification of pore-scale multiphase flow of water and supercritical CO<sub>2</sub> in 2D heterogeneous porous micromodels: flow regimes and interface dynamics, *Water Resources Research*, accepted for publication.

The paper presented a detailed quantification of the pore-scale flow features (*i.e.*, the invasion flow regimes, the interfacial area, and the active flow pathways) that have been obtained by a combination of fluorescence microscopy and pore-scale high-speed imaging. The novel statistical analysis enabled a “visualization” of the pore-scale effect on a much larger scale. The results provided unique experimental insight that address inconsistent observations in the literature and previously unanswered questions about the underlying flow dynamics of this important multi-phase flow scenario directly relevant to CCS applications. These pore-to-core-scale experimental results and analysis are the first of their kind.

### **\*[18] Continuous and accurate monitoring system for injected CO<sub>2</sub>**

\*34. 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. (DOI: 10.1190/INT-2016-0019.1)

This is first achievement of our monitoring study to estimate the temporal variation of seismic velocity using ambient noise. Since this method constructs virtual source signals from noise, we can conduct a time-lapse survey and extract subsurface information using only ambient noise data. The low cost of this approach makes it particularly attractive for long-term monitoring of CCS projects. We have applied this method to seismometer data acquired during fluid-injection. The velocity variation identified in this study can be interpreted as pore pressure increasing due to fluid injection.

\*35. H. Nimiya, T. Ikeda, T. Tsuji (2017) Spatial and temporal seismic velocity changes on Kyushu Island during the 2016 Kumamoto earthquake, *Science Advances*, 3(11), e1700813.

This study first applies spatio-temporal monitoring of seismic velocity using ambient noise in the Kyushu Island. The results revealed spatio-temporal variation of seismic velocity associated with the Mw7.0 Kumamoto earthquake, eruption, and environmental influences. Since such velocity variation can be occurred due to subsurface stress change, the monitoring approach can be used to monitor pore pressure change in CCS project to prevent injection induced seismicity.

\*36. T. Ikeda, T. Tsuji, M. Nakatsukasa, H. Ban, A. Kato, K. Worth, D. White, B. Roberts (2018) Imaging and monitoring of the shallow subsurface using spatially windowed surface-wave analysis with a single permanent seismic source, *Geophysics*, 83(6), EN23-EN38.

The continuous monitoring system using the controlled seismic source has limited spatial resolution because only a single source system is usually installed in monitoring sites. To overcome the limitation, novel seismic processing is proposed. The proposed processing is applied to the CO<sub>2</sub> storage site in Canada. The results demonstrated that spatial variation of seismic velocity can be imaged and monitored with high spatio-temporal resolution using only a single seismic source system. This work shows the potential of our monitoring system to identify spatial distribution of CO<sub>2</sub> leakage.

### **\*[19] Next-generation high-strength, low-cost alloy for hydrogen service**

\*37. 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(33), 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.

\*38. M. Kubota, A. Macadre, K. Mori, R. Mori (2018) Fatigue Properties of Ultra-Fine Grain Austenitic Stainless Steel and the Effect of Hydrogen, *MATEC Web of Conferences*, 165, 03007.

This is the first study that characterized the effect of hydrogen on fatigue failure in ultra-fine grain (UFG) stainless steel. The fatigue crack growth resistance of UFG stainless steel was significantly higher compared to the benchmark 316 stainless steel, dispelling the accepted view that grain refinement is detrimental to fatigue failure. The mechanistic interpretation of this unexpected behavior was based on the interaction between dislocations and UFG boundaries. In addition, although the fatigue limit of UFG stainless steel was not degraded by hydrogen, the crack-nucleating inclusions were significantly smaller compared to those in conventional alloys, offering the opportunity to advance the benchmark mechanics framework associated with the fatigue limit.

### **[20] Mitigation of Hydrogen Embrittlement**

\*39. B.P. Somerday, P. Sofronis, K.A. Nibur, C. San Marchi, R. Kirchheim (2013) Elucidating the Variables Affecting Accelerated Fatigue Crack Growth of Steels in Hydrogen Gas with Low Oxygen Concentrations, *Acta Materialia*, 61(16), 6153-6170.

This paper represents an international, interdisciplinary effort to couple experiments and modeling

to illuminate the variables governing trace oxygen inhibition of hydrogen gas-accelerated fatigue crack growth in steel. For the first time, a physics-based analytical model was developed that quantifies the interplay between several environmental and mechanical variables affecting oxygen-modified, hydrogen-accelerated crack growth. The technological implications of this paper have been recognized, as evidenced by subsequent Air Liquide-sponsored I<sup>2</sup>CNER projects, which are intended to quantify the effectiveness of carbon monoxide to inhibit hydrogen-accelerated cracking of steels in hydrogen production components.

\*40. R. Komoda, M. Kubota, A. Staykov, P. Ginet, F. Barbier, J. Furtado (2019) Inhibitory Effect of Oxygen on Hydrogen-Induced Fracture of A333 Pipe Steel, *Fatigue & Fracture of Engineering Materials & Structures*, 42(6), available on line.  
(DOI:10.1111/ffe.12994)

Extending the study by Somerday et al. (2013), this Air Liquide-sponsored activity investigated the mitigation of hydrogen embrittlement (HE) in pipe line steel through fracture toughness testing in hydrogen gas with trace oxygen. One unexpected insight provided by this activity was that only 1 vppm oxygen can attenuate HE. The mechanism for this HE inhibition was interpreted by expanding the theoretical treatment of impurity-modified HE, as introduced by I<sup>2</sup>CNER. In addition, this research identified the need for strict control of gas impurities during crack-growth testing in hydrogen.

## Appendix 1-2 List of Papers of Representative of Interdisciplinary Research Activities

\* List **up to 20 papers** 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. J. Oh, C.E. Dana, S. Hong, J.K. Román, K.D. Jo, J.W. Hong, J. Nguyen, D.M. Crokek, M. Alleyne, N. Miljkovic (2017) Exploring the Role of Habitat on the Wettability of Cicada Wings, *ACS Applied Materials & Interfaces*, 9(32), 27173-27184.

This interdisciplinary work used bioinspiration to show for the first time that wettability in nature is better correlated with taxonomy, life cycle, and reproductive strategies, rather than habitat. This work not only elucidated the differences between inter- and intra-species topology, wettability, and water shedding behavior, but enabled the development of rational design tools for the manufacture of artificial surfaces for energy and water applications such as anti-icing, self-cleaning, anti-fogging, water harvesting, and enhanced phase change heat transfer.

*Disciplines: Materials science, mechanical engineering, surface science, organic chemistry, analytical chemistry, biology, bioengineering, entomology, evolutionary biology*

2. 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 H<sub>2</sub> Oxidation Reaction, *Angewandte Chemie International Edition*, 53(34), 8895-8898.

The fuel cell comprising [NiFe]-Hydrogenase anode isolated from I<sup>2</sup>CNER 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 benchmark of the first biological fuel cells of O<sub>2</sub>-tolerant hydrogenase, which satisfactorily accomplished the short-term target of H<sub>2</sub>-activation.

*Disciplines: Chemistry, biochemistry, fuel cell engineering*

3. N.D. Muid Noor, H. Matsuura, K. Nishikawa, H. Tai, S. Hirota, J. Kim, J. Kang, M. Tateno, K.S. Yoon, S. Ogo, S. Kubota, Y. Shomura, Y. Higuchi (2018) Redox-dependent Conformational Changes of a Proximal [4Fe-4S] Cluster in Hyb-type [NiFe]-hydrogenase To Protect the Active Site from O<sub>2</sub>, *Chemical Communications*, 54(87), 12385-12388.

Together with the previous studies of the first functional biomimetic [NiFe]hydrogenase (*Science* (2013, 339, 682–684), we set to work on the mid-term targets of H<sub>2</sub>-activation: practical H<sub>2</sub>-catalyst and the crystal structure of O<sub>2</sub>-tolerant [NiFe] hydrogenase. The active site of oxidized enzyme coordinates the six-coordinated Ni geometry that would prevent O<sub>2</sub> from approaching. This interdisciplinary research result is the benchmark of the first crystal structure of NAD<sup>+</sup>-reducing O<sub>2</sub>-tolerant [NiFe] hydrogenase isolated by I<sup>2</sup>CNER.

*Disciplines: Biology, biomimetic chemistry, crystallography*

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. Fe-rich islands forming by HPT are suggested to act as catalysts for hydrogen dissociation, the microcracks and nanograin boundaries act as pathways for hydrogen transport, which is assisted by additional dislocation transport toward the sites of hydride formation. Two commercial processes were developed, cold rolling (2014) and mechanical milling (2015), in which TiFe absorbs hydrogen without any activation.

*Disciplines: Materials engineering, surface science, crystallography*

5. H. Razavi-Khosroshahi, K. Edalati, J. Wu, Y. Nakashima, M. Arita, Y. Ikoma, M. Sadakiyo, Y. Inagaki, A. Staykov, M. Yamauchi, Z. Horita, M. Fuji (2017) High-pressure zinc oxide phase as visible-light-active photocatalyst with narrow band gap, *Journal of Materials Chemistry A*, 5(38), 20298-20303.  
In this study, oxygen vacancies were generated in high-pressure ZnO phase and a low bandgap photocatalyst with visible-light activity was developed. Although chemical modifications were already used to develop visible-light-active ZnO photocatalysts, this study reports the visible-light activity for the first time in pure ZnO. The oxygen vacancies were generated in high-pressure rocksalt-ZnO phase using the high-pressure torsion method and it was found that the visible-light activity is due to the bandgap narrowing down to 1.8 eV in good agreement with predictions of first-principles calculations. This study introduces the high-pressure torsion method as a new processing route to develop visible-light-active photocatalysts even from pure semiconductors.

*Disciplines: Materials engineering, mechanochemistry*

6. K. Matsue, S. Mohan and M. Matalon (2019) Effect of gravity on hydrodynamically unstable flames, will be presented at the 12<sup>th</sup> Asia-Pacific Conference on Combustion, Fukuoka, Japan (July 2019).  
The hydrodynamic instability, due to the large deviation of density between fresh cold mixture and hot combusted products, was discovered by Darrieus and Landau. After seven or eight decades, many aspects of this intrinsic flame instability have been revealed, such as the effects of the flame front curvature and of flow strain rate, its influence on turbulent flames and the self-wrinkling and self-turbulization of expanding flames. In the present study, we focus on the composite effects of thermal expansion, differential diffusion, and gravity on flame dynamics, based on a fully nonlinear, hydrodynamic model obtained by a multi-scale analysis that exploits the distinct length scales associated with such problems. The simulations verify the stabilization effect of gravity on planar flames propagating downwards, known from linear stability theory, and show that in the presence of gravity the nonlinear development beyond the stability threshold leads to cusp-like structures of smaller amplitude that propagate at a reduced speed. Finally, we observe that a judicious choice of the Markstein number, controlled by mixture composition and domain size, and of the Froude number creates richer morphological flame structures than in the absence of gravity

*Disciplines: Applied math, fluid mechanics, aerospace, combustion science, computational science, physics and chemistry*

7. M. Matalon (2019) The Ramifications of the Darrieus-Landau Instability in Turbulent Premixed Flames, *AIAA Journal*, presented at the AIAA Sci-Tech 2019 Forum, San Diego, CA (January 2019). (DOI: 10.2514/6.2019-0182)  
The most prominent intrinsic flame instability is the hydrodynamic, or Darrieus-Landau instability, which arises by virtue of gas expansion that results from the heat released during combustion and is thus ubiquitous to all premixed flames. The Darrieus-Landau instability has many ramifications in premixed combustion; it is responsible for the creation of sharp folds and creases on flame surfaces, for the convex curving of flames propagating in narrow tubes, and for the spontaneous wrinkling that gives outgrowing flames a roughened pebbled-like appearance. The increase in flame surface area creates a commensurate enhancement in fuel consumption or mass-burning rate, which has practical implications in the design of propulsion systems and power generating plants. Although the hydrodynamic instability has been studied extensively, it was not until recently that its effect on turbulent flame propagation began to be examined; it was generally deemed a secondary effect masked by the turbulence and thus largely overlooked. In this paper, we review the main developments that led to the current understanding of the nature of the Darrieus-Landau instability and discuss, in particular, its prominent influence on turbulent flames.

*Disciplines: Applied math, fluid mechanics, aerospace, combustion science, computational science, physics and chemistry*

8. P. Yu, H. Watanabe, W. Zhang, R. Kurose, T. Kitagawa (2019) Flamelet model for a three-feed non-premixed combustion system with diluent stream -Analysis and validation of quasi-two-dimensional flamelet (Q2DF) models, *Energy and Fuels*, 33(5), 4640-4650. (DOI: 10.1021/acs.energyfuels.9b00764)

Three formulations of quasi-two-dimensional flamelet (Q2DF) models are derived from the two-dimensional flamelet formulation on the basis of assumptions regarding the third stream (diluent), and these models are validated by means of two-dimensional direct numerical simulation (DNS) of a three-feed non-premixed combustion system into which diluent is injected as the third stream. DNS combined with the Arrhenius formation (ARF) together with a detailed mechanism is also performed as a reference case and compared with the present models. The characteristics of the flamelets in three-feed non-premixed combustion are discussed in detail for ARF in terms of the three mixture fractions, temperature, major and minor species, and other factors. As the results are not determined solely by a single mixture fraction, one scalar dissipation rate is insufficient for establishing a complete database, and it is considered that an additional scalar dissipation rate is needed to improve the model. Overall, it is confirmed that the three Q2DF models presented in this study capture the fundamental characteristics of flamelets in the three-feed non-premixed combustion system, although further improvement is required.

*Disciplines: Fluid mechanics, mathematical modeling, computational science, combustion*

9. A. N. Madavan, S. Bose, Y. Guo, L. Tong (2019) Risk-Sensitive Security-Constrained Economic Dispatch via Critical Region Exploration, Accepted for presentation at the IEEE Power and Energy Society General Meeting.

This conference paper proposes an alternate formulation of the security-constrained economic dispatch problem that system operators solve to clear day-ahead and real-time markets. The formulation allows for load shedding and penalizes the risk associated with the dispatch decision. In addition, we provide an algorithmic framework to solve it.

*Disciplines: Applied math, power systems, optimization algorithms, operations research.*

10. D. Cai, S. Bose, A. Wierman, S. Low (2018) The Role of a Market Maker in Networked Cournot Competition, Accepted in INFORMS Mathematics of Operations Research.

This paper proposes to alter the market clearing process to limit the effects of strategic interaction among generators in electricity markets.

*Disciplines: Applied math, electricity markets, game theory, mechanism design, operations research.*

11. K. Hirose, H. Masuda (2018) Robust relative error estimation, *Entropy*, 20(9), 632.

Relative error estimation has been recently used in regression analysis. A crucial issue of the existing relative error estimation procedures is that they are sensitive to outliers. To address this issue, we employ the  $\gamma$ -likelihood function, which is constructed through  $\gamma$ -cross entropy with keeping the original statistical model in use. The estimating equation has a redescending property, a desirable property in robust statistics, for a broad class of noise distributions. To find a minimizer of the negative  $\gamma$ -likelihood function, a majorize-minimization (MM) algorithm is constructed. The proposed algorithm is guaranteed to decrease the negative  $\gamma$ -likelihood function at each iteration. We also derive asymptotic normality of the corresponding estimator together with a simple consistent estimator of the asymptotic covariance matrix, so that we can readily construct approximate confidence sets. Monte Carlo simulation is conducted to investigate the effectiveness of the proposed procedure. Real data analysis illustrates the usefulness of our proposed procedure.

*Disciplines: Computational statistics, high-dimensional data analysis, statistical modeling*

12. D. Hoa Nguyen, S. Azuma, T. Sugie (2019) Novel Control Approaches for Demand Response with Real-time Pricing using Parallel and Distributed Consensus-based ADMM, *IEEE Transactions on Industrial Electronics* (In Press).

(DOI: 10.1109/TIE.2018.2881938)

This work first proposes a novel distributed optimization approach named distributed consensus-based Jacobian alternating direction method of multipliers (DCJ-ADMM) for solving grid social welfare maximization problem. The novelty of this DCJ-ADMM approach is on its ability to update the variables in parallel in all agents and the inter-agent communication is sparse, while existing distributed ADMM approaches either update variables in order or update

variables in parallel but with all-to-all, i.e., very dense inter-agent communication structure. Next, the real-time market-clearing electric price is derived, which is equal to the Lagrange multiplier associated with the power supply-demand balance constraint. This real-time electric price is further proved to be a convex combination of local prices in different areas inside the considering grid made by the disconnectivity of the inter-agent communication graph. Based on that result, a novel control architecture is proposed to handle the disconnected communication between agents in the grid.

*Disciplines: Applied math, optimization, power systems, control engineering, computational science*

13. T. T. Doan, S. Bose, D. Hoa Nguyen, C. L. Beck (2019) Convergence of the Iterates in Mirror Descent Methods, *IEEE Control Systems Letters*, 3(1), 114-119.

This paper is the first work to prove the convergence of problem arguments to their optima, for both centralized and distributed agent-based Mirror Descent methods, whereas other works only proved the convergence of the objective function. Mirror Descent is a generalization of the well-known sub-gradient method, and is able to solve optimization problems whose objective functions are not necessarily differentiable nor strongly convex.

*Disciplines: Applied math, power systems, optimization, computational science*

14. M. Murakami, R. Funaki and J. Murata (2017) Design of Incentive-Based Demand Response Programs Using Inverse Optimization, *2017 IEEE International Conference on Systems, Man, and Cybernetics (SMC2017)*, 2754-2759.

This paper introduced probabilistic nature into the consumers' models, which well approximates not-necessarily-optimal decision making done by actual humans. Also, several incentive payment schema were proposed depending on requirements imposed by power utilities.

*Disciplines: Applied math, electrical engineering, computational science*

15. 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, GS01-13*, 2016.

This paper proposed an incentive payment design method for demand response programs with a variety of requirements imposed by power utilities. The design is done by theoretical inverse optimization technique and therefore has no convergence issues that exist in iterative numerical techniques. The paper received an Excellent Paper Award, which was given to three papers out of some 260 papers presented at the conference.

*Disciplines: Applied math, electrical engineering, computational science*

16. D. Triadis, F. Jiang, D. Bolster (2019) Anomalous dispersion in pore-scale simulations of two-phase flow, *Transport in Porous Media*, 126(2), 337-353.  
(DOI: 10.1007/s11242-018-1155-6)

This is the main presentation of the project's research results, demonstrating persistent anomalous dispersion in simulations of non-wetting fluid flow in randomly generated, periodic, 2D porous media with trapped wetting phase fluid present. Anomalous dispersion was found to be strongly dependent upon the assumed molecular diffusivity, initial tracer particle positions, and the induced flow network geometry, but did not vary with fluid-fluid interface slip boundary conditions. The persistence of anomalous dispersion in more realistic, non-periodic porous media is expected to be even greater – insensitivity to fluid-fluid interface slip may simplify analysis of such systems via a primary focus on induced flow network geometries.

*Disciplines: Applied mathematics, fluid mechanics, computational science, environmental engineering*

17. A. Fakhari, Y. Li, D. Bolster, K. T. Christensen (2018) A phase-field lattice Boltzmann model for simulating multiphase flows in porous media: Application and comparison to experiments of CO<sub>2</sub> sequestration at pore scale, *Advances in Water Resources*, 114, 119-134.

This is a related study by project member Diogo Bolster, where the lattice-Boltzmann phase-field numerical method for simulation of two-phase porous media flow is developed, and compared to experimental results designed for consideration of capillary and viscous fingering during CO<sub>2</sub> infiltration of brine-saturated porous media.

*Disciplines: Applied mathematics, fluid mechanics, computational science, environmental engineering*

18. F. Jiang, T. Tsuji, T. Shirai (2018) Pore Geometry Characterization by Persistent Homology Theory, *Water Resources Research*, 54(6), 4150-4163.  
(DOI:10.1029/2017WR021864)

This work relates the persistence diagram derived from digital rock to elastic properties, because persistence diagram includes information of pore geometry. We succeeded to predict elastic properties of natural rock from its persistence diagram.

*Disciplines: Applied math, geology, hydrology, geophysics*

19. T. Tsuji, F. Jiang, A. Suzuki, T. Shirai (2018) Mathematical Modeling of Rock Pore Geometry and Mineralization: Applications of Persistent Homology and Random Walk, *Agriculture as a Metaphor for Creativity in All Human Endeavors*, 95-109.  
(DOI: 10.1007/978-981-10-7811-8\_11)

This work represents the first application of persistence diagram to natural rocks and CO<sub>2</sub> mineralized rocks. This study demonstrates that persistence diagram (i.e. output of this analysis) includes useful information for pore geometry characterization and evaluation.

*Disciplines: Applied math, geology, hydrology, geophysics*

20. S. Koda, Y. Onda, H. Matsui, K. Takahagi, Y. Uehara-Yamaguchi, M. Shimizu, K. Inoue, T. Yoshida, T. Sakurai, H. Honda, S. Eguchi, R. Nishii and K. Mochida (2017) Diurnal transcriptome and gene network represented through sparse modeling in *Brachypodium distachyon*, *Frontiers in Plant Science*, 28, 2055.  
(DOI:10.3389/fpls.2017.02055)

We report the comprehensive identification of periodic genes and their network inference, based on a gene co-expression analysis and an Auto-Regressive model with exogenous variables (ARX model) using a time-series transcriptome dataset in a model grass, *Brachypodium distachyon*. On the basis of the time-series expression patterns of the periodic genes, we constructed a chronological gene co-expression network and identified putative transcription factors encoding genes that might be involved in the time-specific regulatory transcriptional network. Moreover, we inferred a transcriptional network composed of the periodic genes, aiming to identify genes associated with other genes through variable selection by grouping time points for each gene. Based on the ARX model with the group SCAD regularization, we constructed gene networks and found that the networks represent typical scale-free structure. Our findings demonstrate that the diurnal changes in the transcriptome in leaves have a sparse network structure, demonstrating the spatiotemporal gene regulatory network over the cyclic phase transitions diurnal growth.

*Disciplines: Applied math, statistics, genome biology*



## Appendix 1-3

### Major Awards, Invited Lectures, Plenary Addresses (etc.) (within 2 pages)

\*Prepare the information below during the period from the start of the center through March 2019.

#### 1. Major Awards

\*List main internationally-acclaimed awards received/unofficially announced in order from the most recent.

\*For each, write the recipient's name, the name of award, and the date issued.

In case of multiple recipients, underline those affiliated with the center.

	Date	Recipient's name	Name of award
1	Nov. 5, 2018	Takeshi Tsuji	The Early Career Scientist Award of the International Union of Geodesy and Geophysics (IUGG)
2	Sep. 13, 2018	Yukina Takahashi	Incentive Award, The Japan Society for Analytical Chemistry
3	Jun. 21, 2018	Perry, Nicola H.	DOE Early Career Award
4	Jun. 12, 2018	Yasuyuki Takata	ASME ICNMM Outstanding Leadership Award
5	Apr. 10, 2018	Chihaya Adachi	Prize for Science and Technology, The Commendation for Science and Technology by the Minister of Education, Culture, Sports, Science and Technology
6	Mar. 2018	Kaveh Edalati	Scientist Medal for Advanced Energy Materials and Technology by International Association of Advanced Materials
7	May 27, 2017	Arnaud Macadre	Award for Promising Researchers by The Society of Materials Science
8	Feb. 2017	Reiner Kirchheim	Foreign affiliate of the United States National Academy of Engineering
9	Nov. 15, 2016	<u>Tatsumi Ishihara</u> , <u>John A. Kilner</u> , <u>Helena Tellez-Lozano</u> , <u>Aleksandar T. Staykov</u>	Daiwa Adrian Prize
10	Apr. 12, 2016	Naotoshi Nakashima	The Commendation for Science and Technology by MEXT
11	Apr. 12, 2016	Takeshi Tsuji	The Young Scientists' Prize by MEXT
12	Nov. 2, 2015	Zenji Horita	Medal of Honor with Purple Ribbon by Government of Japan
13	Jun. 2015	Toyoki Kunitake	The Kyoto Prize
14	Nov. 3, 2014	Toyoki Kunitake	Order of Culture
15	July 4, 2014	<u>Hellena Téllez-Lozano</u> , <u>John Druce</u> , <u>Ju, Y.-W.</u> , <u>Tatsumi Ishihara</u> , and <u>John Kilner</u>	Christian Friedrich Schonbein Contribution to Science Medal
16	Jun. 17, 2014	Brian Somerday	DOE Hydrogen and Fuel Cells Program Achievement Award
17	Apr. 8, 2013	Seiji Ogo	The Commendation for Science and Technology by MEXT
18	Feb. 8, 2013	Seiji Ogo	The 30th Chemical Society of Japan Award
19	Feb. 2013	Harry L. Tuller	Helmholtz Intl. Fellow Award from the Helmholtz Association of German Research Centers
20	Sep. 27, 2012	<u>Tatsumi Ishihara</u> , <u>John A. Kilner</u> and <u>Harry L. Tuller</u>	Somiya Award

21	May 2011	<u>Ian Robertson</u> , <u>Petros Sofronis</u>	US Department of Energy Hydrogen and Fuel Cells Program Research and Development Award
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## 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)

	Date(s)	Lecturer/Presenter's name	Presentation title	Conference name
1	Jan. 4, 2019	Reiner Kirchheim	Chemomechanics in the context of plasticity and fracture (Keynote)	24th International Conference on Plasticity, Panama City, Panama
2	Sep. 26, 2018	Benjamin McLellan and Andrew Chapman	Equity and Efficacy in Renewable Energy Policy: A Case Study of Australia (Plenary)	World Social Science Forum, Fukuoka, JAPAN
3	Sep. 24, 2018	Joichi Sugimura	Tribology in Hydrogen Environment (Plenary)	59th German Tribology Conference, Göttingen, Germany
4	Jul. 28, 2018	Miho Yamauchi	Inorganic Nanocatalysts for Efficient Power Storage into liquid (Invited)	2018 International Symposium on Advancement and Prospect of Catalysis Science & Technology, Sydney, Australia
5	Jun. 21, 2018	Hiroshige Matsumoto	Intermediate Temperature Steam Electrolysis using Proton Conducting perovskites membrane (Keynote)	15th ICIM 2018, Dresden, Germany
6	May 14, 2018	Takeshi Tsuji	Multi-phase fluid behaviors with various capillary numbers, viscosity and wettability: Insight into effective and safe CO <sub>2</sub> storage (Invited)	InterPore 10th Annual Meeting, New Orleans, USA
7	Oct. 17-18, 2017	Paul Kenis	Electrochemical CO <sub>2</sub> Conversion: Status and Remaining Challenges (Invited)	US National Academy of Sciences / UK Royal Society Sackler Forum: "Dealing with Carbon Dioxide at Scale", Buckinghamshire, UK
8	Sep. 21, 2017	Joichi Sugimura	Tribology and Materials for Hydrogen Energy Society (Plenary)	6th World Tribology Congress, Beijing, China
9	May 28-31, 2017	John Kilner	Ionic and Mixed Conduction Phenomena in Oxides and Their Applications in Devices (Plenary)	ICE 2017 8th International Conference on Electroceramics, Nagoya, Japan
10	Oct. 28, 2016	Ikuo Taniguchi	Effort of I2CNER and the CO <sub>2</sub> capture by membranes (Invited)	New Membrane Technology Symposium 2016, Tokyo, Japan
11	Dec. 2 2015	Masanobu Kubota	Fretting Fatigue in Hydrogen and the Effect of Impurity Addition to Hydrogen on Fretting Fatigue Properties (Plenary)	3rd World Congress on Petrochemistry and Chemical Engineering, Atlanta, USA
12	Jul. 6, 2015	Kenshi Itaoka	Focus groups and stakeholders of the Tomakomai CCS project, International Energy Agency (IEA) Greenhouse Gas R&D Program (Invited)	The 5th Social Research Network Meeting, Cambridge, UK
13	Dec. 15, 2014	Tatsumi Ishihara	New Technology for Carbon Neutral Energy (Plenary)	MSAT-8, Bangkok, Thailand
14	May 29, 2013	Yasuyuki Takata	Wettability Effects in Boiling Heat Transfer (Plenary)	The 8th International Conference on Multiphase Flow (ICMF2013), Jeju, Korea
15	July 8-13, 2012	Petros Sofronis	Recent Advances in Experiments, Modeling and Prognosis of Hydrogen-Induced Fracture (Invited)	GRC on Corrosion-Aqueous, Colby-Sawer College, New London, NH, USA

## Appendix 1-4 2018 List of Center's Research Results

### Refereed Papers

- List only the Center's papers published in 2018. (Note: The list should be for the calendar year, not the fiscal year.)

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

A. WPI papers

List papers whose author(s) can be identified as affiliated with the WPI program (e.g., that state "WPI" and the name of the WPI center (WPI-center name)). (Not including papers in which the names of persons affiliated with the WPI program are contained only in acknowledgements.)

B. WPI-related papers

List papers related to the WPI program but whose authors are not noted in the institutional affiliations as WPI affiliated. (Including papers whose acknowledgements contain the names of researchers affiliated with the WPI program.)

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

(2) Method of listing paper

- List only refereed papers. Divide them into categories (e.g., original articles, reviews, proceedings).
- For each, write the author name(s); year of publication; journal name, volume, page(s), and article title. Any listing order may be used as long as format is consistent. (The names of the center researchers do not need to be underlined.)
- If a paper has many authors (say, more than 20), all of their names do not need to be listed.
- Assign a serial number to each paper to be used to identify it throughout the report.
- If the papers are written in languages other than English, underline their serial numbers.

- Order of Listing

A. WPI papers

1. Original articles
2. Review articles
3. Proceedings
4. Other English articles

B. WPI-related papers

1. Original articles
2. Review articles
3. Proceedings
4. Other English articles

(3) Use in assessments

- The lists of papers will be used in assessing the state of WPI project's progress.
- They will be used as reference in analyzing the trends and whole states of research in the said WPI center, not to evaluate individual researcher performance.
- The special characteristics of each research domain will be considered when conducting assessments.

(4) Additional documents

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

No.	Description
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## Appendix 2 FY 2018 List of Principal Investigators

NOTE:

\*Underline names of principal investigators who belong to an overseas research institution.

\*In the case of researcher(s) not listed in the latest report, attach a "Biographical Sketch of a New Principal Investigator"(Appendix 2a).

<b>&lt;Results at the end of FY2018&gt;</b>							<b>Principal Investigators Total: 27</b>
Name	Age	Affiliation (Position title, department, organization)	Academic degree, Specialty	Effort (%)*	Starting date of project participation	Status of project participation (Describe in concrete terms)	Contributions by PIs from overseas research institutions
Center director <u>Petros Sofronis</u>	61	Prof., International Institute for Carbon- Neutral Energy Research, Kyushu University	Ph.D., Micromechanics of materials, Environmental degradation of materials	90%	2010, Dec. 1st	<ul style="list-style-type: none"> <li>• Directs and administers the Institute</li> <li>• Travels to Kyushu University to participate in events and engage with researchers (42.0% time)</li> <li>• Promotes I<sup>2</sup>CNER's interests worldwide to various universities, government agencies, laboratories, and industries on a daily basis</li> <li>• Intensive trans-Pacific electronic communication via e-mail, Skype, videoconferencing, etc.</li> </ul>	Manages and directs I <sup>2</sup> CNER's operations
Tatsumi Ishihara	57	Prof., International Institute for Carbon- Neutral Energy Research, Kyushu University	Dr. of Engr., Catalyst and solid state electrochemistry	100%	2010, Dec. 1st	<ul style="list-style-type: none"> <li>• Located at I<sup>2</sup>CNER</li> <li>• Executes duties of Associate Director</li> <li>• Lead PI of Molecular Photoconversion Devices Division</li> </ul>	
Chihaya Adachi	55	Prof., Department of Applied Chemistry, Kyushu University	Dr. of Engr., Materials science and device physics	80%	2010, Dec. 1st	<ul style="list-style-type: none"> <li>• Located at I<sup>2</sup>CNER</li> <li>• Leads research activities of his group</li> </ul>	
Atsushi Takahara	63	Prof., Institute for Materials Chemistry and Engineering, Kyushu University	Dr. of Engr., Surface and Interface Characterization	80%	2010, Dec. 1st	<ul style="list-style-type: none"> <li>• Located at I<sup>2</sup>CNER</li> <li>• Leads research activities of his group</li> </ul>	
Seiji Ogo	55	Prof., International Institute for Carbon- Neutral Energy Research, Kyushu University	Dr. of Science, Green Chemistry	100%	2010, Dec. 1st	<ul style="list-style-type: none"> <li>• Located at I<sup>2</sup>CNER</li> <li>• Lead PI of Catalytic Materials Transformations Division</li> </ul>	

Zenji Horita	65	Prof., International Institute for Carbon-Neutral Energy Research, Kyushu University	Ph.D., Dr. of Engr., Materials Science	100%	2010, Dec. 1st	<ul style="list-style-type: none"> <li>• Located at I<sup>2</sup>CNER</li> <li>• Leads research activities of his group</li> </ul>	
Kazunari Sasaki (for engineering next generation fuel cells)	54	Prof., International Institute for Carbon-Neutral Energy Research, Kyushu University	Dr. of Science and technology, Fuel cell materials, Inorganic materials	100%	2010, Dec. 1st	<ul style="list-style-type: none"> <li>• Located at I<sup>2</sup>CNER</li> <li>• Leads research activities of his group</li> </ul>	
<u>Harry L. Tuller</u>	73	Prof., Department of Materials Science and Engineering, Massachusetts Institute of Technology, USA	Engr. Sc. D., Functional electroceramic materials	40%	2010, Dec. 1st	<ul style="list-style-type: none"> <li>• Primarily located at partner institution</li> <li>• Leads research activities of his group</li> <li>• Visited I<sup>2</sup>CNER for four weeks to participate in events and work on collaborative research projects</li> <li>• Participates in research discussions via internet</li> </ul>	Hosted Dr. Dino Klotz from I <sup>2</sup> CNER at MIT three times in FY2018: for (first) 1.5 months, (second) 1 month, and (third) 1 month
<u>John A. Kilner</u>	72	BCH Steele Chair in Energy Materials, Department of Materials, Imperial College, London, UK	Ph.D., Materials for solid oxide fuel cells and electrolyzers	55%	2010, Dec. 1st	<ul style="list-style-type: none"> <li>• Primarily located at partner institution</li> <li>• Leads research activities of his group</li> <li>• Visited I<sup>2</sup>CNER for five weeks to participate in events and work on collaborative projects</li> <li>• Participates in research discussions via internet</li> </ul>	Hosted Dr. Vincent Thoreton from I <sup>2</sup> CNER at the Imperial College London twice in FY2018: once for 2 weeks and another for 3 weeks  Accepted a graduate student from PI Matsumoto's Core-to-Core project at the Imperial College London for one month
Joichi Sugimura	61	Prof., International Institute for Carbon-Neutral Energy Research, Kyushu University	Dr. of Engr., Tribology and Machine Design	100%	2010, Dec. 1st	<ul style="list-style-type: none"> <li>• Located at I<sup>2</sup>CNER</li> <li>• Leads research activities of his group</li> </ul>	
Yasuyuki Takata	62	Prof., International Institute for Carbon-Neutral Energy Research, Kyushu University	Dr. of Engr., Thermal Engineering	100%	2010, Dec. 1st	<ul style="list-style-type: none"> <li>• Located at I<sup>2</sup>CNER</li> <li>• Executes duties of Associate Director</li> <li>• Lead PI of Thermal Sciences and Engineering Division</li> </ul>	
<u>Xinq Zhang</u>	57	Prof., Department of Engineering Mechanics, Tsinghua University, China	Ph.D., Thermal Science	20%	2010, Dec. 1st	<ul style="list-style-type: none"> <li>• Primarily located at partner institution</li> <li>• Leads research activities of his group</li> <li>• Visited I<sup>2</sup>CNER for one week to participate in events and work on collaborative projects</li> <li>• Participates in research discussions via internet</li> </ul>	

<u>Brian P. Somerday*</u>	50	Dr., Southwest Research Institute, USA	Ph.D., Materials Science and Engineering	20%	2010, Dec. 1st	<ul style="list-style-type: none"> <li>• Primarily located at partner institution</li> <li>• Lead PI of Hydrogen Materials Compatibility Division</li> <li>• Visited I<sup>2</sup>CNER for one week to participate in events and work on collaborative projects</li> <li>• Participates in meetings/events via internet and videoconferences</li> </ul>	
<u>Reiner Kirchheim</u>	75	Prof., The Institut für Metallphysik, University of Göttingen, Germany	Ph.D., Hydrogen in Metals, Thermodynamic s of alloys, Interstitial solution and diffusion in glasses	40%	2011, Apr. 1st	<ul style="list-style-type: none"> <li>• Primarily located at partner institution</li> <li>• Leads research activities of his group</li> <li>• Visited I<sup>2</sup>CNER for one week to participate in events and work on collaborative projects</li> <li>• Participates in research discussions via internet</li> </ul>	Organized workshop in Gottingen, Germany on April 1-2, 2018 between Kyushu University and University of Gottingen researchers to explore and discuss plans for a joint International Research Training Group (IRTG)
Miho Yamauchi	45	Prof., International Institute for Carbon- Neutral Energy Research, Kyushu University	Dr. of Science, Chemistry	100%	2012, Jan. 1st	<ul style="list-style-type: none"> <li>• Located at I<sup>2</sup>CNER</li> <li>• Leads research activities of her group</li> </ul>	
Ken Sakai	57	Prof., Department of Chemistry Faculty of Sciences, Kyushu University	Dr. of Science, Inorganic Chemistry	90%	2012, Jan. 16th	<ul style="list-style-type: none"> <li>• Located at both I<sup>2</sup>CNER and the Science Faculty Building.</li> <li>• Leads research activities of his group</li> </ul>	
<u>Ian Robertson</u>	61	Prof., Dean of Engineering, University of Wisconsin-Madison, USA	Ph.D., Metallurgy	15%	2012, April. 1st	<ul style="list-style-type: none"> <li>• Primarily located at partner institution</li> <li>• Participates in research/events as Chief Science Advisor to the Director</li> <li>• Participates in research discussions via internet</li> </ul>	



<u>Andrew A. Gewirth</u>	59	Prof., Department of Chemistry, University of Illinois at Urbana Champaign, USA	Ph.D., Chemistry	25%	2012, April. 1st	<ul style="list-style-type: none"> <li>• Primarily located at partner institution</li> <li>• Leads research activities of his group</li> <li>• Serves as a member of the Illinois Satellite Advisory Committee and IPRC</li> <li>• Participates in research discussions via internet</li> </ul>	
<u>Kenneth T. Christensen</u>	45	Prof., Department Chair, Aerospace and Mechanical Engineering, University of Notre Dame, USA	Ph.D., Theoretical and applied mechanics specializing in experimental fluid mechanics	25%	2012, April. 1st	<ul style="list-style-type: none"> <li>• Primarily located at partner institution</li> <li>• Leads research activities of his group</li> <li>• Serves as a member of IPRC</li> <li>• Visited I<sup>2</sup>CNER for one week to participate in events and work on collaborative projects</li> <li>• Participates in research discussions via internet</li> </ul>	
Shigenori Fujikawa (Associate Professor)	48	Associate Prof., International Institute for Carbon- Neutral Energy Research, Kyushu University	Dr. of Engr., Nanoscience and engineering	100%	2013, June. 1st	<ul style="list-style-type: none"> <li>• Located at I<sup>2</sup>CNER</li> <li>• Lead PI of CO<sub>2</sub> Capture and Utilization Division</li> </ul>	
Takeshi Tsuji	39	Prof., International Institute for Carbon- Neutral Energy Research, Kyushu University	Dr. of Science, Earth and planetary science, Resource engineering, Space exploration	100%	2013, June. 1st	<ul style="list-style-type: none"> <li>• Located at I<sup>2</sup>CNER</li> <li>• Lead PI of CO<sub>2</sub> Storage Division</li> </ul>	

Hiroshige Matsumoto	52	Prof., International Institute for Carbon-Neutral Energy Research, Kyushu University	Dr. of Engr.	100%	2010, Dec. 1st	<ul style="list-style-type: none"> <li>• Located at I<sup>2</sup>CNER</li> <li>• Lead PI of Electrochemical Energy Conversion Division</li> </ul>	
Bidyut B. Saha	53	Prof., International Institute for Carbon-Neutral Energy Research, Kyushu University	Dr. of Engr.	100%	2010, Dec. 1st	<ul style="list-style-type: none"> <li>• Located at I<sup>2</sup>CNER</li> <li>• Leads research activities of his group</li> </ul>	
<u>Thomas Lippert</u>	56	Prof., Department of Chemistry and Applied Biosciences, Laboratory of Inorganic Chemistry, Swiss Federal Institute of Technology Zurich, and Paul Scherrer Institut, Thin Films & Interfaces Group, Villigen-PSI, Switzerland	Dr. of Science, Physical Chemistry	25%	2016, Aug. 1st	<ul style="list-style-type: none"> <li>• Primarily located at partner institution</li> <li>• Leads research activities of his group</li> <li>• Visited I<sup>2</sup>CNER for two weeks to participate in events and work on collaborative projects</li> <li>• Participates in research discussions via internet</li> </ul>	<p>Hosted a group of researchers from I<sup>2</sup>CNER at the Paul Scherrer Institut twice in FY2018 for PSI-I<sup>2</sup>CNER joint research workshops</p> <p>Hosted Dr. Kulbir Ghuman and Dr. Luo Sijun from I<sup>2</sup>CNER at PSI for multiple months in FY2018</p>
Tsuyohiko Fujigaya	41	Prof., Department of Applied Chemistry, Kyushu University	Ph.D. Engr., Polymer chemistry	80%	2018, Apr. 1st	<ul style="list-style-type: none"> <li>• Located at I<sup>2</sup>CNER</li> <li>• Leads research activities of his group</li> </ul>	
Aleksandar Staykov	39	Associate Prof., International Institute for Carbon-Neutral Energy Research, Kyushu University	Ph.D., Physical and theoretical chemistry	100%	2018, Apr. 1st	<ul style="list-style-type: none"> <li>• Located at I<sup>2</sup>CNER</li> <li>• Leads research activities of his group</li> </ul>	
Hiroaki Watanabe	46	Associate Prof., Department of Mechanical Engineering, Kyushu University	Ph.D. Engineering	80%	2018, Oct. 1st	<ul style="list-style-type: none"> <li>• Located at I<sup>2</sup>CNER</li> <li>• Leads research activities of his group</li> </ul>	

**Principal investigators unable to participate in project in FY 2018**

Appendix 2

Name	Affiliation (Position title, department, organization)	Starting date of project participation	Reasons	Measures taken
Setsuo Takaki	N/A	2011, Apr. 1st	Retirement from the PI position as of March 31, 2018	

## Appendix 2a Biographical Sketch of a New Principal Investigator

(within 3 pages per person)

**Name (Age)** Tsuyohiko Fujigaya (41)  
**Affiliation and position** (Position title, department, organization, etc.)  
 Professor, Department of Applied Chemistry, Graduate School of Engineering, Kyushu University  
**Academic degree and specialty** Ph.D. Engineering  
**Effort** 80%

### Research and education history

#### <Education>

- Ph. D. Department of Chemistry and Biotechnology School of Engineering, Tokyo University
- M. S. Department of Organic and Polymeric Materials, Tokyo Institute of Technology
- B. S. Department of Polymer Chemistry, Tokyo Institute of Technology

#### <Research>

- Professor, Dept. of Applied Chemistry, Kyushu University, 2018-present
- Associate Professor, Dept. of Applied Chemistry, Kyushu University, 2011 – 2017
- Guest Associate Professor, Dept. of Applied Chemistry, Kyushu University, 2007 – 2011
- Postdoctoral Associate, Kyushu University, 2006 – 2007
- Post-doctoral Associate, Chemistry Department, Northwestern University, 2005 – 2006

### 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.)

(1) A highly efficient and durable carbon nanotube-based anode electrocatalyst for water electrolyzers

Iridium (Ir) nanoparticles with a uniform diameter of  $1.1 \pm 0.2$  nm were homogeneously deposited on multi-walled carbon nanotubes (MWNTs) wrapped by polybenzimidazole (PBI), in which PBI enables efficient anchoring of the Ir nanoparticles. The Ir nanoparticles were electrochemically oxidized to afford Ir oxide (IrO) and evaluated as an oxygen evolution reaction catalyst by half-cell measurements. The composite was also used as an anode electrocatalyst for proton exchange membrane water electrolyzers (PEMWEs). It was revealed that the IrO<sub>2</sub> on the PBI-wrapped MWNTs exhibited a very high electrocatalytic mass activity and durability even compared to the other state-of-the-art Ir-based catalysts, while the IrO<sub>2</sub> deposited on conventional carbon black showed only a poor durability.

(Sources: *J. Mater. Chem. A* 5, 10584 -10590, 2017)

(2) A highly durable carbon nanotube-based electrocatalyst for polymer electrolyte fuel cell

Improvement of the durability of the polymer electrolyte fuel cell (PEFC) is the one of the urgent target of the I<sup>2</sup>CNER. We developed novel PEFC using polymer-wrapped carbon nanotube (CNT) as the catalyst supporting material (CNT-based PEFC) showing a remarkable high durability (single cell test: >400,000 cycles) at 80 °C under humidified condition. Such a remarkable durability has not been achieved yet and we found the conventional PEFC using carbon black (commercial PEFC) only showed the durability below 5,000 cycles at the same operation condition. Our dramatic improvement was achieved by the use of the novel preparation method named 'PBI-wrapping method' developed by our group, in which the PBI stand for polybenzimidazole. Owing to this achievement, one of the important milestone in I<sup>2</sup>CNER was realized.

(Sources: Sci. Rep. 5, art. No.16711, 2015, *Adv. Mater.*, 25, 1666-1681, 2013. *J. Mater.*

*Chem.* 21, 1187-1190, 2011. *ChemCatChem.* 5, 1701-1704, 2013. *Polym. J.* 45, 326-330, 2013. *ChemPlusChem.*, 79, 400-405, 2014, *J. Mater. Chem. A*, 2, 3888-3893, 2014, *Sci. Rep.*, 3, Art. No. 1764, 2013, *ChemCatChem.*, 6, 567-571, 2014, *J. Mater. Chem. A*, 2, 19053-19059, 2014)  
(Sources: *Sci. Rep.* 5, art. No.16711, 2015)

## Achievements

### (1) International influence \* Describe the kind of attributes listed below.

#### a) Recipient of international awards

Iijima Award, The Fullerenes, Nanotubes and Graphene Research Society, 2014  
Best Paper Award, International Photopolymer Science & Technology, 2003

#### b) Member of a scholarly academy in a major country

Member, American Chemical Society (ACS)  
Member, The Electrochemical Society (ECS)  
Member, Thermoelectrics Society of Japan (TSJ)  
Member, The Society of Fiber Science and Technology, Japan  
Member, The Materials Research Society of Japan  
Member, The Electrochemical Society of Japan  
Member, The Chemical Society of Japan  
Member, The Japan Society of Applied Physics  
Member, The Fullerenes and Nanotubes Research Society  
Member, The Society of Polymer Science, Japan

#### c) Guest speaker or chair of related international conference and/or director or honorary chairman of a major international academic society in the subject field

Invited speaker. 233rd Electrochemical Society Spring Meeting, Seattle USA, May, 2018.  
Invited speaker. The 9th A3 Symposium on Emerging Materials, Kyoto, Oct, 2018  
Invited speaker. International Conference on Organic and Hybrid Thermoelectrics, Valencia, Spain, January, 2018,  
Invited speaker. The 8th A3 Symposium on Emerging Materials, Suzhou, China, 2018.  
Invited speaker. International Conference on Organic and Hybrid Thermoelectrics, Kyoto, Japan, January 2016  
Invited speaker. The 9th Japan-China Joint Symposium on Functional Supramolecular Architectures at IMS, Okazaki, Japan, February, 2016  
Invited speaker. Japan-UK Collaboration in Chemistry, London, June 2016  
Invited speaker. The International Conference on Flexible and Printed Electronics, Yamagata, Japan. September, 2016  
Invited speaker. The 7th A3 Symposium on Emerging Materials, South Korea, November, 2016  
Invited speaker. The 6th A3 Symposium on Emerging Materials, Tenjin, China, Oct. 2014  
Invited speaker. The 15th IUMRS-International Conference in Asia, Fukuoka, Aug. 2014  
Invited speaker. The Second Japan-Korea Joint Symposium on Polymer Nanohybrid Materials, Kyoto Aug. 2012  
Invited speaker. 1st NUS-IMCE Workshop, Fukuoka, 2012  
Invited speaker. International Conference on Materials for Advanced Technologies, Singapore, June 2011  
Invited speaker. International Conference on Science and Application of Nanotubes, Satellite Symposium, Cambridge, UK, July, 2011

Invited speaker. International Symposium for Young Organic Chemists, Tsukuba, Mar 2011.  
 Invited speaker. China-Japan Young Chemists Forum, Xiamen, China June 2010.  
 Invited speaker. International Hydrogen Energy Development Forum, Fukuoka, Feb 2010.  
 Invited speaker. Advanced Polymeric Materials and Technology Symposium, Jeju Korea, Jan 2010.  
 Invited speaker. 3rd German-Japanese Young Researchers Workshop, Karlsruhe, Germany, July 2009

d) Editor of an international academic journal

N/A

e) Peer reviewer for an overseas competitive research program (etc.)]

N/A

## (2) Receipt of major large-scale competitive funds (over the past 5 years)

- T. Fujigaya (Coordinator) Grant-in-Aid for Scientific Research (A), Japan Society for the Promotion of Science, duration: 2016-2018, amount: JP Yen 21 million
- T. Fujigaya (Coordinator) Precursory Research for Embryonic Science and Technology, Japan Science and Technology Agency, duration: 2015-2018, amount: JP Yen 40 million
- T. Fujigaya (Coordinator), K. Ito, A. Hayashi and H. Nakajima, Advanced Low Carbon Technology Research and Development Program, Japan Science and Technology Agency, duration: 2013-2018, amount: JP Yen 120 million
- T. Fujigaya (Coordinator), Grant-in-Aid for Challenging Exploratory Research, Japan Society for the Promotion of Science, duration: 2016-2017, amount: JP Yen 3.3 million.

## (3) Major publications (Titles of major publications, year of publication, journal name, number of citations)

1. Design of an Assembly of Polybenzimidazole, Carbon Nanotubes and Pt Nanoparticles for a Fuel Cell Electrocatalyst with an Ideal Interfacial Nanostructure, *Small* 5, 735-740 (2009). (citation; 143)
2. Biologically Active Protein Nanoarrays Generated Using Parallel Dip-Pen Nanolithography *Adv. Mater.*, 18, 1133-1136 (2006). (citation; 112)
3. Fuel Cell Electrocatalyst Using Polybenzimidazole-Modified Carbon Nanotubes as Support Materials, *Adv. Mater.*, 25, 1666-1681 (2013). (citation: 105)
4. Switching of Spin States Triggered by a Phase Transition: Spin Crossover Properties of Self-Assembled Iron(II) Complexes with Alkyl-Tethered Triazole Ligands *J. Am. Chem. Soc.*, 125, 14690-14691 (2003). (citation: 102)
5. Non-covalent polymer wrapping of carbon nanotubes and the role of wrapped polymers as functional dispersants *Sci. Technol. Adv. Mater.* 16, 024802 (2015) (citation: 96)
6. Design of an assembly of pyridine-containing polybenzimidazole, carbon nanotubes and Pt nanoparticles for a fuel cell electrocatalyst with a high electrochemically active surface area *Carbon* 47, 3227-3232 (2009). (citation: 96)
7. Very-High-Performance Alkali Anion-Exchange Membrane Fuel Cells" *Adv. Funct. Mater.* 21, 1089-1094 (2011). (citation: 93)
8. Near-IR Laser-Driven Reversible Volume Phase Transition of Single-Walled Carbon Nanotubes/Poly(N-isopropylacrylamide) Composite gels *Adv. Mater.* 20, 3610-3614 (2008). (citation: 88)

## (4) Others (Other achievements indicative of the PI's qualification as a top-world researcher, if any.)

N/A

## Appendix 2a Biographical Sketch of a New Principal Investigator

(within 3 pages per person)

**Name (Age)** Aleksandar Tsekov Staykov (39)

**Affiliation and position** (Position title, department, organization, etc.)

Associate Professor, Molecular Photoconversion Division, International Institute for Carbon-Neutral Energy Research, Kyushu University

**Academic degree and specialty** Ph.D. Physical and theoretical chemistry

**Effort** 100%

\* Percentage of time that the principal investigator will devote to working for the center vis-à-vis his/her total working hours.

### Research and education history

#### <Education>

- Ph.D. Wilhelm-Ostwald Institute for Physical and Theoretical Chemistry, Leipzig University, 2006
- M.Sc. Organic chemistry, Faculty of chemistry, Sofia University, Bulgaria, 2002
- B.Sc. Chemistry, Faculty of chemistry, Sofia University, Bulgaria, 2000

#### <Research>

- Associate Professor, Molecular Photoconversion Devices Division, International Institute for Carbon Neutral Energy Research, Kyushu University, Japan, 2015-present
- Assistant Professor, Hydrogen Production Division, International Institute for Carbon Neutral Energy Research, Kyushu University, Japan, 2011-2014
- JSPS Fellowship for Postdoctoral Research in Japan, Institute for Materials Chemistry and Engineering, Kyushu University 2008-2010
- Postdoctoral research associate, Institute for Materials Chemistry and Engineering, Kyushu University 2006-2008

### 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.)

1) Diarylethenes are a class of photoswitching molecules developed by M. Irie (Kyushu University) that quickly became promising candidates for control units in the fields of molecular electronics and molecular machines. In 2005, B. Feringa group (University of Groningen) has demonstrated the ability to control the diarylethene switching electrochemically. This result significantly expanded the fields of application of diarylethenes, however, the control of switching for linked diarylethene molecules remained unclear. In 2011, a joint research of A. Staykov (theory) and B. Feringa (experiment) proved that the photochemical and electrochemical switching of diarylethenes are one process based on the occupation of their frontier orbitals (ACS Nano 2011, 5, 1165). This outcome led to the design of predictive theory for switching of single and linked diarylethenes. In 2016, B. Feringa received Noble Prize in Chemistry.

2) SOFC are promising devices for electrochemical conversion of chemical energy into electricity. Their electrodes are usually made from perovskites (complex oxides of two or more metallic cations) which are characterized with ionic conductivity, electronic conductivity, and surface oxygen exchange. A major reason for the insufficient industrial application of SOFCs is the electrodes' durability, which suffers from various degradation mechanisms. Thus, it is crucial to elucidate the electrodes' surface structure and catalytic activity. J. Kilner (Imperial College London) and T. Ishihara (Kyushu University)

proved that perovskite surfaces are always terminated with their "A-site" elements. The oxygen reduction reaction (ORR) depends on the type of A-site element (earth alkaline or rare earth). A. Staykov proved that rare earth elements on A-sites possess supreme catalytic activity, owing to partial covalency within the crystal structure. The use of rare earth elements on A-sites of perovskites limits the possible electrode degradation. The joint work (Kilner, Ishihara, Staykov) is awarded with Daiwa-Adrian Prize for Japan-UK collaboration (2016).

c) Hydrogen embrittlement of metals is a problem that significantly endangers the acceptance of hydrogen as safe and reliable energy source. When H-atoms are dissolved in the lattices of structural components, the result is materials' fatigue and failure. For decades the problem has been addressed from the fields of mechanical engineering and metallurgy with design of hydrogen resistant steels and coatings. Recently, B. Somerday (South West Research Institute) and A. Staykov proved a chemical concept for mitigation of hydrogen embrittlement of metals based on impurities in the hydrogen gas. The mitigation mechanism is based on the poisoning of the catalytic activity of metal surfaces towards the molecular hydrogen dissociation reaction. Thus, by controlling the impurities in the hydrogen gas one can control the safety of structural components in hydrogen transport and storage.

## Achievements

**(1) International influence** \* Describe the kind of attributes listed below.

a) Recipient of international awards

Daiwa-Adrian Prize for Japan-UK collaboration (2016)

b) Member of a scholarly academy in a major country

c) Guest speaker or chair of related international conference and/or director or honorary chairman of a major international academic society in the subject field

1. Aleksandar Staykov. Air Liquide Conferences. Chemical processes at surfaces and interfaces. Air Liquide Laboratories, Tsukuba, Japan. June 2018.
2. Aleksandar Staykov. Chemical processes at surfaces and interfaces. EMRS Spring meeting, Lille, France. May 2016.
3. Aleksandar Staykov. Application of the Non-equilibrium Green's function method in Chemistry, IMI-La Trobe Joint Conference "Mathematics for Materials Science and Processing," La Trobe University, Melbourne, February 15-17 2016.
4. Aleksandar Staykov. The Stability of Titania-Silica Interface. 14<sup>th</sup> meeting of Brazilian Materials Research Society, Rio de Janeiro, Brazil. October 2015.
5. Aleksandar Staykov, Yuuki Ooishi, Tatsumi Ishihara. Immobilizing Metal Nanoparticles on Single Wall Nanotubes. Effect of Surface Curvature. 10th Congress of the World Association of Theoretical and Computational Chemists (WATOC), Santiago, Chile, October 2014.
6. Aleksandar Staykov, Yuuki Ooishi, Tatsumi Ishihara. Immobilizing Metal Nanoparticles on Single Wall Nanotubes. Effect of Surface Curvature. Catalysis Research Center International symposium, Hokkaido University, March 17, 2014, Sapporo, Japan.
7. Aleksandar Staykov, Yuuki Ooishi, Tatsumi Ishihara. Immobilizing Metal Nanoparticles on Single Wall Nanotubes. Effect of Surface Curvature. Energy Material Nanotechnology Spring meeting 2014, March 2, 2014, Las Vegas, USA.
8. Aleksandar Staykov, Junichiro Yamabe, Brian Somerday. Theoretical Study of the Co-adsorption of Hydrogen and Unsaturated Molecules on Iron Surface. ACS Fall meeting. September 8-12, 2013, Indianapolis, USA.
9. Aleksandar Staykov. Current Rectifying Properties of Mono- and Bi-layered Graphene Nanomaterials, International Conference on Emerging Advanced Nanomaterials, October 22-25, 2012, Brisbane, Australia.



10. Aleksandar Staykov, Xinqian Li, Yuta Tsuji, Kazunari Yoshizawa. Theory of Rectification Applied on Nitrogen and Boron Doped Nanographenes and Cyclophanes. International Conference for Young Researchers on Advanced Materials, July 6-th, 2012, Singapore.
11. Aleksandar Staykov. Electrochemical and Photochemical Switching of Diarylethenes and Diarylethene-capped Sexithiophene Wires. 28th Symposium on Chemical Kinetics and Dynamics, June 2012, Fukuoka, Japan.

d) Editor of an international academic journal

e) Peer reviewer for an overseas competitive research program (etc.)

**(2) Receipt of major large-scale competitive funds (over the past 5 years)**

1. Air Liquide "CO Interaction with Ni and Fe surfaces. Multiscale modeling." 7.5 million yen over 3 years 2014-2017. PI
2. Grant-in-Aid for Young Scientists (B); Molecular spin-switch for effective electron-hole separation at hybrid interfaces for application in photocatalysis. 4.2 million yen in two years; 2016-2018. PI
3. Grant-in-Aid for Scientific Research (C); Environmental Degradation of Perovskite Electrode Surfaces in Solid Oxide Fuel Cells; 4.2 million yen in three years. 2018-2020. PI

**(3) Major publications (Titles of major publications, year of publication, journal name, number of citations)**

1. A Staykov, D Nozaki, K Yoshizawa. Theoretical study of donor–  $\pi$ -bridge– acceptor unimolecular electric rectifier. *J. Phys. Chem. C* 111, 11699-11705, 2007. Cited 118 times.
2. A Staykov, T Kamachi, T Ishihara, K Yoshizawa. Theoretical study of the direct synthesis of H<sub>2</sub>O<sub>2</sub> on Pd and Pd/Au surfaces. *J. Phys. Chem. C* 112, 19501-19505, 2008. Cited 95 times.
3. A Staykov, D Nozaki, K Yoshizawa. Photoswitching of conductivity through a diarylperfluorocyclopentene nanowire. *J. Phys. Chem. C* 111, 3517-3521, 2007. Cited 75 times.
4. A Staykov, J Areephong, WR Browne, BL Feringa, K Yoshizawa. Electrochemical and photochemical cyclization and cycloreversion of diarylethenes and diarylethene-capped sexithiophene wires, *ACS nano* 5, 1165-1178, 2011. Cited 64 times.
5. A Staykov, H Téllez, T Akbay, J Druce, T Ishihara, J Kilner. Oxygen activation and dissociation on transition metal free perovskite surfaces. *Chem. Mater.* 27, 8273-8281, 2015. Cited 33 times.
6. A Staykov, M Watanabe, T Ishihara, K Yoshizawa. Photoswitching of conductance through salicylidene methylamine. *J. Phys. Chem. C* 118, 27539-27548. 2014. Cited 25 times.
7. A Staykov, Y Ooishi, T Ishihara. Immobilizing metal nanoparticles on single wall nanotubes. Effect of surface curvature. *J. Phys. Chem. C* 118, 8907-8916. 2014. Cited 17 times.

**(4) Others (Other achievements indicative of the PI's qualification as a top-world researcher, if any.)**

## Appendix 2a Biographical Sketch of a New Principal Investigator

(within 3 pages per person)

**Name (Age)** Hiroaki Watanabe (46)  
**Affiliation and position** (Position title, department, organization, etc.)  
 Associate Professor, Department of Mechanical Engineering, Faculty of Engineering, Kyushu University  
**Academic degree and specialty** Ph.D. Engineering  
**Effort** 80%

### Research and education history

2018-present	Principal Investigator, Thermal Science and Engineering Division, International Institute for Carbon-Neutral Energy Research (I <sup>2</sup> CNER), Kyushu University
2014-present	Associate Professor, Department of Mechanical Engineering, Faculty of Engineering, Kyushu University
2011-2014	Visiting Associate Professor, Department of Human and Engineered Environmental Studies, Graduate School of Frontier Sciences, The University of Tokyo
2010-2011	Senior Research Fellow, Center for Turbulence Research, Stanford University
2013-2014	Senior Research Scientist, Energy Engineering Research Laboratory, Central Research Institute of Electric Power Industry
2002-2013	Research Scientist, Energy Engineering Research Laboratory, Central Research Institute of Electric Power Industry
1998-2002	Researcher, Department of Energy Machinery, Central Research Institute of Electric Power Industry
2008	Doctor of Philosophy in Engineering, Department of Mechanical Engineering and Science, Kyoto University
1998	Master Degree in Engineering, Department of Mechanical Engineering, Waseda University
1996	Bachelor Degree in Engineering, Department of Mechanical Engineering, Waseda University

### 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.)

1. A clarification of characteristics of conserved and non-conserved scalars, radiation and soot formation and a proposal of a new turbulent combustion model by means of DNS. This work made a breakthrough to account the effect of interphase heat transfer including radiation and was essential to perform high accurate LES. Developed model was validated on a gas turbine combustor.
2. A clarification of characteristics of heat and mass transfer within a coal particle taking nano-scale pore forming and molecular diffusion into account and a proposal of a new model. This model can essentially capture the mechanism of solid particle combustion physics with much lower computational cost. Modeling of devolatilization process considering solid phase elementary reactions. This is the first model coupled with elementary reactions to account for detailed chemistry of polycyclic aromatic hydrocarbons and soot formation. These works are new and make a breakthrough to account molecular level interaction in a computation of heterogeneous combustion.
3. Application of state-of-the-art models in RANS to clarification of gasification characteristics

on semi-industrial or practical scale gasifier. This work has been cited in 248 papers at present and is regarded as a benchmark in this research area.

4. First papers in the world to investigate capability of LES for pulverized coal combustion and this work excited the researchers in LES modeling of coal combustion at present.

## Achievements

### (1) International influence \* Describe the kind of attributes listed below.

- a) Recipient of international awards
  1. Certificate of Appreciation from American Chemical Society (2011)
  2. Feature Article from Combustion and Flame (Combustion Institute) (2007)
- b) Member of a scholarly academy in a major country
  1. The Japan Society of Mechanical Engineers (JSME)
  2. Combustion Society of Japan
  3. Gas Turbine Society of Japan
  4. The Japan Institute of Energy
  5. Society of Automotive Engineers of Japan
  6. The Society of Powder Technology, Japan
  7. American Geophysical Union
  8. European Geosciences Union
- c) Guest speaker or chair of related international conference and/or director or honorary chairman of a major international academic society in the subject field
  1. Plenary Lecture at the 11th Asia-Pacific Conference on Combustion (2017)
  2. Co-chair at International Conference on Polygeneration (2019)
- d) Editor of an international academic journal
  1. Advanced Powder Technology
  2. Journal of Vibration Testing and System Dynamics
  3. Proceedings of the Combustion Institute
- e) Peer reviewer for an overseas competitive research program (etc.)  
N/A

### (2) Receipt of major large-scale competitive funds (over the past 5 years)

1. MEXT FLAGSHIP 2020 Project, Post K, A Priority Issue 6, Accelerated Development of Innovative Clean Energy Systems, Energy Conversion Systems Accompanied by High-pressure Combustion and Gasification, 34,500,000JPY (2015-2019).
2. METI Technical Investigation of Production of Shallow Methane Hydrate, 13,650,000JPY (2016-2018).
3. Grants-in-aid for Scientific Research (C), JSPS, Modeling of elementary reactions in multiphase turbulence based on physical and chemical structures of pulverized coal, 3,700,000JPY (2016-2019).
4. Grants-in-aid for Scientific Research (C), JSPS, Analysis of ignition process of a pulverized coal particle and modeling of multiphase turbulent combustion, 4,000,000JPY (2013-2015).
5. Research Fund from JFE 21st Century Foundation, Development of numerical simulation of gas-particle two-phase reacting flow on raceway in a blast furnace for evaluation of durability of cokes, 2,000,000JPY (2019).

**(3) Major publications (Titles of major publications, year of publication, journal name, number of citations)**

1. Watanabe, H., Otaka, M., Numerical simulation of coal gasification in entrained flow coal gasifier, 2006, *Fuel*, 85, 1935-1943, Citation: 403.
2. Watanabe, H., Kurose, R., Hwang, S.-M., Akamatsu, F., Characteristics of flamelets in spray flames formed in a laminar counterflow, 2007, *Combustion and Flame*, 148, 234-248, Citation: 101.
3. Watanabe, H., Kurose, R., Komori, S., Pitsch, H., Effects of radiation on spray flame characteristics and soot formation, 2008, *Combustion and Flame*, 152, 2-13, Citation: 75.
4. Kurose, R., Watanabe, H., Makino, H., Numerical simulation of pulverized coal combustion, 2009, *KONA Powder and Particle Journal*, 27, 144-156, Citation: 66.
5. Muto, M., Watanabe, H., Kurose, R., Komori, S., Balusamy, S., Hochgreb, S., Large-eddy simulation of pulverized coal jet flame -Effect of oxygen concentration on NO<sub>x</sub> formation-, 2015, *Fuel*, 142, 152-163, Citation: 50.
6. Fujita, A., Watanabe, H., Kurose, R., Komori, S., Two-dimensional direct numerical simulation of spray flames -Part 1: Effects of equivalence ratio, fuel droplet size and radiation, and validity of flamelet model, 2013, *Fuel*, 104, 515-525, Citation: 46.
7. Hayashi, J., Watanabe, H., Kurose, R., Akamatsu, F., Effects of fuel droplet size on soot formation in spray flames formed in a laminar counterflow, 2011, *Combustion and Flame*, 152, 2559-2568, Citation: 45.

**(4) Others (Other achievements indicative of the PI's qualification as a top-world researcher, if any.)**

N/A

## Appendix 3-1 FY 2018 Records of Center Activities

### 1. Researchers and other center staffs, satellites, partner institutions

#### 1-1. Number of researchers and other center staffs

\* Fill in the number of researchers and other center staffs in the table below.

\* Describe the final goals for achieving these numbers and dates when they will be achieved described in the last "center project."

#### a) Principal Investigators

(full professors, associate professors or other researchers of comparable standing)

(number of persons)

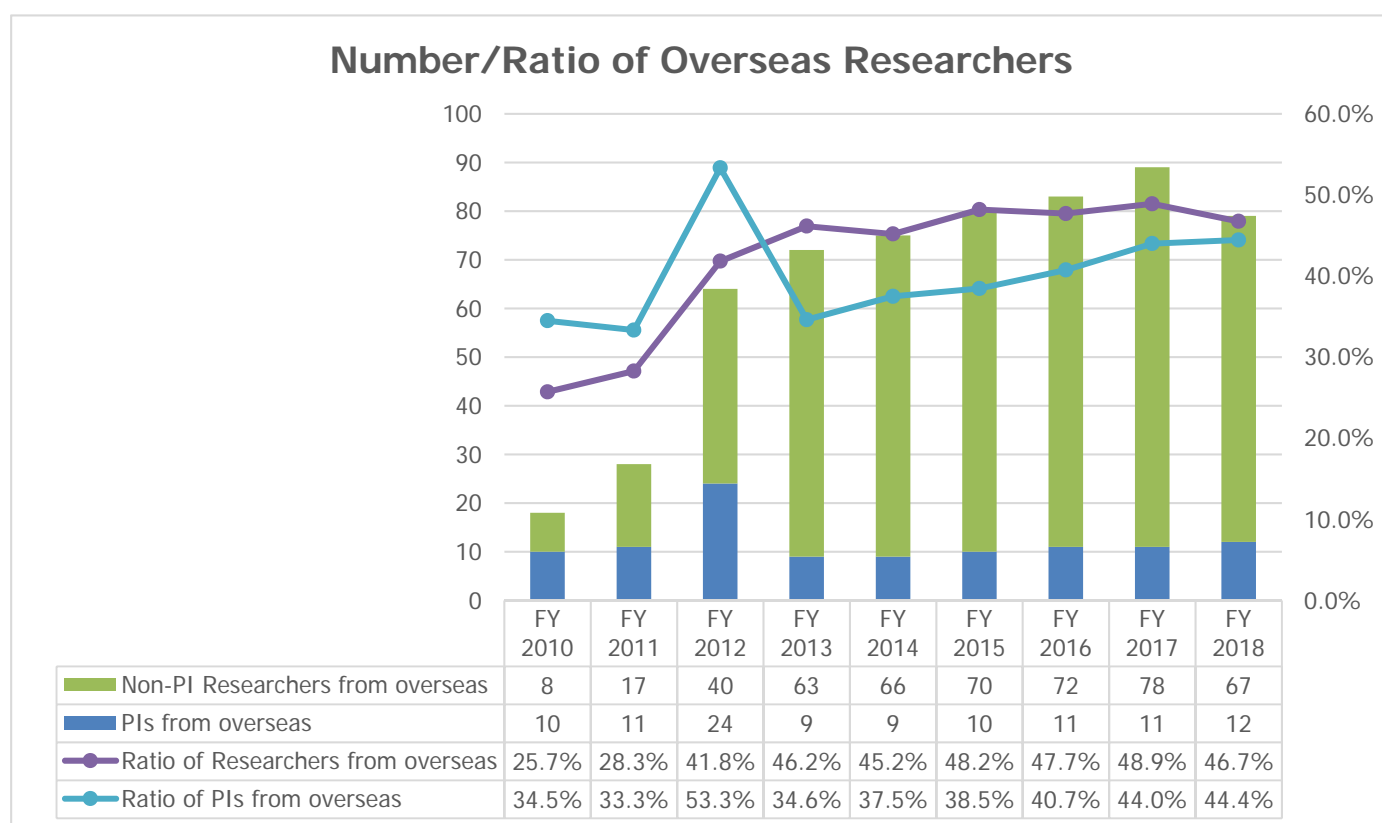
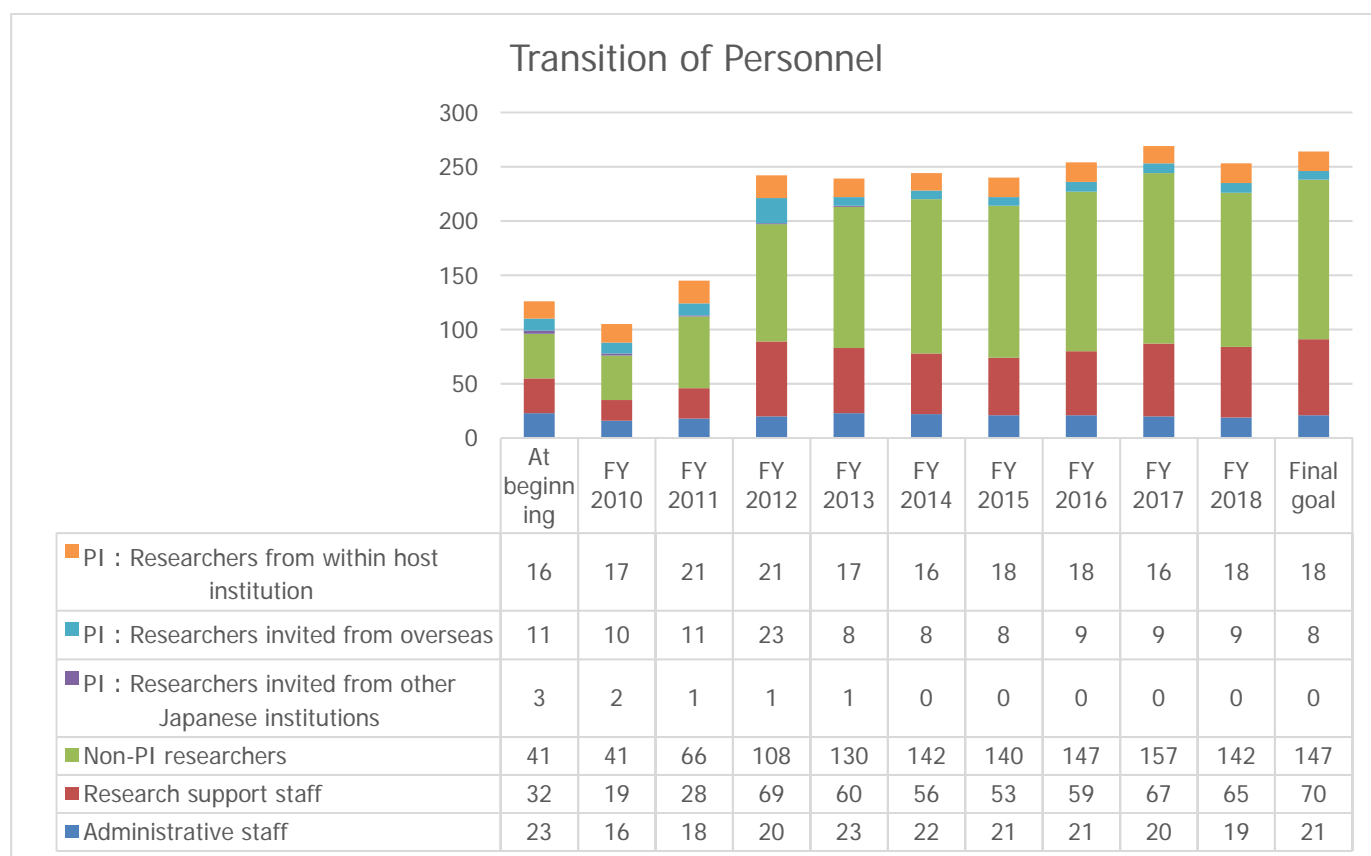
	At the beginning of project	At the end of FY 2018	Final goal (Date: month, year)
Researchers from within the host institution	16	18	18
Researchers invited from abroad	11	9	8
Researchers invited from other Japanese institutions	3	0	0
Total principal investigators	30	27	26

#### b) Total members

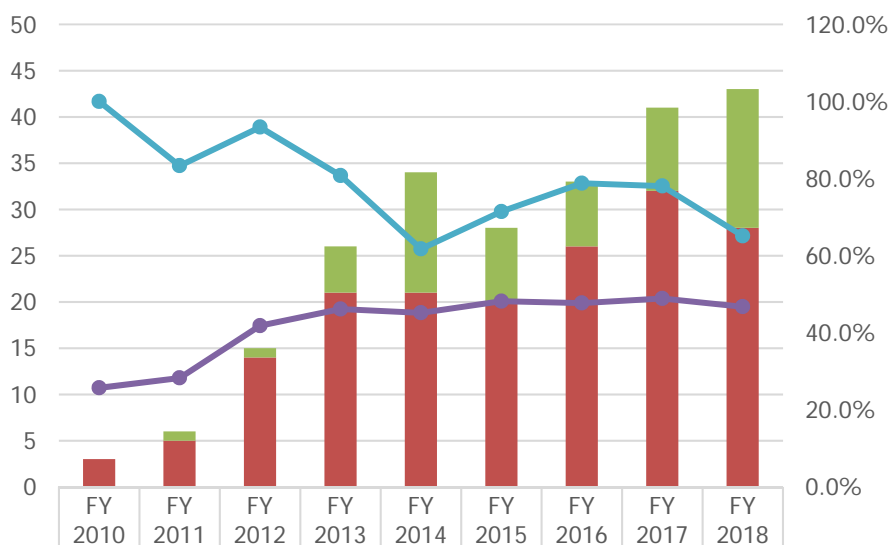
	At the beginning of project		At the end of FY2018		Final goal (Date: month, year)	
	Number of persons	%	Number of persons	%	Number of persons	%
Researchers	71	/	169	/	173	/
Overseas researchers	21	30%	79	47%	80	46%
Female researchers	4	6%	26	15%	29	17%
Principal investigators	30	/	27	/	26	/
Overseas PIs	11	37%	12	44%	8	31%
Female PIs	1	3%	1	4%	1	4%
Other researchers	41	/	142	/	147	/
Overseas researchers	10	24%	67	47%	72	49%
Female researchers	3	7%	25	18%	28	19%
Research support staffs	32	/	65	/	70	/
Administrative staffs	23	/	19	/	21	/
Total number of people who form the "core" of the research center	126	/	253	/	264	/

## Appendix 3-2 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.

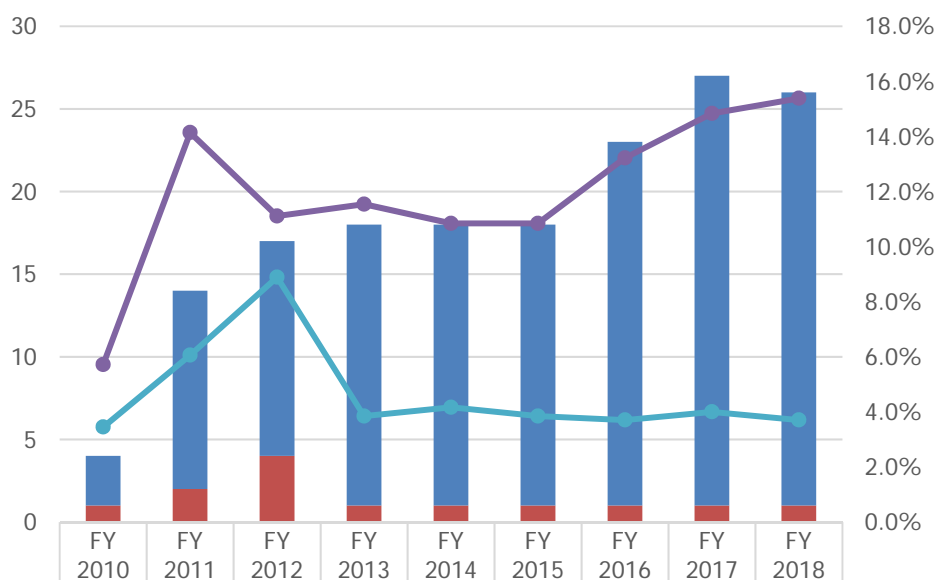


### Number/Ratio of Overseas Postdoc



Japanese Postdocs	0	1	1	5	13	8	7	9	15
Overseas Postdocs	3	5	14	21	21	20	26	32	28
Ratio of Researchers from overseas	25.7%	28.3%	41.8%	46.2%	45.2%	48.2%	47.7%	48.9%	46.7%
Ratio of Postdocs from overseas	100%	83%	93%	81%	62%	71%	79%	78%	65%

### Number/Ratio of Female Researchers



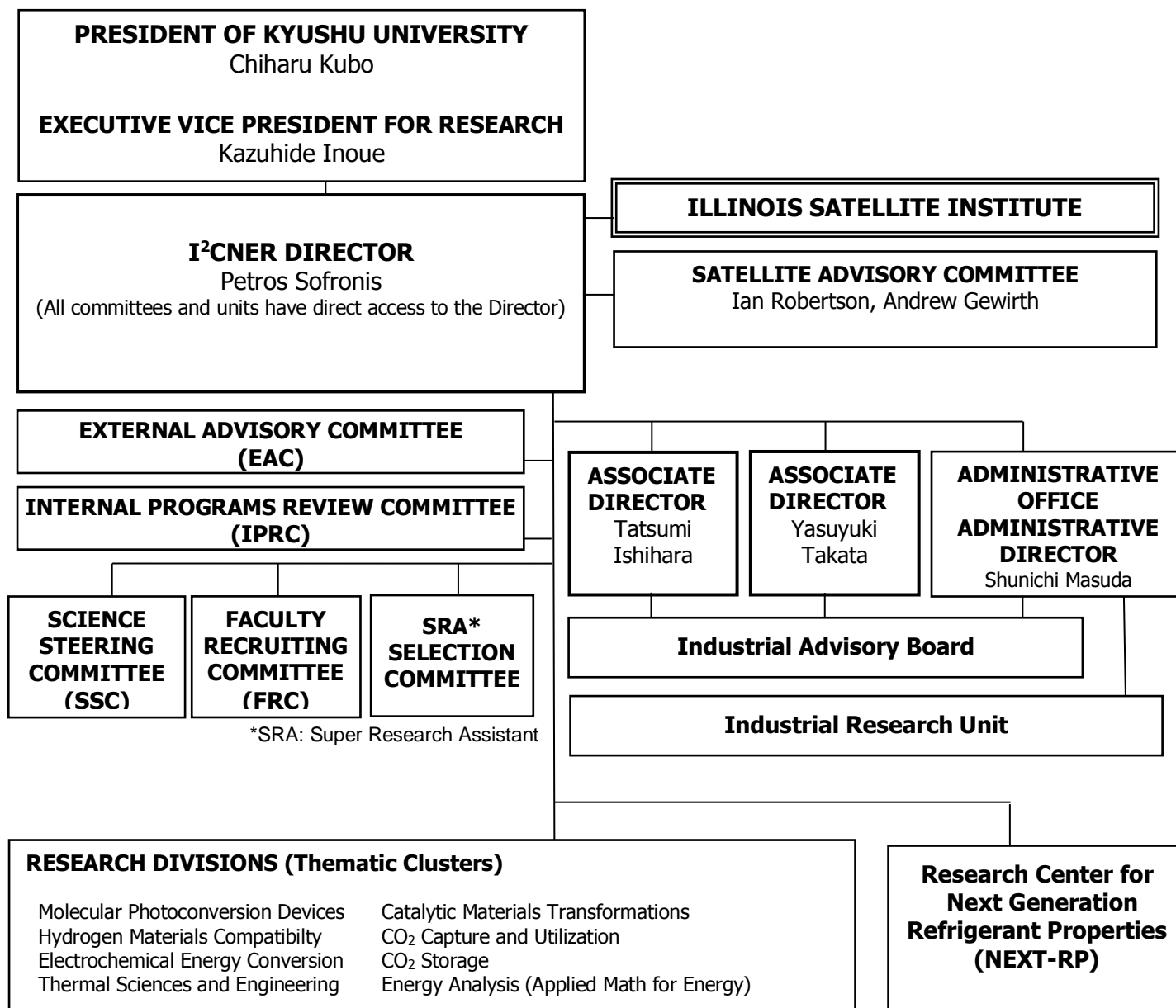
Non-PI Female Researchers	3	12	13	17	17	17	22	26	25
Female PIs	1	2	4	1	1	1	1	1	1
Ratio of Female Researchers	5.7%	14.1%	11.1%	11.5%	10.8%	10.8%	13.2%	14.8%	15.4%
Ratio of Female PIs	3.4%	6.1%	8.9%	3.8%	4.2%	3.8%	3.7%	4.0%	3.7%

## Appendix 3-3 Diagram of Management System

- Diagram the center's management system and its position within the host institution in an easily understood manner.
- If any changes have been made in the management system from that in the latest "center project" last year, describe them. Especially describe any important changes made in such as the center director, administrative director, head of host institution, and officer(s) in charge at the host institution (e.g., executive vice president for research).

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

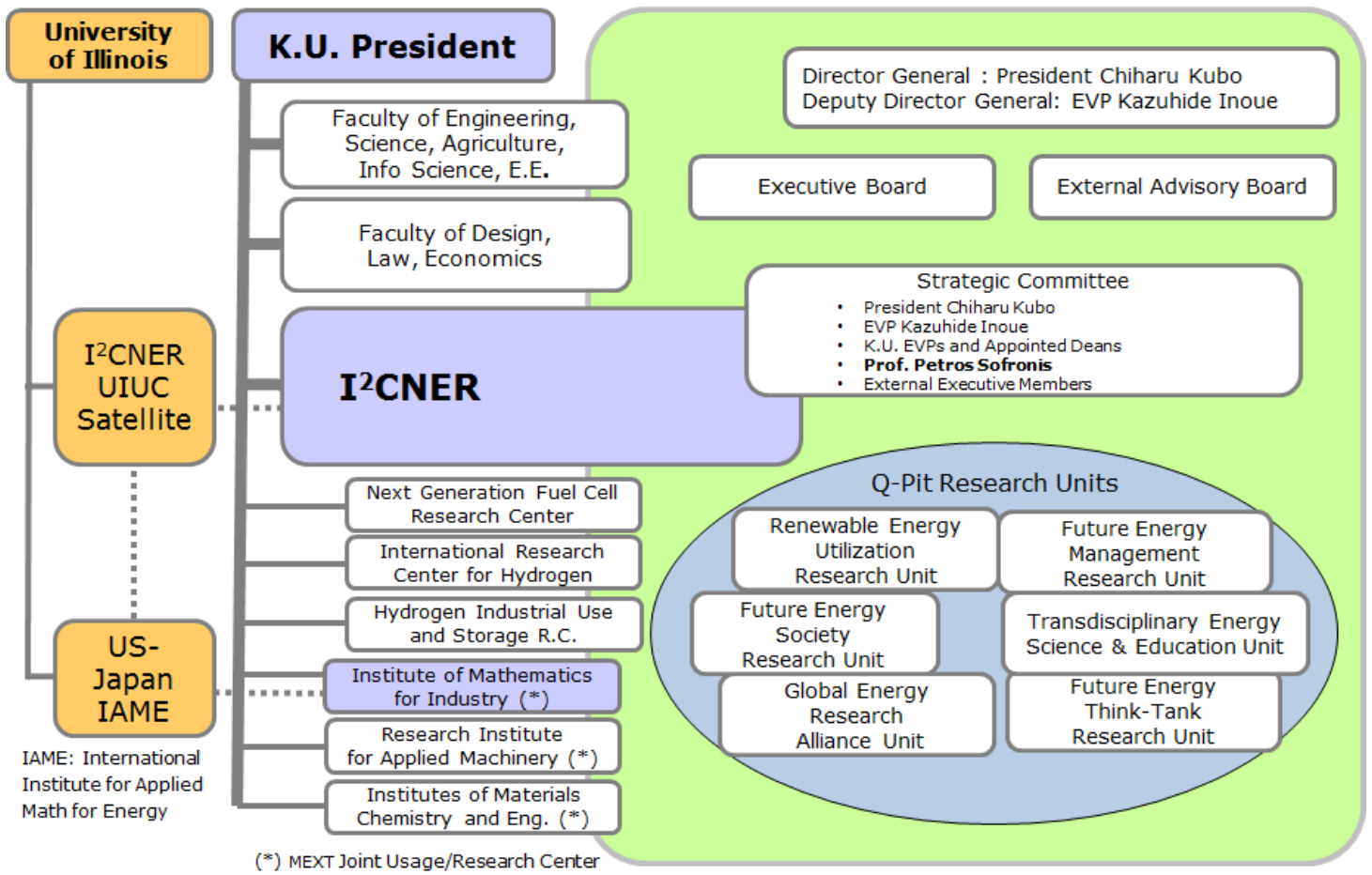
(As of March 31, 2019)



As of April 1, 2018, Professor Kazuhide Inoue replaced Professor Masato Wakayama as Executive Vice President (EVP) for Research. Prof. Inoue, concurrently holds the post of executive vice president for finance, oversees I<sup>2</sup>CNER's interactions with all of Kyushu University.

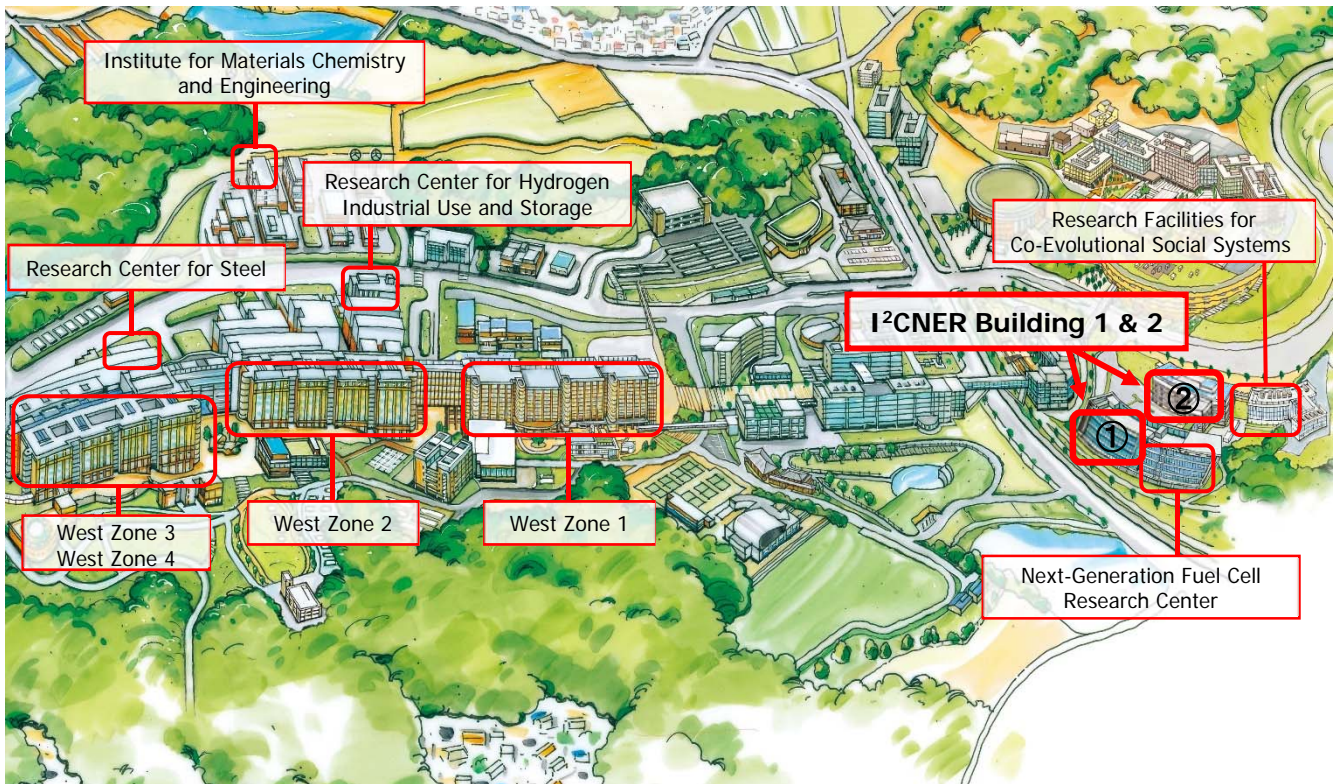


**I<sup>2</sup>CNER within Kyushu University**  
(As of March 31, 2019)



## Appendix 3-4 Campus Map

- Draw a simple map of the campus showing where the main office and principal investigator(s) are located.



### Appendix 3-5 Project Expenditures in FY2018

#### 1) Overall project funding

\* In the "Total costs" column, enter the total amount of funding required to implement the project, without dividing it into funding sources.

\* In the "Amount covered by WPI funding" column, enter the amount covered by WPI within the total amount.

\* In the "Personnel," "Project activities," "Travel," and "Equipment" blocks, the items of the "Details" column may be changed to coincide with the project's actual content.

Cost items	Details (For Personnel - Equipment please fill in the breakdown of fiscal expenditure, and the income breakdown for Research projects.)	(Million yens)		Costs (Million yens)	
		Total costs	Amount covered by WPI funding		
				<b>WPI grant in FY 2018</b>	1080
Personnel	Center director and administrative director	22	22		
	Principal investigators (no. of persons):17	188	166	Costs of establishing and maintaining facilities	1
	Other researchers (no. of persons):75	372	269		
	Research support staffs (no. of persons):18	44	44		
	Administrative staffs (no. of persons):23	91	46		
	Subtotal	717	547		
Project activities	Gratuities and honoraria paid to invited principal investigators (no. of persons):40	4	3		
	Cost of dispatching scientists (no. of persons):0	0	0		
	Research startup cost (no. of persons):17	37	13	Costs of equipment procured	294
	Cost of satellite organizations (no. of satellite organizations):1	145	145		
	Cost of international symposiums (no. of symposiums):1	1	1		
	Rental fees for facilities	250	250		
	Cost of consumables	15	13		
	Cost of utilities	35	35		
	Other costs	35	15		
Subtotal	522	475			
Travel	Domestic travel costs	13	10		
	Overseas travel costs	38	36		
	Travel and accommodations cost for invited scientists (no. of domestic scientists):41 (no. of overseas scientists):33	13	10		
	Travel cost for scientists on transfer (no. of domestic scientists):0 (no. of overseas scientists):2	1	1		
	Subtotal	65	57		
Equipment	Depreciation of buildings	81	1		
	Depreciation of equipment	683	171		
	Subtotal	764	172		
Research projects (Detail items must be fixed)	Project supported by other government subsidies, etc. *1	103			
	KAKENHI	177			
	Commissioned research projects, etc.	346			
	Joint research projects	137			
	Others (donations, etc.)	159			
Subtotal	922	0			
<b>Total</b>		<b>2990</b>	<b>1251</b>		

\*1. Funding sources that include government subsidies (including Enhancements promotion expenses (機能強化促進経費), National university reform reinforcement promotion subsidy (国立大学改革強化推進補助金) etc.), indirect funding, and allocations from the university's own resources.

\*2 When personnel, travel, equipment (etc.) expenses are covered by KAKENHI or under commissioned research projects or joint research projects, the amounts should be entered in the "Research projects" block.

## 2) Costs of satellites

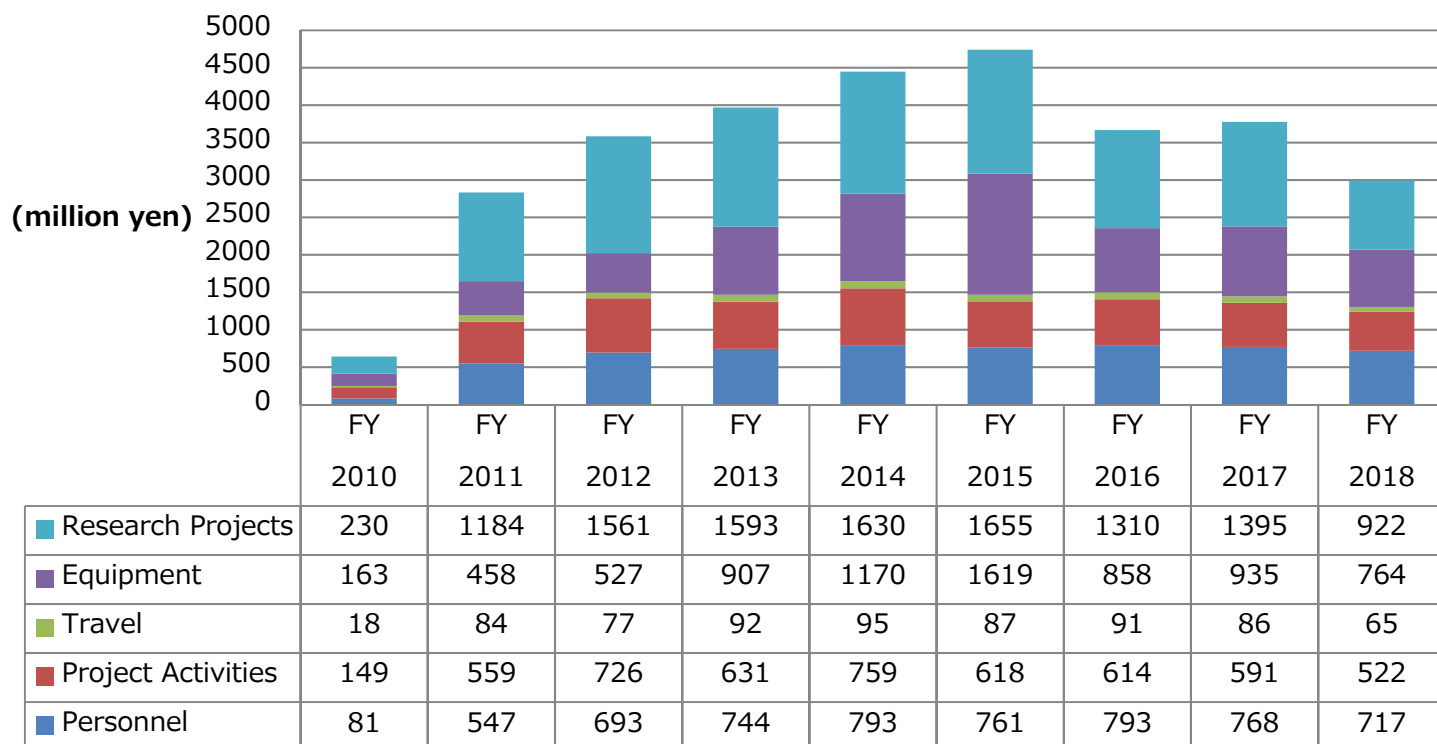
(Million yens)			
Cost items	Details	Total costs	Amount covered by WPI funding
Personnel	Principal investigators (no. of persons):2	/	/
	Other researchers (no. of persons):8		
	Research support staffs (no. of persons):12		
	Administrative staffs		
	Subtotal		
Project activities	Subtotal	37	37
Travel	Subtotal	6	6
Equipment	Subtotal	0	0
Research projects	Subtotal	0	0
Total		145	145

## Appendix 3-6 Annual Transition in the Amounts of Project Funding

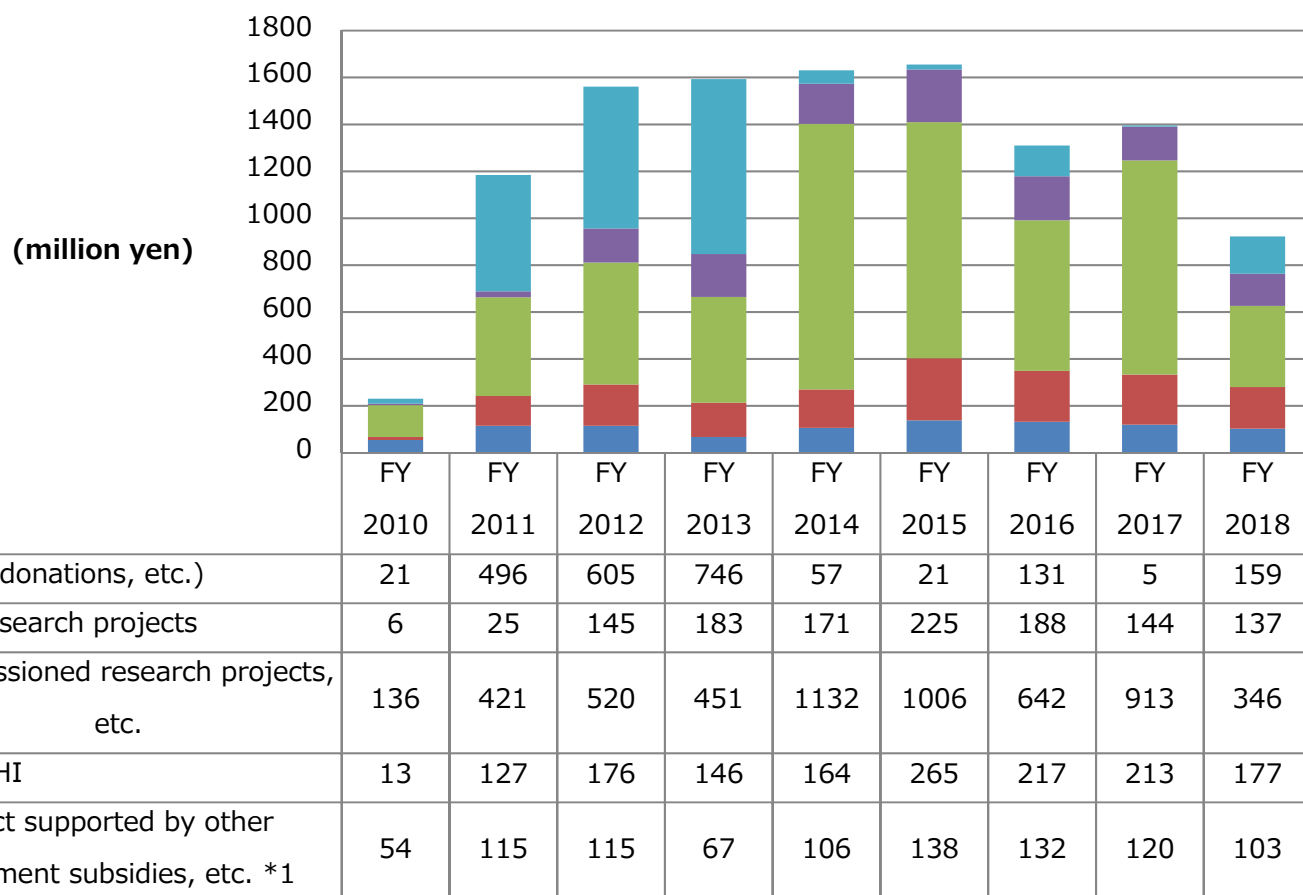
\*Make a graph of the transition in the number of overall project funding.

\*1 Definition is as shown in Appendix 3-5 (Project Expenditures)

### Transition of Project Expenditures



### Transition of Research Project Expenditures



## Appendix 4-1 FY 2018 Status of Collaboration with Overseas Satellites

- If satellite and partner institutions have been established, fill in required items of the form below.

### 1. Satellites and partner institutions

- List the satellite and partner institutions in the table below (including the domestic satellite institutes).  
- Indicate newly added and deleted institutions in the "Notes" column.

#### <Satellite institutions>

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

#### < Partner institutions>

Institution name	Principal Investigator(s), if any	Notes
Bandung Institute of Technology, Indonesia		
California Air Resources Board (CARB), USA		
Colorado School of Mines, USA		
Department of Energy (Office of Energy Efficiency and Renewable Energy), USA		
Helmholtz Institute Forschungszentrum Juelich, Germany		
Imperial College London, UK	John Kilner	
Massachusetts Institute of Technology, USA	Harry Tuller	
Norwegian University of Science and Technology (NTNU), Norway		
Paul Scherrer Institute (PSI), Switzerland	Thomas Lippert	
RMIT (Royal Melbourne Institute of Technology) University		New
Southwest Research Institute, USA	Brian Somerday	
Tsinghua University, China	Xing Zhang	
Universiti Teknologi Malaysia, Malaysia		
University of Bergen, Norway		
University of California, Berkeley, USA		
University of California, Irvine (National Fuel Cell Research Center), USA		
University of Göttingen, Germany	Reiner Kirchheim	
University of Edinburgh, UK		
University of New South Wales, Australia		
University of Notre Dame, USA,	Kenneth Christensen	
University of Oxford, UK		
University of Texas at Austin, USA		
University of Thessaly, Greece		
University of Wisconsin-Madison, USA	Ian Robertson	

- If overseas satellite institutions have been established, fill in required items on the form below. If overseas satellite institutions have not been established, it is not necessary to complete the form.

## 2. Coauthored Papers

- List the refereed papers published in FY 2018 that were coauthored between the center's researcher(s) in domestic institution(s) (include satellite institutions) and overseas satellite institution(s). List them by overseas satellite institution in the below blocks.
- Transcribe data in same format as in Appendix 1-4. Italicize the names of authors affiliated with overseas satellite institutions.
- For reference write the Appendix 1-4 item number in parentheses after the item number in the blocks below. Let it free, if the paper is published in between Jan.-Mar. 2019 and not described in Appendix 1-4.

### Overseas Satellite: University of Illinois at Urbana-Champaign, USA (Total: 10 papers)

- (116) Ida, S; Sato, K; Nagata, T; Hagiwara, H; Watanabe, M; Kim, N; Shiota, Y; Koinuma, M; Takenaka, S; Sakai, T; *Ertekin, E*; Ishihara, T (2018), A Cocatalyst that Stabilizes a Hydride Intermediate during Photocatalytic Hydrogen Evolution over a Rhodium-Doped TiO<sub>2</sub> Nanosheet, *Angew. Chem.-Int. Edit.*, 57 (29), 9073-9077.
- (133) Nygren, KE; Wang, S; Bertsch, KM; Bei, HB; Nagao, A; *Robertson, IM* (2018), Hydrogen embrittlement of the equi-molar FeNiCoCr alloy, *Acta Mater.*, 157, 218-227.
- (155) *Kearney, K*; Seo, G; Matsushima, T; Adachi, C; *Ertekin, E*; *Rockett, A* (2018), Computational Analysis of the Interplay between Deep Level Traps and Perovskite Solar Cell Efficiency, *J. Am. Chem. Soc.*, 140 (46), 15655-15660.
- (191) *Hosseini, ZS*; *Dadfarnia, M*; Somerday, BP; Sofronis, P; Ritchie, RO (2018), On the theoretical modeling of fatigue crack growth, *J. Mech. Phys. Solids*, 121, 341-362.
- (246) Kitamura, K; Nishizawa, O; *Christensen, KT*; Ito, T; Finley, RJ (2018), Seismic and strain detection of heterogeneous spatial distribution of CO<sub>2</sub> in high-permeable sandstone, *Int. J. Greenh. Gas Control*, 72, 65-73.
- Martin, ML; *Dadfarnia, M*; Nagao, A; Wang, S; Sofronis, P (2019), Enumeration of the hydrogen-enhanced localized plasticity mechanism for hydrogen embrittlement in structural materials, *Acta Mater.*, 165, 734-750.
- Harrington, GF; Sun, LX; Yildiz, B; Sasaki, K; *Perry, NH*; Tuller, HL (2019), The interplay and impact of strain and defect association on the conductivity of rare-earth substituted ceria, *Acta Mater.*, 166, 447-458.
- Chen, T; Harrington, GF; Masood, J; Sasaki, K; *Perry, NH* (2019), Emergence of Rapid Oxygen Surface Exchange Kinetics during in Situ Crystallization of Mixed Conducting Thin Film Oxides, *ACS Appl. Mater. Interfaces*, 11 (9), 9102-9116.
- Dadfarnia M.*, Sofronis P., Brouwer J., Sosa S. (2019), Assessment of resistance to fatigue crack growth of natural gas line pipe steels carrying gas mixed with hydrogen, *International Journal of Hydrogen Energy*.
- Wang S., Nygren K.E., Nagao A., Sofronis P., *Robertson I.M.* (2019), On the failure of surface damage to assess the hydrogen-enhanced deformation ahead of crack tip in a cyclically loaded austenitic stainless steel, *Scripta Materialia*, 166, 102-106.

## 3. Status of Researcher Exchanges

- Using the below tables, indicate the number and length of researcher exchanges in FY 2018. Enter by institution and length of exchange.
- Write the number of principal investigator visits in the top of each space and the number of other researchers in the bottom.

### Overseas Satellite 1: University of Illinois at Urbana-Champaign, USA

<To satellite>

	Under 1 week	From 1 week to 1 month	From 1 month to 3 months	3 months or longer	Total
FY2018	2	0	0	0	2
	1	1	0	2	4

&lt;From satellite&gt;

	Under 1 week	From 1 week to 1 month	From 1 month to 3 months	3 months or longer	Total
FY2018	1	0	0	0	1
	1	4	0	0	5



## Appendix 4-2 FY 2018 Visit Records of Researchers from Abroad

\* If researchers have visited/ stayed at the Center, provide information on them in the below table.

**Total: 42**

	Name	Age	Affiliation (Position title, department, organization)	Academic degree, specialty	Record of research activities (Awards record, etc.)	Time, duration	Summary of activities during stay at center (e.g., participation as principal investigator; short-term stay for joint research; participation in symposium)
1	Kim Schumacher		Postdoctoral Research Associate, Smith School of Enterprise and the Environment, University of Oxford	Ph.D., Environmental Sciences	<ul style="list-style-type: none"> <li>Selected Publication: Schumacher, K. (2019) Approval procedures for large-scale renewable energy installations: comparison of national legal frameworks in Japan, New Zealand, the EU and the US. Energy Policy, 129: 139-152.</li> </ul>	April 5, 2018	Participation in I <sup>2</sup> CNER Laboratory Tour
2	Yves Brechet	57	High Commissioner, CEA (The French Alternative Energies and Atomic Energy Commission)	Ph.D., Materials Science	<ul style="list-style-type: none"> <li>Chevalier de la legion d'honneur (2010)</li> <li>Max Planck Lecture, Germany (2009)</li> <li>Silver medal CNRS (2009)</li> <li>D.K.McDonald Lecture, Canada (2007)</li> </ul>	April 24, 2018	Participation in I <sup>2</sup> CNER Laboratory Tour
3	Laurent Antoni		Hydrogen and Fuel Cells Programme Manager, CEA Liten	Ph.D., Electrochemistry and Surface Sciences	<ul style="list-style-type: none"> <li>President of N.ERGHY European Association on Hydrogen and Fuel Cells gathering more than 65 and research organizations.</li> <li>Member of the Governing Board of the JU FCH2, European Joint technology initiative on H2FC</li> <li>French representative on International governmental agreements at IPHE (International Partnership on Hydrogen Economy) and executive committee member of AFC (Advanced Fuel Cells) of International Energy Agency (IEA)</li> </ul>	April 24, 2018	Participation in I <sup>2</sup> CNER Laboratory Tour
4	Bernard Niclot		Technical Director, International Automobile Federation	Ph.D., Applied Mathematics	<ul style="list-style-type: none"> <li>Joined the FIA (2010-)</li> <li>Head of Innovation Chassis, Transmission and Safety at PSA Peugeot Citroën (2003)</li> <li>General Director of Vallourec Composants Automobiles (VCA), a producer of automotive components (1998)</li> </ul>	April 24, 2018	Participation in I <sup>2</sup> CNER Laboratory Tour

5	Kenneth T. Christensen	45	Prof., Department Chair, Aerospace and Mechanical Engineering, University of Notre Dame, USA	Ph.D., Theoretical and applied mechanics specializing in experimental fluid mechanics	<ul style="list-style-type: none"> <li>• Dean's Award for Excellence in Research from the College of Engineering, UIUC (2012)</li> <li>• François Frenkiel Award for Fluid Mechanics from APS-DFD (2011)</li> <li>• NSF CAREER Award (2007)</li> </ul>	April 30, 2018-May 3, 2018	Joint Research
6	Thirumalai S Neeraj		Researcher, ExxonMobil Research & Engineering	Ph.D., Materials	<ul style="list-style-type: none"> <li>• Selected Publication: Hydrogen embrittlement of ferritic steels: Observations on deformation microstructure, nanoscale dimples and failure by nanovoiding, Acta Materialia, Volume 60, Issues 13–14, August 2012, Pages 5160-5171</li> </ul>	June 7, 2018	Participation in I <sup>2</sup> CNER Laboratory Tour
7	James Stubbins		Prof., Department Head of Nuclear, Plasma, and Radiological Engineering, University of Illinois, USA	Ph.D., Materials Science	<ul style="list-style-type: none"> <li>• Donald Biggar Willett Professor (2013)</li> <li>• Outstanding Achievement Award, Materials Science and Technology Division (2012)</li> <li>• Engineering Council Award for Excellence in Advising (2011)</li> <li>• Glenn Murphy Award (2010)</li> <li>• International Scientist of the Year (2004)</li> </ul>	<p>(1) June 25, 2018-June 30, 2018</p> <p>(2) January 26, 2019-February 3, 2019</p>	<p>(1) Joint Research</p> <p>(2) Joint Research and Participation in I2CNER Annual Symposium and International Workshops as Satellite Faculty</p>
8	Nenad Miljkovic		Prof., The Institut für Metallphysik, University of Göttingen, Germany	Ph.D., Hydrogen in Metals, Thermodynamics of alloys, Interstitial solution and diffusion in glasses	<ul style="list-style-type: none"> <li>• ASME ICNMM Outstanding Early Career Award</li> <li>• ASME Pi Tau Sigma Gold Medal, 2018 (2018)</li> <li>• National Academy of Sciences Arab-American Frontiers Fellowship, 2018 (2018)</li> <li>• United Kingdom Royal Society of Engineering Distinguished Visiting Fellow, 2017 (2017)</li> <li>• ONR Young Investigator Award, 2017 (2017)</li> <li>• NSF CAREER Award, 2016 (2016)</li> </ul>	June 27, 2018-July 2, 2018	Joint Research and Participation in Site Visit as Satellite Faculty
9	Khellil Sefiane		Prof., Head of the Institute for Materials and Processes, School of Engineering, University of Edinburgh, UK	Ph.D., Chemical Engineering	<ul style="list-style-type: none"> <li>• Elected member of the UK Heat transfer Committee</li> <li>• Elected member of the Scientific Council of the International Centre for Heat and Mass Transfer (2010)</li> <li>• Elected UK representative on EURO THERM committee (2011)</li> <li>• Fellow of the Royal Society of Chemistry, FRSC, Cambridge, UK (2011).</li> <li>• Exxon-Mobil fellow, awarded (in 2000) by the Royal Academy of Engineering (RAEng), London, UK</li> </ul>	<p>(1) June 25, 2018-July 7, 2018</p> <p>(2) September 23, 2018-October 6, 2018</p> <p>(3) February 15, 2019, February 23, 2019</p>	Joint Research

10	Nicholas Kotov	52	Professor, Department of Chemical Engineering, University of Michigan, USA	Ph.D., Chemical and Reaction Kinetics	<ul style="list-style-type: none"> <li>• 2017 Colloid Chemistry Award (American Chemical Society, ACS)</li> <li>• 2016 UNESCO Medal for Development of Nanoscience and Nanotechnologies</li> <li>• 2014 Fellow of the Materials Research Society (MRS)</li> <li>• 2013 Fellow of the Royal Society of Chemistry (RSC)</li> <li>• 2011 Top 100 Materials Scientists in 2000-2010 (Thomson Reuter)</li> <li>• 2011 Top 100 Chemists in 2000-2010 (Thomson Reuter)</li> </ul>	August 2, 2018	I <sup>2</sup> CNER Seminar Series Presentation
11	Ashok Kumar Nanjundan		Research Fellow, The University of Queensland	Ph.D., Engineering	<ul style="list-style-type: none"> <li>• Selected Publication: Biomass derived carbon nanoparticle as anodes for high performance sodium and lithium ion batteries, Nano Energy, 26 346-352.</li> </ul>	September 7, 2018	Participation in I <sup>2</sup> CNER Laboratory Tour
12	John Kilner	72	Prof., Department of Materials, Imperial College, London, UK	Ph.D., Materials for solid oxide fuel cells and electrolysers	<ul style="list-style-type: none"> <li>• Daiwa Adrian Prize (2016)</li> <li>• Imperial College Medal (2016)</li> <li>• Christian Friedrich Schonbein Contribution to Science Medal (2014)</li> <li>• Platinum Medal, Institute of Materials Minerals and Mining (2012)</li> <li>• Somiya Award, International Union of Materials Research Societies (2012)</li> </ul>	(1) October 1, 2018- October 12, 2018  (2) January 22, 2019-February 4, 2019	(1) Joint Research  (2) Joint Research and Participation in I <sup>2</sup> CNER Annual Symposium, International Workshops, and the Electrochemical Energy Conversion Division retreat as Principal Investigator
13	Pailin Ngaotrakanwivat		Assistant Professor, Burapha University, Thailand	Ph.D., Applied Chemistry	<ul style="list-style-type: none"> <li>• 2012 EMA2- Erasmus Mundus programme, Italy</li> <li>• 2008 Short-term Visit Program to Japan Granted by AUN/SEED-Net, JICA</li> <li>• 2006 Asian Youth Fellowship (AYF) Returnees Network Support Program</li> <li>• 2001-2003 Scholarship Grantee of Asian Youth Fellowship (Japan Foundation)</li> </ul>	October 10, 2018	I <sup>2</sup> CNER Seminar Series Presentation
14	Yang Tian	49	Visiting professor, East China Normal University, China	Ph.D., Electronic Chemistry	<ul style="list-style-type: none"> <li>• 2013 The Distinguished Lectureship Award (<i>Chemical Society of Japan</i>)</li> <li>• 2011 The First Prize in Science and Technology, China Association for Instrumental Analysis.</li> </ul>	October 10, 2018	I <sup>2</sup> CNER Seminar Series Presentation
15	Espen Steinseth Hamborg		Principal Researcher, Equinor	Ph.D., Chemical Engineering	<ul style="list-style-type: none"> <li>• Selected Patent: Method for Enhancing the Performance of Processes for the Removal of Acid Gas, Publication number: 20120090466</li> </ul>	October 23, 2018	Participation in I <sup>2</sup> CNER Laboratory Tour

16	John Andrews		Professor, RMIT University, Australia	Ph.D., Engineering	<ul style="list-style-type: none"> <li>Special Recognition award at the Institution of Engineers Australia Awards Ceremony, 2011</li> <li>RMIT Research Award in 2007</li> <li>National Energy Award from the Commonwealth Government in 1997</li> <li>A Business/Higher Education Round Table Award for Outstanding Achievement in Collaborative R&amp;D in 1998</li> </ul>	November 7, 2018	I <sup>2</sup> CNER Seminar Series Presentation
17	Reiner Kirchheim	75	Prof., The Institut für Metallphysik, University of Göttingen, Germany	Ph.D., Hydrogen in Metals, Thermodynamics of alloys, Interstitial solution and diffusion in glasses	<ul style="list-style-type: none"> <li>Foreign Affiliate of the United States National Academy of Engineering (2017)</li> <li>Leibniz-Medaille of the IFW Dresden (2013)</li> <li>Hydrogen &amp; Energy Award, H&amp;E-Symposium (2010)</li> <li>Lee Hsun Lecture Award, IMR Shenyang, Chinese Academy of Sciences (2007)</li> <li>Heyn-Denk Münze (highest award of the German Materials Society, DGM) (2004)</li> </ul>	December 1, 2018- December 8, 2018	Joint Research (Principal Investigator)
18	Luca Brandt		Professor, KTH Royal Institute of Technology, Sweden	Ph.D., Fluid Mechanics	<ul style="list-style-type: none"> <li>2013 ERC Consolidator Grant TRITOS, from April 2014</li> <li>2009 Ranked second for Chair of Applied Mechanics, University of Uppsala.</li> <li>2008 The Senior Researcher Position (Rådsforskartjänt) from the Swedish Research Council (VR) in Mechanics.</li> <li>2006 The Göran Gustafsson Fellowship for young researchers</li> </ul>	December 5, 2018	I <sup>2</sup> CNER Seminar Series Presentation
19	Janusz Szmyd	65	Department Head, Dept. of Fundamental Research in Energy Engineering, AGH University of Science and Technology, Poland	Ph.D., Energy Engineering	<ul style="list-style-type: none"> <li>2015 Doctor Honoris Causa, Shibaura Institute of Technology, Tokyo, Japan</li> <li>2011 GCOE (Global 21st Century Center of Excellence) lectureship, Japan</li> <li>2011 President of AGH University Awards</li> <li>2003 "Złoty krzyż zasługi" - Medal given by President of Poland</li> </ul>	December 7, 2018	I <sup>2</sup> CNER Seminar Series Presentation
20	Harry L. Tuller	73	Prof., Department of Materials Science and Engineering, Massachusetts Institute of Technology, USA	Engr. Sc. D., Functional electroceramic materials	<ul style="list-style-type: none"> <li>Distinguished Life Membership in American Ceramic Society (2016)</li> <li>Senior Member, IEEE (2016)</li> <li>President, International Society of Solid State Ionics (2015)</li> <li>Helmholtz International Fellow Award (2012)</li> <li>Somiya Award of the International Union of Materials Research Society (2012)</li> </ul>	(1) January 22, 2019- February 5, 2019  (2) March 6, 2019- March 17, 2019	(1) Joint Research and Participation in I <sup>2</sup> CNER Annual Symposium, International Workshops, and the Electrochemical Energy Conversion Division retreat as Principal Investigator  (2) Joint Research
21	Xing Zhang	57	Prof., Department of Engineering Mechanics, Tsinghua University, China	Ph.D., Thermal Science	<ul style="list-style-type: none"> <li>Significant Contribution Awards from the 10th Asian Thermophysical Properties Conference (2013)</li> <li>National Nature Science Award (Second Class) from the State Council of the People's Republic of China (2011)</li> <li>Best Paper Award from the Heat Transfer Society of Japan (2008)</li> </ul>	January 24, 2019- February 2, 2019	Joint Research (Principal Investigator)

22	Thomas Lippert	56	Prof., Department of Chemistry and Applied Biosciences, Laboratory of Inorganic Chemistry, Swiss Federal Institute of Technology Zurich, and Paul Scherrer Institut, Thin Films & Interfaces Group, Villigen-PSI, Switzerland	Dr. of Science, Physical Chemistry	<ul style="list-style-type: none"> <li>• President of the Senate of the European-Materials Research Society (E-MRS) (from 1/2016 to 2/2017)</li> <li>• President of the European-Materials Research Society (E-MRS) (from 1/2014 to 12/2015)</li> <li>• Dr. honoris causa, University of Bucharest, Romani (2014)</li> <li>• Vice-President of the European-Materials Research Society (E-MRS) (from 6/2011 to 12/2013)</li> <li>• Member of the E-MRS Executive Committee (from 2008)</li> </ul>	January 27, 2019- February 9, 2019	Joint Research and Participation in I2CNER Annual Symposium, International Workshops, and the Molecular Photoconversion Devices Division retreat as Principal Investigator
23	Paul Kenis		Prof., Department Head of Chemical and Biomolecular Engineering, University of Illinois, USA	Ph.D., Chemistry	<ul style="list-style-type: none"> <li>• University Scholar, University of Illinois, UC (2011)</li> <li>• Beckman Fellow, Center for Advanced Study (2007-2008)</li> <li>• CAREER Award, National Science Foundation (2006)</li> <li>• Xerox Award for Faculty Research, College of Engineering, University of Illinois, UC (2006)</li> </ul>	January 27, 2019- February 2, 2019	Joint Research and Participation in I2CNER Annual Symposium and International Workshops as Satellite Faculty
24	Brian P. Somerday	50	Dr., Southwest Research Institute, USA	Ph.D., Materials Science and Engineering	<ul style="list-style-type: none"> <li>• DOE Hydrogen and Fuel Cell Program Achievement Award (2014)</li> <li>• Best Poster Award, ASME 12th Fuel Cell Science, Engineering, and Technology Conference (2014)</li> </ul>	January 28, 2019- February 3, 2019	Joint Research and Participation in I2CNER Annual Symposium, International Workshops, and the Hydrogen Materials Compatibility Division retreat as Principal Investigator
25	Anutosh Chakraborty	45	Associate Professor, Assistant Chair (Graduate Studies), Nanyang Technological University, Singapore	Ph.D., Mechanical Engineering	<ul style="list-style-type: none"> <li>• Best Paper Award, IV International Symposium on Innovative Materials for Processes in Energy Systems, October 23 – 26, Taormina, Sicily, Italy, 2016.</li> <li>• Research Award: IES Prestigious Engineering Achievement Awards 2009 (Absorption desalination development).</li> </ul>	January 30, 2019	HYDROGENIUS & I <sup>2</sup> CNER Joint Research Symposium
26	Kelly Elizabeth Nygren	29	Postdoctoral Research Associate, Cornell High Energy Synchrotron Source, Cornell University	Ph.D., Materials Science and Engineering	<ul style="list-style-type: none"> <li>• Selected Publication: K. E. Nygren , K. M. Bertsch, S. Wang, H. Bei, A. Nagao, I. M. Robertson, "Hydrogen embrittlement in compositionally complex FeNiCoCrMn FCC solid solution alloy." Current Opinion in Solid State and Materials Science, Vol 22 Issue 1 (2018) 1-7</li> </ul>	January 30, 2019	HYDROGENIUS & I <sup>2</sup> CNER Joint Research Symposium
27	Geert Verbong	64	Professor, Eindhoven University of Technology (TU/e) Eindhoven, the Netherlands	Ph.D., History of Technology	<ul style="list-style-type: none"> <li>• Selected publication: Manders, T. N., Wieczorek, A. J. &amp; Verbong, G. P. J (2018), Understanding smart mobility experiments in the Dutch automobility system: who is involved and what do they promise?, Futures. 96, 90-103.</li> </ul>	January 31, 2019	I <sup>2</sup> CNER Annual Symposium

28	Jill Engel-Cox	52	Director, Joint Institute for Strategic Energy Analysis (JISEA) at the U.S. National Renewable Energy Laboratory (NREL)	Ph.D., Philosophy in Environmental Science	<ul style="list-style-type: none"> <li>• Excellence in Teaching Award, Johns Hopkins University, Whiting School of Engineering (2015)</li> <li>• Women's History Month Honoree, Battelle (2013)</li> <li>• Pollution Prevention Award, U.S. Department of Energy (2000,1998)</li> <li>• Key Contributor Award, Pacific Northwest National Laboratory (1999)</li> </ul>	January 31, 2019	I <sup>2</sup> CNER Annual Symposium
29	Michael A. Celia	62	Theodora Shelton Pitney Professor of Environmental Studies, Princeton University  Director, Princeton Environmental Institute, Princeton University	Ph.D., Civil Engineering	<ul style="list-style-type: none"> <li>• Honorary Doctoral Degree, University of Stuttgart (2018)</li> <li>• Elected to the US National Academy of Engineering (2016)</li> <li>• 2014 Honorary Lifetime Membership Award, International Society of Porous Media, presented (2014)</li> <li>• Elected Fellow of the American Association for the Advancement of Science (AAAS) (2008)</li> <li>• One of many IPCC contributing authors who share in the 2007 Nobel-Peace Prize (Contributing author to IPCC Working Group III Special Report on Carbon Dioxide Capture and Storage).</li> </ul>	January 31, 2019	I <sup>2</sup> CNER Annual Symposium
30	David Michael Reiner	51	University Senior Lecturer in Technology Policy, University of Cambridge  Assistant Director, Energy Policy Research Group, University of Cambridge  Assistant Director (Systems & Policy), UK Carbon Capture and Storage Research Centre	Ph.D., Political Science	<ul style="list-style-type: none"> <li>• Selected Publications:</li> </ul> <p>D Guan et al (2018) Structural decline in China's CO<sub>2</sub> emissions through transitions in industry and energy systems, Nature Geoscience 11, 551–555 (2018)</p> <p>M Honegger, D Reiner, (2018) The political economy of negative emissions technologies: consequences for international policy design, Climate Policy 18 (3), 306-321</p> <p>DMG Newbery, DM Reiner, and RA Ritz, When is a carbon price floor desirable? Energy Journal (In press).</p>	January 31, 2019	I <sup>2</sup> CNER Annual Symposium

31	Lane W. Martin	36	Professor & Associate Chair, Materials Science and Engineering, University of California, Berkeley  Faculty Scientist, Materials Sciences Division, Lawrence Berkeley National Laboratory	Ph.D., Materials Science and Engineering	<ul style="list-style-type: none"> <li>• 2018 Highly Cited Researcher – Ranked in the top 1% by citations for field and publication year in Web of Science (Nov. 2018)</li> <li>• 2017 Excellence in Laboratory Safety Grand Prize, UC Berkeley Environmental, Health, and Safety (EHS) (Feb. 2018)</li> <li>• Robert L. Coble Award for Young Scholars, American Ceramic Society (Oct. 2016)</li> <li>• American Association for Crystal Growth (AACG) Young Author Award (Aug. 2015)</li> <li>• Presidential Early Career Award for Scientists and Engineers, President of the United States of America (Dec.</li> </ul>	February 1, 2019	I <sup>2</sup> CNER International Workshop
32	Romain Chassagne	38	Research Fellow, Infrastructure and Society Heriot-Watt University, Edinburgh, Scotland - UK	Ph.D., Applied Mathematics	<ul style="list-style-type: none"> <li>• Sasakawa Foundation award, 2016.</li> <li>• Sasakawa Foundation award, 2015.</li> <li>• Selected Publication: ZHANG Q., CHASSAGNE R. and MACBETH C., European Conference on the Mathematics of Oil Recovery, Seismic History Matching Uncertainty With Weighted Objective Functions, 2018.</li> </ul>	February 1, 2019	I <sup>2</sup> CNER International Workshop
33	Daniele Pergolesi	48	Senior Scientist, Paul Scherrer Institute, Switzerland	Ph.D., Materials Science	<ul style="list-style-type: none"> <li>• Selected Publication: A. Fluri, D. Pergolesi, A. Wokaun, T. Lippert, Stress evolution in oxide epitaxy. (2018) Phys. Rev. B, 97, 125412</li> </ul>	February 1, 2019	I <sup>2</sup> CNER International Workshop
34	Jihui Jia		Assistant Professor, China University of Petroleum-Beijing, China	Ph.D., Earth Resources and Environmental Engineering	<ul style="list-style-type: none"> <li>• Selected Publication: Chanmaly Chhun, Arata Kioka, Jihui Jia, Tsuji Takeshi, 2018, Characterization of hydrate and gas reservoirs in plate convergent margin by applying rock physics to high resolution seismic velocity model. Marine and Petroleum Geology, 92, 719-732.</li> </ul>	February 1, 2019	I <sup>2</sup> CNER International Workshop
35	Yuliy Baryshnikov		Professor, University of Illinois at Urbana-Champaign, USA	Ph.D., Applied Mathematics	<ul style="list-style-type: none"> <li>• Alexander von Humboldt Fellow (1992)</li> <li>• Lady Davis Professorship, Technion (2003)</li> <li>• Selected Publication: Arnold, Maxim; Baryshnikov, Yuliy; LaValle, Steven M; Convex hull asymptotic shape evolution Algorithmic Foundations of Robotics X 349-364 2013 Springer Berlin Heidelberg</li> </ul>	February 1, 2019	I <sup>2</sup> CNER International Workshop
36	Mohamed Mahmoud Nasef		Professor, Chemical Engineering Department Universiti Teknologi Petronas, Malaysia	Ph.D., Chemical Engineering	<ul style="list-style-type: none"> <li>• Represented Malaysia in Coordinated Research Project (CRP) organized by IAEA in period 2007-2010.</li> <li>• Active member of European Membrane Society, Electrochemical Society and Materials Research Society and Asian Polymer Federation</li> </ul>	February 12, 2019	I <sup>2</sup> CNER Seminar Series Presentation

37	Carsten Cremers		Researcher (Group Leader), Fraunhofer Institute for Chemical Technology, Germany	Ph.D., Theoretical Chemistry	<ul style="list-style-type: none"> <li>Selected Publication: Functionalization of multi-walled carbon nanotubes with indazole, Electrochimica Acta, Volume 298, 1 March 2019, Pages 884-892.</li> </ul>	February 25, 2019	Participation in I <sup>2</sup> CNER Laboratory Tour
38	Kwan Young Lee		Professor, Korea University, South Korea	Ph.D., Chemistry	<ul style="list-style-type: none"> <li>Selected Publication: Three-dimensional crystal structure of novel aluminophosphate PST-5 solved using a powder charge flipping method, RSC Advances 7(61):38631-38638.</li> </ul>	February 27, 2019	Participation in I <sup>2</sup> CNER Laboratory Tour
39	Sea-fue Wang		President, National Taipei Institute of Technology, Taiwan	Ph.D., Materials Science	<ul style="list-style-type: none"> <li>Selected Publication: Facile Synthesis of Copper Sulfide Decorated Reduced Graphene Oxide Nanocomposite for High Sensitive Detection of Toxic Antibiotic in Milk, Ultrasonic Sonochemistry, December 2018.</li> </ul>	March 1, 2019	Participation in I <sup>2</sup> CNER Laboratory Tour
40	Thomas Chung-Kuang Yang		Vice president, National Taipei Institute of Technology, Taiwan	Ph.D., Materials	<ul style="list-style-type: none"> <li>Selected Publication: Wei-Han Tao, Thomas C.-K. Yang*, Li-Kai Chang and Tsair-Wang Chung, "Modeling the effects of moistures on the vapor phase adsorption of organic compounds by zeolite 13X", in press, J. of Environmental Engineering, 2003 [SCI] (1999 Impact Factor:1.373 )</li> </ul>	March 1, 2019	Participation in I <sup>2</sup> CNER Laboratory Tour
41	Steven S.C. Chuang		Professor, Department of Polymer Science, The University of Akron, USA	Ph.D., Chemical Engineering	<ul style="list-style-type: none"> <li>2007 Outstanding Researcher Award of the College of Engineering at the University of Akron.</li> <li>2006 Distinguished Alumni Award, National Taipei University of Technology, Taipei, Taiwan.</li> <li>1998 Louis A. Hill Award for the outstanding achievement. College of Engineering at the University of Akron.</li> </ul>	March 1, 2019	Participation in I <sup>2</sup> CNER Laboratory Tour
42	Jian Chen	30	Assistant Research Fellow, Peking University, China	Ph.D., Material Science and Engineering	<ul style="list-style-type: none"> <li>Research Administrator, Assistant Research Fellow, Division for Institutional Affairs, Office of Scientific Research, Peking University (2017.07-now)</li> <li>Research Administrator, Division for Science and Technology, Department of Science and Education, Ministry of Finance (2017.07-2018.03)</li> </ul>	March 28, 2019	Participation in I <sup>2</sup> CNER Laboratory Tour



### Appendix4-3 Postdoctoral Positions through Open International Solicitations

\* In the column of number of applications and number of selection, put the total number (upper), the number and percentage of overseas researchers in the < > brackets (lower).

<b>Fiscal year</b>	<b>number of applications</b>	<b>number of selection</b>
<b>FY 2010</b>	75	1
	< 71, 95%>	< 0, 0%>
<b>FY 2011</b>	95	2
	< 62, 65%>	< 2, 100%>
<b>FY 2012</b>	13	3
	< 12, 92%>	< 2, 67%>
<b>FY 2013</b>	12	2
	< 11, 92%>	< 1, 50%>
<b>FY 2014</b>	16	2
	< 15, 93%>	< 2, 100%>
<b>FY 2015</b>	71	2
	< 64, 90%>	< 2, 100%>
<b>FY 2016</b>	0	0
	< 0, 0%>	< 0, 0%>
<b>FY 2017</b>	60	2
	<54, 90%>	< 2, 100%>
<b>FY 2018</b>	0	0
	<0, 0%>	< 0, 0%>

## Appendix 4-4 Status of Employment of Postdoctoral Researchers

\* Prepare the information below during the period from the start of the center through March 2019.

\* 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 affiliation, position title (Country)
Apr. 1, 2011-May. 31, 2012	PhD Student, Kyoto University (Japan)	Asstant Professor, Nagoya University (Japan)
Apr. 1, 2013-Mar. 31, 2014	Postdoc, Hokkaido University (Japan)	Asstant 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)	Asstant 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)	Asstant Professor, I2CNER (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 <sup>2</sup> CNER )
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)	Asstant Professor, Okayama University (Japan)
May. 1, 2015-Mar. 31, 2018	Researcher, Asahi Intecc (Japan)	Postdoc, Kyushu University (Japan)
Apr. 1, 2016-Mar. 31, 2017	PhD Student, Kyushu University (Japan)	ADECA CORPORATION (Japan)
Nov. 1, 2016-Mar. 31, 2018	Postdoc, Kyushu University (Japan)	Tanaka Kikinzoku Kogyo K.K, (Japan)
Apr. 1, 2017-Mar. 31, 2018	Postdoc, Kyushu University (Japan)	Postdoc, Kyushu University (Japan)
Apr. 1, 2017-Sep. 30, 2018	Postdoc, Kyushu University (Japan)	Assistant Professor, Fukuoka University (Japan)
May. 1, 2017-Present	Researcher, I-Cems, Kyoto Universiy (Japan)	(Currently at I <sup>2</sup> CNER )
Apr. 1, 2018-Present	Postdoc, Kyushu University (Japan)	(Currently at I <sup>2</sup> CNER )
Jul. 16, 2018-Present	Postdoc, Kyushu University (Japan)	(Currently at I <sup>2</sup> CNER )

## Overseas Postdocs

Period of project participation	Previous affiliation, position title (Country)	Next affiliation, position title (Country)	Nationality
Jan. 16, 2012-Nov. 14, 2017	Postdoc, Imperial College London (UK)	TBD	UK
Apr. 1, 2012-Mar. 31, 2018	Postdoc, Kyushu University (Japan)	Associate Professor, Yamaguchi University, Japan	French
Sep. 1, 2012-Dec. 31, 2017	Postdoc, Northwestern University (USA)	Assistant Professor, University of Illinois at Urbana-Champaign (USA)	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 University (Japan)	Professor, Huazhong 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 <sup>2</sup> CNER (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-Nov. 30, 2018	PhD Student, University of Edinburgh (Scotland)	Lecturer, University of Edinburgh (Scotland)	Spanish
Oct. 1, 2013-Present	JSPS Postdoc, Kyushu University (Japan)	(Currently at I <sup>2</sup> CNER )	Cameroonian
Nov. 1, 2013-Dec. 30, 2013	Lecturer, Sriwijaya University (Indonesia)	Researcher, Sriwijaya University (Indonesia)	Indonesian
Jan. 1, 2014-Feb. 28, 2019	Postdoc, University of Kitakyushu (Japan)	Assistant Professor, I <sup>2</sup> CNER (Japan)	Ukrainian
Feb. 1, 2014-Oct. 30, 2018	Postdoc, Kyushu University (Japan)	Assistant Professor, I <sup>2</sup> CNER (Japan)	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, Pukyong 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 <sup>2</sup> CNER )	Indian
Apr. 1, 2015-Mar. 31, 2018	PhD Student, Kyushu University (Japan)	TBD	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 <sup>2</sup> CNER )	Romanian
Jan. 16, 2016-Dec. 22, 2017	PhD Student, Jawaharlal Nehru Centre for Advanced Scientific Research (India)	Research Fellow, University of Warwick (UK)	Indian
Mar. 1, 2016-Sep. 30, 2016	Postdoc, Kyushu University (Japan)	Assistant Professor, Nanjing Tech University (China)	Chinese
Mar. 1, 2016-Oct. 10, 2017	Researcher, Sebelas Maret Univesity (Indonnesia)	Assistant Professor, Sebelas Maret University (Indonesia)	Indonesian
Apr. 1, 2016-May. 31, 2017	PhD Student, Kyoto Institute of Technology, (Japan)	TBD	Thai
May 1, 2016-Jul. 14, 2017	Postdoc, Kyushu University (Japan)	Research Professor, Ningbo Institute of Industrial Technology, (China)	Chinese

May 16, 2016-Oct. 11, 2017	PhD Student, Indian Institute of Science, Bangalore (India)	Postdoc, Indian Institute of Technology Kharagpur, (India)	Indian
May 16, 2016-Nov. 8, 2018	PhD Student, Imperial College London (UK)	Postdoc, University of Bath (UK)	Chinese
Jun. 1, 2016-Aug. 31, 2017	Postdoc, Kyushu University (Japan)	Assistant Professor, China University of Petroleum (China)	Chinese
Sep. 1, 2016-Nov. 30, 2018	Assistant Professor, Jagannath University (Bangladesh)	Associate Professor, Jagannath University (Bangladesh)	Bangladeshi
Oct. 1, 2016-Mar. 31, 2018	Research Assistant Professor, Hangyang University (Korea)	Assistant Professor, Hokkaido University (Japan)	Chinese
Nov. 1, 2016-Mar. 31, 2018	Postdoc, Kyushu University (Japan)	Yanmar Co. Ltd., Japan (Japan)	German
Nov. 16, 2016-Mar. 31, 2019	Postdoc, Norwegian University of Science and Technology (Norway)	Postdoc, Universitetet i Oslo (Norway)	French
Dec. 1, 2016-Aug. 9, 2018	Postdoc, Kyushu University (Japan)	Lecturer, University of East Anglia in Norwich (UK)	Greece
Dec. 1, 2016-Sep. 30, 2018	Postdoc, Kyushu University (Japan)	Postdoc, Kyushu University (Japan)	Bulgarian
Jan. 1, 2017-Present	Researcher, University of Toronto (Canada)	(Currently at I <sup>2</sup> CNER )	Indian
Jan. 1, 2017-Present	PhD Student, University of Girona (Spain)	(Currently at I <sup>2</sup> CNER )	Spanish
Apr. 1, 2017-Present	Postdoc, Kyushu University (Japan)	(Currently at I <sup>2</sup> CNER )	Thai
May. 1, 2017-Mar. 31, 2018	Researcher, National Central University (Taiwan)	Postdoc, Academia Sinica (Taiwan)	Taiwanese
Jun. 1, 2017-Present	PhD Student, Huazhong University of Science and Technology (China)	(Currently at I <sup>2</sup> CNER )	Chinese
Jun. 1, 2017-Present	Postdoc, Karlsruhe Institute of Technology (Germany)	(Currently at I <sup>2</sup> CNER )	German
Oct. 1, 2017-Present	Research Support Staff, I <sup>2</sup> CNER (Japan)	(Currently at I <sup>2</sup> CNER )	South Korean
Oct. 1, 2017-Present	PhD Student, Daegu Gyeongbuk Institute of Science and Technology (South Korea)	(Currently at I <sup>2</sup> CNER )	Indian
Dec. 1, 2017-Mar. 31, 2018	Postdoc, Kyushu University (Japan)	Postdoc, Kyushu University (Japan)	Swiss
Dec. 1, 2017-Dec. 31, 2018	Postdoc, Kyushu University (Japan)	Research associate, Imperial college (London)	Chinese
Dec. 16, 2017-Present	PhD Student, Tulane University (USA)	(Currently at I <sup>2</sup> CNER )	Chinese
Dec. 16, 2017-Jan. 31, 2019	Postdoc, Sungkyunkwan University (South Korea)	TBD	South Korean
Mar. 1, 2018-Present	Research Associate, Akita University (Japan)	(Currently at I <sup>2</sup> CNER )	Iranian
Apr. 1, 2018-Present	Postdoc, University of Tokyo (Japan)	(Currently at I <sup>2</sup> CNER )	Chinese
May. 16, 2018-Present	Postdoc, National Taiwan University (Taiwan)	(Currently at I <sup>2</sup> CNER )	Indian
Jun. 16, 2018-Present	Lecturer and Researcher, Institute of Technology Bandung (Indonesia)	(Currently at I <sup>2</sup> CNER )	Indonesian

## Appendix4-5 List of the Cooperative Research Agreements with Overseas Institutions

\*Prepare the information below during the period from the beginning of the Center through March 2019.

### 1. Name of Agreement

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

#### Dates of Agreement

(Start) April 27, 2012

(End) April 26, 2015

#### Counterpart of Agreement

The UK QICS Project Consortium

#### Summary of Agreement

The purpose of this MOU is to jointly improve our understanding of the potential impacts of a leak from offshore CO<sub>2</sub> storage on the marine ecosystems. For this purpose, the Japanese Parties will conduct complementary tasks in the Work Packages (WPs) of the Project and the UK Project Consortium will facilitate the involvement of the Japanese Parties in the Project. All Parties will also exchange knowledge and information to achieve the overall aims for the WPs and the Knowledge Exchange in the Project. Each party shall be responsible for all the expenses incurred related to their own research contribution to this collaboration under this MOU.

### 2. Name of Agreement

Visiting Research Agreement

#### Dates of Agreement

(Start) September 25, 2012

(End) December 19, 2012

#### Counterpart of Agreement

VTT Technical Research Centre of Finland

#### Summary of Agreement

The agreement specifies the terms and conditions of the working relationship between the Visiting Researcher from VTT Technical Research Centre of Finland and the Host Organization, the International Institute for Carbon Neutral Energy Research (I<sup>2</sup>CNER). The aim of the visit is to establish a collaborative relationship and introduce the Visiting Researcher to the scientific research work performed by the Host Organization. The Visiting Researcher is willing to carry out research activities as part of the Supervisor's team during his stay at the Host Organization.

### 3. Name of 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 Agreement

(Start) October 1, 2013

(End) September 30, 2017

#### Counterpart of Agreement

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

#### Summary of 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."

**4. Name of 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 Agreement**

(Start) December 31, 2013,

(Renewed) January 15, 2019

(End) January 14, 2024

**Counterpart of Agreement**

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

**Summary of Agreement**

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

**5. Name of Agreement**

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

**Dates of Agreement**

(Start) March 17, 2014

(Renewed) March 17, 2019

(End) March 16, 2024

**Counterpart of Agreement**

The Norwegian University of Science and Technology (NTNU)

**Summary of 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.

**6. Name of Agreement**

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

**Dates of Agreement**

(Start) May 26, 2014

(End) May 25, 2019

**Counterpart of Agreement**

The University of Illinois at Urbana-Champaign, USA

**Summary of Agreement**

The purpose of this university-wide agreement is to develop scientific, academic, and educational cooperation on the basis of equality and reciprocity. This agreement also promotes mutual understanding and helps strengthen the relationship between KU and Illinois in the form of joint research, student exchanges, faculty exchanges and sabbaticals, etc. This agreement is currently in the process of being revised and renewed as part of the “Kyushu-Illinois Strategic Partnership”.

**7. Name of Agreement**

Letter of Understanding

**Dates of Agreement**

January 20, 2015 - Current

**Counterpart of Agreement**

California Air Resources Board (CARB), USA

**Summary of Agreement**

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

**8. Name of Agreement**

Consortium Agreement concerning the project “Direct electrocatalytic conversion of CO<sub>2</sub> into chemical energy carriers in a co-ionic membrane reactor (eCOCO<sub>2</sub>)”

**Dates of Agreement**

Pending

**Counterpart of Agreement**

eCOCO<sub>2</sub> project participants (Parties) such as Agencia Estatal Consejo Superior de Investigaciones Científicas (Spain), University of Oslo (Norway), CoorsTek Membrane Sciences AS (Norway), SINTEF (Norway), Polytechnic University of Valencia (Spain), RWTH Aachen University (Germany), HERA HOLDING, Hábitat, Ecología y Restauración Ambiental, S.L. (Spain), CEMEX Research Group AG (Switzerland), Arcelormittal Belgium NV (Belgium), Shell Global Solutions International B.V., and Xiamen University (China).

**Summary of 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.

## Appendix4-6 Holding International Research Meetings

\* Indicate up to twenty of most representative international research conferences or symposiums held from the start of the center through March 2019 and give the number of participants using the table below.

	Date	Meeting title and Place held	Number of participants
1	February 1, 2011	Kick-Off Symposium Kyushu University, Japan	From domestic institutions: 128 From overseas institutions: 26
2	March 6-7, 2012	I <sup>2</sup> CNER Satellite Kick-Off Symposium University of Illinois at Urbana-Champaign, U.S.	From domestic institutions: 70 From overseas institutions: 30
3	December 7, 2012	I <sup>2</sup> CNER Tokyo Symposium National Center of Sciences (Hitotsubashi Hall etc.), Japan	From domestic institutions: 130 From overseas institutions: 20
4	January 29, 2013	I <sup>2</sup> CNER Annual Symposium Kyushu University, Japan	From domestic institutions: 159 From overseas institutions: 66
5	January 30, 2014	I <sup>2</sup> CNER & ACT-C Joint Symposium Kyushu University, Japan	From domestic institutions: 119 From overseas institutions: 58
6	December 12, 2014	I <sup>2</sup> CNER Tokyo Symposium TKP Garden City Shinagawa, Tokyo, Japan	From domestic institutions: 98 From overseas institutions: 27
7	February 4, 2015	I <sup>2</sup> CNER International Workshops 2015 Kyushu University, Japan	From domestic institutions: 321 From overseas institutions: 83
8	February 4, 2016	I <sup>2</sup> CNER International Workshops 2016 Kyushu University, Japan February 4, 2016	From domestic institutions: 304 From overseas institutions: 76
9	March 13-17, 2016	The First Pacific Rim Thermal Engineering Conference, Hawaii, U.S.	Total 500 - 600
10	September 11-14, 2016	2016 International Hydrogen Conference Jackson Lake Lodge, U.S.	From domestic institutions: 25-30 From overseas institutions: 100-125
11	October 7, 2016	I <sup>2</sup> CNER NEXT-RP Kick-Off Meeting Kyushu University, Japan	From domestic institutions: 48 From overseas institutions: 29



12	October 23-26, 2016	International Symposium on Innovative Materials for Processes in Energy Systems 2016, Hotel Villa Diodoro, Italy	From domestic institutions: 40 From overseas institutions: 160
13	November 18-20, 2016	Asia Pacific Innovation Conference ACROS Fukuoka, Japan	From domestic institutions: 25 From overseas institutions: 75
14	February 2-3, 2017	University of New South Wales-I <sup>2</sup> CNER 2nd Energy Workshop Kyushu University, Japan	From domestic institutions: 22 From overseas institutions: 8
15	May 17-19, 2017	NanoMat2017: 12th Japan-France Workshop on Materials Science (3rd WPI-Workshop on Materials Science), Kyushu University, Japan	From domestic institutions: 39 From overseas institutions: 40
16	September 2-5, 2017	International Workshop on Giant Straining Process for Advanced Materials 2017 (GSAM 2017) Reference Dai-Hakata building, Fukuoka, Japan	From domestic institutions: 50 From overseas institutions: 20
17	February 2, 2018	2018 I <sup>2</sup> CNER International Workshops, Kyushu University, Japan	From domestic institutions: 282 From overseas institutions: 114
18	March 12-15, 2018	The 10th International Conference on Boiling and Condensation Heat Transfer (ICBCHT 2018), Nagasaki Brick Hall, Nagasaki, Japan	From domestic institutions: 150 From overseas institutions: 60
19	January 31, 2019	I <sup>2</sup> CNER Annual Symposium Kyushu University, Japan	From domestic institutions: 124 From overseas institutions: 26
20	February 1, 2019	I <sup>2</sup> CNER International Workshops Kyushu University, Japan	From domestic institutions: 287 From overseas institutions: 69

## Appendix 5 List of Media Coverage of Projects Carried out between FY 2010 – 2018

\* Select main items of press releases, media coverage, and reports for FY 2010-2018 (especially by overseas media)

### 1) Japan

No.	Date	Type of the media (e.g., newspaper, magazine, television)	Description
1	Jul. 6, 2018	Newspaper	<b>Nikkei Sangyo Shimbun</b> Newspaper article covering the press release "Exploiting singlet fission in organic light-emitting diodes" (Profs. Chihaya Adachi, Hajime Nakanotani)
2	Jul. 19, 2018	Newspaper website	<b>Nihon Keizai Shimbun</b> Newspaper article covering the press release "An analysis of urban environmental Kuznets curve of CO <sub>2</sub> emissions: Empirical analysis of 276 global metropolitan areas" (Prof. Andrew Chapman)
3	Jan. 8-9, 2019	Television	<b>Kyushu Asahi Broadcasting</b> (Jan. 8) <b>NHK Fukuoka</b> (Jan. 8 and 9) <b>RKB Mainichi Broadcasting</b> (Jan. 8) TV news covering a new electric vehicle made of a newly-developed, light and tough polymer. (Prof. Atsushi Takahara)
4	Mar. 8, 2018	Newspaper	<b>Nishi-Nippon Shimbun</b> Special edition for elementary school students: An interview article by kids reporters focusing on hydrogen energy research at Kyushu University (Prof. Kazunari Sasaki)
5	Jan. 2018	Newspaper, Website	<b>Kumamoto Nichinichi Shimbun</b> (Jan. 20), <b>Asahi Shimbun Digital</b> (Jan. 24) Newspaper/web news articles entitled, "Horizontal sliding observed at the Uchinomaki hot spring area" and "Hot spring dormant during the 2016 earthquake," respectively (Prof. Takeshi Tsuji)

No.	Date	Type of the media (e.g., newspaper, magazine, television)	Description
6	Dec. 2017-Jan. 2018	Newspaper	<b>Nikkei Sangyo Shimbun</b> (Dec. 28), <b>Kagaku Shimbun</b> (Jan. 19) Newspaper articles covering the press release "Continuous synthesis of glycolic acid as a next generation fuel" (Profs. Masaaki Sadakiyo et al)
7	Nov. 25, 2017	Newspaper	<b>Nihon Keizai Shimbun</b> (Nov. 25), <b>Nishi-Nippon Shimbun</b> (Nov. 26) Newspaper article introducing the research on the crust damage caused by the 2016 Kumamoto earthquake (Prof. Takeshi Tsuii)
8	Nov. 10, 2017	Newspaper, Website	<b>Kyodo News,</b> <b>Jiji.com,</b> <b>Nihon Keizai Shimbun,</b> <b>Asahi Shimbun Digital,</b> <b>Sankei News,</b> <b>Sankei Biz,</b> <b>Kyoto Shimbun,</b> <b>Saga Shimbun,</b> <b>Nishi-Nippon Shimbun</b> Nishina Memorial Award for the contribution to the development of OLEDs (Prof. Chihaya Adachi)
9	Nov. 2, 2017	Newspaper	<b>Nikkei Sangyo Shimbun</b> (Nov. 2) Newspaper article covering the press release "NIR-driven H <sub>2</sub> evolution from water: Expanding wavelength range for solar energy conversion" (Prof. Ken Sakai)

No.	Date	Type of the media (e.g., newspaper, magazine, television)	Description
10	Oct. 2017	Newspaper, Website	<b>Nihon Keizai Shimbun</b> (Oct. 17), <b>Science Portal</b> (Oct. 24) Newspaper/web news articles entitled, "Reveal structures related to the size of the earthquake in the Nankai Trough" and "Reveal the relationship between 2016 earthquake and 1944 Tonankai mega earthquake," respectively (Prof. Takeshi Tsuji)
11	Oct. 2017	Newspaper, Website	<b>Nikkei Sangyo Shimbun</b> (Oct. 12), <b>National Institute for Environmental Studies' (NIES) website</b> (Oct. 17) Newspaper/web news articles covering the press release "A Fusion of Biomimetic Fuel and Solar Cells Based on Hydrogenase, Photosystem II, and Cytochrome c Oxidase" (Prof. Seiji Ogo)
12	Sep. 28, 2017	Newspaper	<b>Kagaku Kogyo Nippo</b> Newspaper article featuring a special lecture at the Fullerenes-Nanotubes-Graphene General Symposium in Kyoto (Prof. Tsuyohiko Fujigaya)
13	Sep. 2017	Television, Newspaper, Website	<b>NHK Fukuoka</b> (Sep. 14), <b>TVQ Kyushu Broadcasting</b> (Sep. 14), <b>Itosima Shimbun</b> (Sep. 21), <b>Fukuoka Internet TV</b> (Sep. 28) TV/newspaper/web news covering local junior high school students' visit to I <sup>2</sup> CNER as part of a field trip organized by the Fukuoka prefectural government (Profs. Motonori Watanabe, Keigo Kitamura, and Dr. Thomas Bayer)

No.	Date	Type of the media (e.g., newspaper, magazine, television)	Description
14	Sep. 1, 2017	Website	<b>Nihon Keizai Shimbun's website</b> Web news article introducing the research on the structural basis of the redox switches in the NAD+-reducing soluble [NiFe]-hydrogenase (Prof. Seiji Ogo et al.)
15	Aug. 2017	Newspaper, Website	<b>Nihon Keizai Shimbun's website</b> (Aug. 29), <b>Nikkan Kogyo Shimbun</b> (Aug. 30), <b>Shinano Mainichi Shimbun's website</b> (Aug. 30) Newspaper/web news articles covering the press release "Cutting-edge technology for mass production of highly formable Ni-based superalloy" (Prof. Zenji Horita)
16	Jun. 2017	Television, Newspaper, Website, Magazine	<b>Television Nishi-Nippon Corporation</b> (Jun. 6), <b>Asahi Shimbun Digital</b> (Jun. 7), <b>Nihon Keizai Shimbun</b> (Jun. 7), <b>Nishi-Nippon Shimbun</b> (Jun. 8), <b>Sankei News</b> (Jun. 8), <b>Nikkei Sangyo Shimbun</b> (Jun. 8), <b>Phys.org</b> (Jun. 22), <b>AZoCleantech</b> (Jun. 23) <b>DWV-Mitteilungen</b> (Sep. 14) Newspaper/web news/magazine articles covering the press release "One Model, Two Enzymes: Activation of Hydrogen and Carbon Monoxide" (Prof. Seiji Ogo)

No.	Date	Type of the media (e.g., newspaper, magazine, television)	Description
17	Apr.-May 2017	Newspaper	<b>Nikkei Sangyo Shimbun</b> (Apr. 11), <b>New Energy News</b> (May 1) Newspaper articles introducing the development of high performance inorganic metal oxide hybrid catalysts using carbon nanotubes (Profs. Naotoshi Nakashima and Tsuyohiko Fujigaya)
18	Feb. 21, 2017	Newspaper	<b>Yomiuri Shimbun, others</b> Horizontal sliding of kilometer-scale hot spring area during the 2016 Kumamoto earthquake (Takeshi Tsuji, CO <sub>2</sub> Storage division)
19	Nov. 20, 2016	Newspaper	<b>Yomiuri Shimbun</b> Organic electroluminescence: Next-generation lighting devices (Chihaya Adachi, Molecular Photoconversion Devices division)
20	Oct. 2, 2016	Newspaper	<b>Nihon Keizai Shimbun</b> CO <sub>2</sub> catch by ultrathin membrane (Shigenori Fujikawa, CO <sub>2</sub> Capture and Utilization division)

No.	Date	Type of the media (e.g., newspaper, magazine, television)	Description
21	Sep. 15, 2016	Newspaper	<b>Nihon Keizai Shimbun</b> 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)
22	Jul. 11, 2016	Newspaper	<b>Nikkei Sangyo Shimbun</b> Chemically-Modified Carbon Nanotubes Emit New Near-Infrared Light (Naotoshi Nakashima, Electrochemical Energy Conversion division)
23	Jul. 8, 2016	Newspaper	<b>Nikkan Kogyo Shimbun</b> 12 Scientists Recognized at Thomson Reuters "Japan Research Front Awards" (Chihaya Adachi, Molecular Photoconversion Devices division)
24	Jun. 6, 2016	Newspaper	<b>Nihon Keizai Shimbun</b> 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)
25	Apr. 15, 2016	Newspaper	<b>Nihon Keizai Shimbun</b> Comment on Kumamoto Earthquakes: 3rd largest number of inland earthquakes in history possibly affected by the near-surface epicenter (Takeshi Tsuji, CO <sub>2</sub> Storage division)
26	Apr. 2016	Newspaper	<b>Nikkan Sangyo Shimbun</b> (Apr. 13, 2016), <b>Nikkan Kogyo Shimbun</b> (Apr. 28, 2016) Increasing efficiency in underground CO <sub>2</sub> storage: KU researchers analyze rocks to detect suitable areas (Takeshi Tsuji, CO <sub>2</sub> Storage division)

No.	Date	Type of the media (e.g., newspaper, magazine, television)	Description
27	Nov. 26, 2015	Newspaper	<b>Nikkan Kogyo Shimbun</b> Durability enhancement of polymer electrolyte fuel cells (Naotoshi Nakashima, Electrochemical Energy Conversion Devices division)
28	Nov. 9, 2015	Newspaper	<b>Nihon Keizai Shimbun</b> Breakthrough in continuous monitoring of CO <sub>2</sub> leaks from storage sites (Takeshi Tsuji and Tatsunori Ikeda, CO <sub>2</sub> Storage division)
29	Nov. 4, 2015	Newspaper	<b>Nikkei Sangyo Shimbun, Asahi Shimbun</b> Enzyme for both sides of fuel cells (Seiji Ogo, Catalytic Materials Transformations division)
30	Nov. 2, 2015	Newspaper	<b>Nishinippon Shimbun, Asahi Shimbun, Yomiuri Shimbun, Nihon Keizai Shimbun</b> Medal with Purple Ribbon (Zenji Horita, Hydrogen Storage division)
31	Oct. 20, 2015	Newspaper	<b>Nikkei Sangyo Shimbun</b> Organic Electroluminescence, Cheap But Brilliant Light (Chihaya Adachi, Molecular Photoconversion Devices division)



No.	Date	Type of the media (e.g., newspaper, magazine, television)	Description
32	Oct. 1, 2015	Newspaper, Website	<b>Sankei Shimbun,</b> <b>Nihon Keizai Shimbun,</b> <b>Science Portal,</b> <b>excite news,</b> <b>zakzak,</b> <b>Sankei News</b> Found new geological formation controlling earthquake off the Kii peninsula (Takeshi Tsuji, CO <sub>2</sub> Storage division)
33	Jul. 29, 2015	Newspaper	<b>Nihon Keizai Shimbun</b> Increasing the efficiency of the electric power generation of fuel cells (Kazunari Sasaki, Electrochemical Energy Conversion division)
34	Jul. 2, 2015	Newspaper	<b>Mainichi Shimbun</b> Mechanism of cell membrane (Toyoki Kunitake CO <sub>2</sub> Capture and Utilization division)
35	Jun. 2015, Nov. 2015	Newspaper	<b>Asahi Shimbun</b> (Jun. 20, 2015), <b>Nishinippon Shimbun</b> (Jun. 23, 2015), <b>Yomiuri Shimbun</b> (Nov. 23, 2015) Kyoto Prize (Toyoki Kunitake, CO <sub>2</sub> Capture and Utilization division)
36	Apr. 20, 2015	Newspaper	<b>Nihon Keizai Shimbun</b> Vision and challenge of hydrogen society (Kazunari Sasaki, Electrochemical Energy Conversion division)
37	Apr. 7, 2015	Newspaper	<b>Nihon Keizai Shimbun</b> Interview about usage of hydrogen (Etsuo Akiba, Hydrogen Storage division)

No.	Date	Type of the media (e.g., newspaper, magazine, television)	Description
38	Oct., 2014	Newspaper	<b>Zaikei Shimbun</b> (Oct. 6, 2014), <b>Nikkei Sangyo Shimbun</b> (Oct. 8, 2014), <b>Nikkan Kogyo Shimbun</b> (Oct. 10, 2014), <b>Kagaku Shimbun</b> (Oct. 10, 2014) Semiconducting carbon nanotube sorting (Naotoshi Nakashima, Fuel Cells division)
39	Sep. 29, 2014	Newspaper	<b>Denki Shimbun,</b> <b>Nikkan Kogyo Shimbun,</b> <b>Nikkei Shimbun</b> World-first experiment on a controlled sub-seabed CO <sub>2</sub> leak demonstrates minimal environmental impact and rapid recovery (Kiminori Shitashima, CO <sub>2</sub> Storage division)
40	Jun. 4, 2014- Jun. 5, 2014	Television, Newspaper	<b>NHK,</b> <b>Yomiuri Shimbun,</b> <b>Mainichi Shimbun,</b> <b>Nikkei Shimbun</b> [NiFe]Hydrogenase from <i>Citrobacter</i> sp. S-77 Surpasses Platinum as an Electrode for H <sub>2</sub> Oxidation Reaction (Seiji Ogo, Catalytic Materials Transformations division)
41	May 2014-Jun. 2014	Newspaper, Website	<b>Nikkei Technology Online</b> (May 30, 2014), <b>Nishinippon Shimbun</b> (May 31, 2014), <b>Nikkan Kogyo Shimbun</b> (Jun. 2, 2014) Development of EL devices with 100% of luminous efficiency (Chihaya Adachi, Hydrogen Production division)

No.	Date	Type of the media (e.g., newspaper, magazine, television)	Description
42	Apr. 2014, Sep. 2014	Newspaper	<b>Nikkei Shimbun</b> (Apr. 11, 2014), <b>Nishinippon Shimbun</b> (Sep. 6, 2014), <b>Nikkan Kogyo Shimbun</b> (Sep. 8, 2014), <b>Nikkei Sangyo Shimbun</b> (Sep. 9, 2014) Development of a future-generation of PEFCs using a minimal amount of Pt (Naotoshi Nakashima, Fuel Cells division)
43	Oct. 2, 2013	Newspaper	<b>Nikkei Business Daily</b> Newspaper article introducing an idea that fuel cell is expected to be downsized and solid oxide fuel cells can operate at 300°C (Tatsumi Ishihara, Hydrogen Production division)
44	May 27, 2013	Magazine	<b>Nikkei Business</b> Magazine article introducing groundbreaking organic materials (Chihaya Adachi, Hydrogen Production division)
45	May 4, 2013	Newspaper, Website	<b>Nikkei Shimbun,</b> <b>Yomiuri Shimbun,</b> <b>Nishinippon Shimbun,</b> <b>Nikkan Kogyo Shimbun,</b> <b>Kyodo Tsushin (online),</b> <b>Shikoku Shimbun (online),</b> <b>Shizuoka Shimbun (online)</b> 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)

No.	Date	Type of the media (e.g., newspaper, magazine, television)	Description
46	Feb. 2013-Mar. 2013	Website, Newspaper	<b>NIKKEI.com</b> (Feb. 26, 2013), <b>Yahoo Japan! News</b> (Feb. 26, 2013), <b>Optronics Web Journal</b> (Feb. 26, 2013), <b>Nikkei Shimbun</b> (Feb. 26, 2013), <b>Sustainablejapan.net</b> (Feb. 28, 2013), <b>Nanotech Japan</b> (Mar. 11, 2013), <b>Yomiuri Shimbun</b> (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)
47	Feb., 2013-Mar. 2013	Newspaper	<b>Nikkei Shimbun</b> (Feb. 22, 2013), <b>Nikkei Sangyo Shimbun</b> (Feb. 26, 2013), <b>Science News</b> (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)
48	Feb. 2013	Newspaper	<b>Yomiuri Shimbun</b> (Feb. 8, 2013), <b>Asahi Shimbun</b> (Feb. 8, 2013), <b>Mainichi Shimbun</b> (Feb. 8, 2013), <b>Nikkei Shimbun</b> (Feb. 8, 2013), <b>Nishinippon Shimbun</b> (Feb. 8, 2013), <b>Science News</b> (Feb. 15, 2013), <b>Nikkei Shimbun</b> (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)
49	Dec. 12, 2012	Newspaper	<b>Nikkan Kogyo Shimbun</b> Newspaper article introducing the success in the fabrication of dual carbon batteries with high capacity (Tatsumi Ishihara, Hydrogen Production division)

No.	Date	Type of the media (e.g., newspaper, magazine, television)	Description
50	Oct., 2012-Nov. 2012	Newspaper	<b>Nikkei Sangyo Shimbun</b> (Oct. 24, 2012), <b>Nikkan Kogyo Shimbun</b> (Oct. 25, 2012), <b>Kagaku Kogyo Nippo</b> (Oct. 25, 2012), <b>Denki Shimbun</b> (Oct. 25, 2012), <b>Kagaku Shimbun</b> (Nov. 2, 2012) Newspaper article introducing the reason of high oxygen permeation rate of a praseodymium nickel oxide (Tatsumi Ishihara, Hydrogen Production division)
51	May 24, 2012	Television	<b>"Today's Close-up" on NHK</b> Television article introducing a front-line waste heat utilization technology (Tatsumi Ishihara, Hydrogen Production division)
52	Mar. 11, 2012	Newspaper	<b>Nikkei Shimbun</b> Newspaper article introducing the latest research on solid oxide fuel cell and its unique technology (Tatsumi Ishihara, lead of Hydrogen Production division)
53	Dec. 21, 2011	Television	<b>NHK Fukuoka Broadcasting Office</b> TV coverage featuring the next generation fuel cell (Kazunari Sasaki, lead of Fuel Cells division)
54	Sep., 2011	Newspaper, Website	<b>Yomiuri Shimbun</b> (Sep. 13, 2011), <b>Kyodo News</b> (Sep. 13, 2011), <b>Nikkan Kogyo Shimbun</b> (Sep. 14, 2011), <b>Nikkei Sangyo Shimbun</b> (Sep. 14, 2011), <b>Asahi.com</b> (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)

No.	Date	Type of the media (e.g., newspaper, magazine, television)	Description
55	Jun. 5, 2011	Newspaper	<b>Asahi Shimbun</b> Newspaper featured an interview with Prof. Petros Sofronis, Director of I <sup>2</sup> CNER, reviewing his future perspective from hiring excellent young brains worldwide to the achievement of the hydrogen society.
56	May 7, 2011	Website	<b>NIKKEI.com</b> Web Article introducing an interview with Prof. Yukitaka Murakami, Vice Director of I <sup>2</sup> CNER. Risk of the concentration of power stations, and proposal of dispersed power sources by the usage of hydrogen fuel cell are mentioned.

## 2) Overseas

No.	Date	Type of the media (e.g., newspaper, magazine, television)	Description
1	Jul. 2017	Website	<b>New Electronics</b> (Jul. 13), <b>Photonics Media</b> (Jul. 13) Web news articles entitled, "Harnessing hydrogens for high efficiency OLEDs" and "Hydrogen Could Provide Path to High-Efficiency OLEDs," respectively (Prof. Chihaya Adachi)
2	Apr.-May 2017	Website	<b>Bloomberg Technology</b> (Apr. 24), <b>The Science Times</b> (May 2) Web news articles entitled, "New iPhone screen puts blue-colored spotlight on Japan Supplier" and "Organic Laser: Recent Development For Longer Light Emissions," respectively (Prof. Chihaya Adachi)
3	Aug. 7, 2016	Radio	<b>COPE</b> Interview by Spanish National Radio (Helena Téllez-Lozano, Electrochemical Energy Conversion division)

No.	Date	Type of the media (e.g., newspaper, magazine, television)	Description
4	Jul. 13, 2016	Newspaper	<b>Diario Cordoba</b> Press release covering the 9th Shiseido Female Researcher Grant Award (Helena Téllez-Lozano, Electrochemical Energy Conversion division)
5	Jul. 8, 2016	Radio	<b>Cadena Sur</b> Interview by Spanish National Radio (Helena Téllez-Lozano, Electrochemical Energy Conversion division)
6	Jul. 8, 2016	Digital newspaper	<b>Europa Press, La Vanguardia, El Confidencial</b> Press release covering the 9th Shiseido Female Researcher Grant Award (Helena Téllez-Lozano, Electrochemical Energy Conversion division)
7	Dec. 11, 2015	Television	<b>Bangladesh Sangbad Sangstha</b> Japanese Team meets DU VC (Bidyut Baran Saha, Thermal Science and Engineering division)
8	Feb., 2015	Newspaper	<b>Economist, Seattle Times, Washington Times</b> Wendy Schmidt Ocean Health XPRIZE: selected as Team SINDEN Japan Team Leader (Kiminori Shitashima, CO <sub>2</sub> Storage division)

No.	Date	Type of the media (e.g., newspaper, magazine, television)	Description
9	Nov. 21, 2013	Webpage	<b>Helmholtz-Zentrum Geesthacht</b> Web article introducing international ECOSTORE project (Etsuo Akiba, Hydrogen Storage division)
10	Aug. 29, 2013	Webpage	<b>Helmholtz Zentrum Berlin</b> Massachusetts Institute of Technology/Materials Processing Center (Sep. 24 ) Interview of Prof. Harry Tuller (Fuel Cells division)
11	Jan. 17, 2013	Website	<b>CHEMICAL &amp; ENGINEERING NEWS</b> Polymer Gets Sticky When Hit with Light (Atsushi Takahara, Hydrogen Production division)
12	Jun. 2012-Aug. 2012	Website	<b>The Guardian</b> (Jun. 29, 2012), <b>Fish Update</b> (Jun. 29, 2012), <b>Planet Earth Online</b> (Jun. 29, 2012), <b>This is Cornwall</b> (Jun. 30, 2012), <b>International Business Time</b> (Jul. 1, 2012), <b>Responding to Climate Change</b> (Aug. 14, 2012) Web article introducing the world-first field experiment of CO <sub>2</sub> leakage in CCS (Kiminori Shitashima, CO <sub>2</sub> Storage division)
13	Nov. 8, 2011	Website	<b>MRS Bulletin Website</b> Japan funds new international energy center, I <sup>2</sup> CNER, led by the University of Illinois
14	May 12, 2011	Website	<b>Sandia National Laboratories</b> Japanese collaboration promises to put Sandia hydrogen program on global track (Brian Somerday, Hydrogen Materials Compatibility division)



No.	Date	Type of the media (e.g., newspaper, magazine, television)	Description
15	May 11, 2011	Website	<b>U.S. Department of Energy</b> DOE Hydrogen and Fuel Cells Program Team Awards with special recognition for outstanding technical contributions (Petros Sofronis, Director)

## Appendix 5 List of Achievements of Center's Outreach Activities between FY 2010 – 2018

\* Using the table below, show the achievements of the Center's outreach activities from FY2010 through FY2018 (number of activities, times held).

\*If there are any rows on activities the center didn't implement, delete that (those) row(s). If you have any activities other than the items stated below, fill in the space between parentheses after "Others" on the bottom with the name of those activities and state the numbers of activities and times held in the space on the right. A row of "Others" can be added, if needed.

Activities	FY2010	FY2011	FY2012	FY2013	FY2014	FY2015	FY2016	FY2017	FY2018
	(number of activities, times held)								
PR brochure, pamphlet	0	4	6	5	5	5	5	7	3
Lectures, seminars for the general public	0	3	6	11	14	12	17	23	15
Teaching, experiments, training for elementary, secondary and high school students	0	11	10	9	16	22	15	44	8
Science cafe	0	1	0	0	1	2	1	1	1
Open house	0	1	0	1	1	1	1	1	1
Participating, exhibiting in events	0	3	1	4	5	7	7	4	10
Press releases	0	1	7	10	14	14	8	13	4
Publications of the popular science books	0	1	1	0	1	2	1	0	1
Others ( )	0	0	0	0	0	0	0	0	0

## Appendix6-1 Host Institution's Commitment (Fund, Personnel)

### 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)

<b>(FY 2010-2018)</b>									
<b>&lt;Fund&gt; (million yen)</b>									
<b>Fiscal Year</b>	<b>2010</b>	<b>2011</b>	<b>2012</b>	<b>2013</b>	<b>2014</b>	<b>2015</b>	<b>2016</b>	<b>2017</b>	<b>2018</b>
Personnel	58	351	379	226	243	227	211	186	169
Faculty members	44	299	330	187	199	180	158	137	125
Full-time	44	299	330	187	199	180	158	137	125
Concurrent	0	0	0	0	0	0	0	0	0
Postdocs	0	0	0	0	0	0	0	0	0
RA etc.	0	0	0	0	0	0	0	0	0
Research support staff	0	0	0	0	0	0	0	0	0
Administrative staff	14	52	49	39	44	47	53	49	44
Full-time	14	52	49	39	44	47	53	49	44
Concurrent	0	0	0	0	0	0	0	0	0
Project activities	1	7	12	22	128	74	79	81	47
Travel	0	2	1	3	4	3	7	6	7
Equipment	0	0	819	10	1957	34	8	1	1
Research projects	720	1570	2238	2557	2838	2128	1543	1733	1215
<b>Total</b>	<b>779</b>	<b>1930</b>	<b>3449</b>	<b>2818</b>	<b>5170</b>	<b>2466</b>	<b>1848</b>	<b>2007</b>	<b>1439</b>
<b>&lt;Personnel&gt; (person)</b>									
<b>Fiscal Year</b>	<b>2010</b>	<b>2011</b>	<b>2012</b>	<b>2013</b>	<b>2014</b>	<b>2015</b>	<b>2016</b>	<b>2017</b>	<b>2018</b>
Personnel	49	62	65	48	49	47	45	39	41
Faculty members	43	56	59	42	41	39	36	31	34
Full-time	43	56	59	42	41	39	36	31	34
Concurrent	0	0	0	0	0	0	0	0	0
Postdocs	0	0	0	0	0	0	0	0	0
RA etc.	0	0	0	0	0	0	0	0	0
Research support staff	0	0	0	0	0	0	0	0	0
Administrative staff	6	6	6	6	8	8	9	8	7
Full-time	6	6	6	6	8	8	9	8	7
Concurrent	0	0	0	0	0	0	0	0	0

## Appendix6-1 Host Institution's Commitment

### 1. Contributions from host institution

#### (2) Provision of land and/or building(s), lab space, etc.

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

Kyushu University offers space/land free for the I<sup>2</sup>CNER building 2, which was built at the end of February 2015. The building has 4 stories and a total floor space of 5,014 m<sup>2</sup>, 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.

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

#### **I<sup>2</sup>CNER's Permanent Position within Kyushu University**

Effective April 1, 2013, with the revision of the "Regulations of Kyushu University," I<sup>2</sup>CNER's position is clearly defined as a permanent Research Institute of Kyushu University.

#### **Director's Authority**

I<sup>2</sup>CNER's governing documents have been developed to assure that the Institute Director is responsible for making decisions and propose to the President 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 directly report to the President 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 I<sup>2</sup>CNER and another unit of Kyushu University to facilitate their engagement in I<sup>2</sup>CNER's activities in coordination with their home departments, such as making request for cooperation and arrangements with the head of his/her home department.

#### **Tenured Positions**

So far, Kyushu University has allotted a total of 11 tenured faculty positions to I<sup>2</sup>CNER. Additionally, as a result of a joint proposal that I<sup>2</sup>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<sup>2</sup>CNER has been utilizing the system and had 7-9 senior-level faculty transferred from other units of the university in FY2013-2018.

### 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**

I<sup>2</sup>CNER follows a special salary system which deviates from the established salary ranges. Individual faculty and proposed salaries for researchers are determined based on their accomplishments and contributions to the interests of the Institute. In order to finalize researchers salaries the Director reports to the President, 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 case is considered as a pilot program for KU's cross appointment system. Later, KU introduced its official cross appointment system in FY2016.

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

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

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

I<sup>2</sup>CNER building 1 (approximately 3,290 m<sup>2</sup>) 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 I<sup>2</sup>CNER members.

## **6. Support for other types of assistance**

### **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 platform for future energy research and education. I<sup>2</sup>CNER is expected to become a primary research entity within this organization.

## Appendix6-2 The Host Institution's Mid-term Plan

\* Excerpt the places in the host institution's "Mid-term objectives" and/or "Mid-term plan" that clearly show the positioning of the WPI center within its organization.

### [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<sup>2</sup>CNER) 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<sup>2</sup>CNER) 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<sup>2</sup>CNER and other diverse fields/domains, such as natural science (especially theory), mathematics, humanities, and social sciences, etc.

# World Premier International Research Center Initiative (WPI) Progress Plan (For Final Evaluation)

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

\* Write your report **within 6 pages**.

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

## 1. Mid- to Long-term Research Objectives and Strategies Based on the Center's Results during Funded Period

Describe new challenges in the Center's research objectives and plans after the funding period ends. If major adjustments will be made in the Center's operation, such as newly set research themes/objectives or a change in the director, describe the strategic background to the adjustments.

### A Vision for Future Impact

I<sup>2</sup>CNER has amassed a remarkable record of accomplishments over the past 10 years. It has defined and embraced the development of the science to dramatically reduce Japan's CO<sub>2</sub> emissions while strengthening Japan's energy security. I<sup>2</sup>CNER's many accomplishments have been built on the development and growth of extremely strong research teams at Kyushu University (KU) and at the Satellite Center at the University of Illinois at Urbana-Champaign. The capabilities of these research teams are further strengthened by a high level of engagement with other of the world's best scientist in I<sup>2</sup>CNER's areas of technical expertise. I<sup>2</sup>CNER's mission and accomplishments are directly in line with Japan's vision for a robust energy future which optimizes energy resources in concert with Japan's overarching energy vision: energy security, economic efficiency, and environmental protection without compromising safety (3E+S). I<sup>2</sup>CNER has moved its science accomplishments forward through largescale interactions with industry where I<sup>2</sup>CNER developments can be directly implanted for use in society.

While I<sup>2</sup>CNER's accomplishments have propelled Japan to the international forefront of carbon-neutral energy research and associated technology development, there are still major challenges ahead. In fact, from the very beginning, I<sup>2</sup>CNER recognized the need for the development of Roadmaps to guide its science initiatives toward the long-term 2050 CO<sub>2</sub> emissions reduction goal. These Roadmaps set milestones at each technology evolution point to better focus and define the necessary accomplishments to meet the long-term carbon-neutrality goal. This process includes establishing aggressive research accomplishment targets for each of the I<sup>2</sup>CNER research divisions. Each division's progress is tracked by continuous assessment of research efforts toward their research milestones. This approach also allows for determination of the most promising scientific directions to meet the overall CO<sub>2</sub> reduction target. This process has also guided the use of I<sup>2</sup>CNER's resource allocations to have the highest impact on its long-term mission. To ensure the highest overall impact, I<sup>2</sup>CNER developed a research portfolio which includes high-risk high-payoff science balanced with science with clearly identifiable directions and outcomes. This approach allowed I<sup>2</sup>CNER to invest in breakthrough and high impact science, and avoid incremental steps involving small advances in existing technologies. *I<sup>2</sup>CNER sees that this approach, which has proven highly successful in the past, should direct the science and resource planning for the future.*

Our vision for the future will also ensure that Japan remains at the forefront of international science addressing carbon emissions. Additionally, it ensures that Japan will lead the technology transfer process to implement the best new energy developments that help reduce carbon impact. Engaging the world's best scientists in this mission is critical to success. Built on I<sup>2</sup>CNER's impressive record of attracting the best science minds, future success will require the continued involvement and interactions with the best international scientists across I<sup>2</sup>CNER's fields of research. I<sup>2</sup>CNER has earned an international reputation for involvement of the best scientists to address an issue of major importance to all of humanity. The future I<sup>2</sup>CNER efforts will continue to develop and grow these relationships as a central, overarching element of all future activities.

This vision for the future of I<sup>2</sup>CNER is captured in the table below. To make best use of resources in the talented research teams, I<sup>2</sup>CNER will streamline its research portfolio by reshaping its strongest research themes and phasing out those that are less impactful. I<sup>2</sup>CNER will continue to invest in disruptive, high-risk high-payoff science as well as directed, discovery research. This approach has served I<sup>2</sup>CNER well and

## I<sup>2</sup>CNER 2020 and Beyond

### Platform for International Collaborations and Partnerships

Support international collaborative research of KU researchers, international and national universities, research institutes, and laboratories

### Streamlined Thematic Research Clusters

Advanced Energy Materials	Advanced Energy Systems	Energy Future and Environment
Develop innovative materials for energy production, conversion, transport, and utilization (new alloys, catalysts, semiconductors, etc.)	Develop new systems for efficient energy generation and utilization (power generation, thermal systems, PV, solar-hydrogen, fuel and electrolyzer cells, batteries, etc.)	Technoeconomics of energy, policy and planning in Japan; CO <sub>2</sub> management (social impact, advanced membranes for CO <sub>2</sub> capture, CO <sub>2</sub> storage, next generation refrigerants, etc.)

### Platform for Societal Implementation and Industrial Collaboration

Place research output to use in society through open innovation and collaboration with industry

will be an efficient, effective way to move forward for the future. Our focus continues to address basic science and engineering research with the overall goal of reduced CO<sub>2</sub> emissions. Moving forward, the three streamlined thematic research clusters or '**Thrusts**' will be **Advanced Energy Materials**, **Advanced Energy Systems**, and **Energy Future and Environment**. This structure allows us to capture all of the most relevant existing capabilities and to organize them for the best future impact. It also provides an efficient mechanism for top international and Japanese researchers to work interactively to accomplish common goals which cut across disciplines. I<sup>2</sup>CNER will continue to rely on the central role of the current Energy Analysis Division (EAD) that will be integrated in the Energy Future and Environment Thrust, in close cooperation with the science divisions, to set near, medium, and long-term goals to meet I<sup>2</sup>CNER's mission. *This includes the continued use of Roadmaps to set research goals and assess progress.*

The Advanced Energy Materials Thrust combines the best features of the development of materials for hydrogen transport and storage, materials for selective CO<sub>2</sub> capture, and materials for efficient energy conversion, particularly for fuel cell and regenerative energy applications. These efforts require coordinated interactions between I<sup>2</sup>CNER's major experimental capabilities and I<sup>2</sup>CNER's excellent materials modeling capabilities. The cooperation of these two research approaches will continue to lead to modeling-informed experiments which are highly effective in developing and evolving new science discoveries.

The Advanced Energy Systems Thrust combines the efforts of multiple I<sup>2</sup>CNER researchers to develop systems approaches and capabilities for efficient energy conversion and applications. This will be accomplished with the evolution of systems which either lower carbon emission, increase energy efficiency, or both, as identified in I<sup>2</sup>CNER's main research themes. Progress in these areas requires systems-level approaches which can also make use of new materials developed in Advanced Energy Materials Thrust.

The Energy Future and Environment Thrust pulls together the range of challenges facing Japan's and the world's energy transition, namely the transition from largely fossil fueled energy technology to a carbon-neutral or a carbon-free energy supply. This represents a major challenge for Japan, but an even larger international challenge. Japan's leadership in this area is crucial and I<sup>2</sup>CNER provides the basis for understanding and directing this transition. This Thrust enables the coordination of carbon reduction technologies, energy efficiency technologies, and guidance for social, political, and investment strategies to coordinate this transition.

The three research Thrusts will be interwoven with the **Platform for International Collaborations and Partnerships**. This platform is intended to maintain and foster I<sup>2</sup>CNER's international identity. The members of this platform, who are world experts, will continue to collaborate with I<sup>2</sup>CNER's researchers from all three Thrusts. Since the Platform for International Collaborations and Partnerships and the three Thrusts are interwoven and the Thrusts' themes overlap, this will be an effective way to promote interdisciplinary collaborations across the institute and the world. I<sup>2</sup>CNER currently has 25 partnering institutes and these collaborations will continue to grow. More specifically, the aim is to expand on the substantive collaborations that already exist with institutes such as: Illinois, MIT, Paul Scherrer Institute at



ETH, Imperial College, London, Goettingen, and the University of Edinburgh. Given I<sup>2</sup>CNER's portfolio on non-engineering aspects of energy, some of these partnerships may then grow into strategic partnerships with KU to involve various departments (e.g. Economics, Law, Humanities, and Mathematics). As a prime example, a delegation of 11 executives and faculty from various KU departments, led by KU's Executive Vice President for International Affairs, Prof. Masato Wakayama, visited Illinois on May 8-10, 2019 to work on a joint vision statement for the future of the Kyushu-Illinois strategic partnership.

The three major Research Thrust Clusters will all contribute directly to the transition of future I<sup>2</sup>CNER science advances to applicable technology transfer through a large and growing network of I<sup>2</sup>CNER industrial interactions. The **Platform for Societal Implementation and Industrial Collaboration** will ensure this high level of tech transfer. This coordination with Japan's energy and transportation industries will provide a means to directly implement carbon-saving energy technologies to reduce emissions and improve efficiencies. These technological applications will also have an impact on Japan's international markets where energy technologies are lagging behind Japan's efforts.

The future I<sup>2</sup>CNER Platform for Societal Implementation and Industrial Collaboration will also provide policy guidance for science and technology investments, as well as, addressing possible social acceptance and social impact issues. This is an important aspect of I<sup>2</sup>CNER's future vision and impact. The recent experiences of energy transitions to lower carbon emissions in other countries have alerted the rest of the world that the transition must include social acceptance and social equity. Disruptive changes in energy transition elsewhere in the world have led to unforeseen higher carbon emissions and higher electricity prices, both of which are contrary to the intended outcome. With its strengths in both advanced energy science and energy analysis, I<sup>2</sup>CNER will provide critical direction and support to Japan's energy transition over the next 30 years to meet the 2050 carbon reduction goals with minimal social and economic disruptions.

### Building on I<sup>2</sup>CNER's Accomplishments

In the first ten years, I<sup>2</sup>CNER has compiled remarkable number of technical achievements which, in combination, have impacted the progress toward a carbon-neutral society in a major way. These accomplishments are the result of extensive international collaborations and high-level scientific achievements. The accomplishments have also invigorated a large number of young scientists who will build on I<sup>2</sup>CNER's past accomplishments as I<sup>2</sup>CNER leads the way to a carbon neutral society over the next 30 years. In addition, the growth of interaction with industry to best couple I<sup>2</sup>CNER's science to technology transfer to industry, where I<sup>2</sup>CNER science is already producing results for carbon reduction and energy efficiency, increases. This cycle of continuously evolving and building on I<sup>2</sup>CNER's strengths is represented in the following figure. This model shows how basic science will continue to empower societal impact and Japan's energy goals while building new generations of scientist and leading world science in this field.

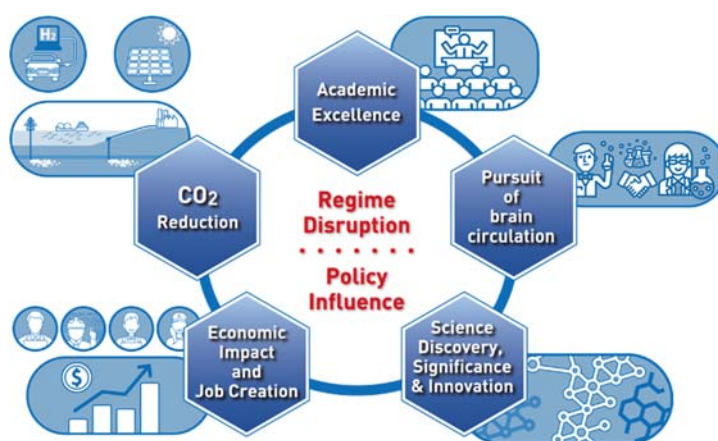


Fig. 1. I<sup>2</sup>CNER's Contribution to 2050 CO<sub>2</sub> Reductions (as of April 2019)

### The grand challenge and moving forward

I<sup>2</sup>CNER has built an effective, world-leading research and development program that exemplifies the WPI vision in international reputation, infrastructure, research standards and productivity, open research platform, and education. Additionally, I<sup>2</sup>CNER increased diversity, provided a new culture for young scientists to thrive independently and to foster collaborations for interdisciplinary research around the world.

This altogether is directed toward solving Japan's energy and carbon challenge. This is the goal around which I<sup>2</sup>CNER coalesced from the very early stages, and the goal toward which I<sup>2</sup>CNER has taken great strides over the past 10 years. This goal is supported by Japan's energy policy: energy security, economic efficiency, and environmental protection without compromising safety (3E+S). The drastic reduction of carbon emissions in concert with the 3E+S remains the Grand Challenge which will require a continued, concerted, focused effort to meet that goal. Fortunately, I<sup>2</sup>CNER has set a clear path toward this goal. In the future, I<sup>2</sup>CNER will continue on this path with full engagement of all parties, domestic and international. Japan's leadership in this Grand Challenge, supported by the efforts and capabilities of I<sup>2</sup>CNER, will continue to grow in international impact. Japan's leadership in this area will open new international markets and have a positive impact on international societal evolution to a more carbon-free world. *The support for this effort through I<sup>2</sup>CNER's induction into the WPI Academy is critical to fulfilling this Grand Challenge.*

## 2. Management System of the Research Organization

### 2-1. Describe the Center's Research Organizational Management System that will Execute the Research Strategy and Plan Described above.

- In Appendix 1, list the PIs who will ensure that the Center's project is sustained and advanced after the funding period ends.
- In Appendix 2, diagram the Center's organizational management system.

The organizational structure of I<sup>2</sup>CNER beyond 2020 can be described as the "*Three Thrust, Two Platform*" approach. I<sup>2</sup>CNER will maintain its international identity through the *platform for international collaborations and partnerships*. This platform will involve the academic institutions of the international PIs, namely Illinois, MIT, Paul Scherrer Institute at ETH, Imperial College, London, Goettingen, Tsinghua and institutions with which we developed research interactions and collaborations during the past 10 years of operation, e.g. the University of Edinburgh. Through this platform, I<sup>2</sup>CNER will continue its successful program on graduate student, and postdoc exchanges, and faculty sabbaticals.

The research programs of our 26 PIs presently in I<sup>2</sup>CNER will continue to operate beyond 2020 under the umbrella of three research thrusts with the following composition:

- Advanced Energy Materials (AEM)*: Tenured I<sup>2</sup>CNER PIs Yamauchi, Kubota, Staykov, Sofronis tenured I<sup>2</sup>CNER Associate Professors Yoon, Takahashi, and M. Watanabe; and PIs Ogo and Sakai, Sugimura, and Takahara. The research activities of the thrust will be supported by the international PIs Kirchheim and Somerday of the platform for international collaborations and partnerships.
- Advanced Energy Systems (AES)*: Tenured I<sup>2</sup>CNER PI Matsumoto; and PIs Adachi, Ishihara, Takata, Fujigaya, and Sasaki. The research activities of the thrust will be supported by the international PIs Tuller, Kilner, Lippert, and Gewirth of the platform for international collaborations and partnerships.
- Energy Future and Environment (EFE)*: Tenured I<sup>2</sup>CNER PIs Saha and Fujikawa; tenured I<sup>2</sup>CNER Associate Professor Chapman, PIs Tsuji and Watanabe; non-tenured faculty Prof. Itaoka; and international PIs Zhang, Christensen, and Stubbins. (Prof. Stubbins will be a new proposed PI for FY20.)

It should be mentioned that there is a substantial thematic overlap between the Thrusts, which has already been demonstrated by the joint publications amongst the researchers. By way of example, whereas organizationally Prof. Fujikawa will carry out his research on membrane materials for CO<sub>2</sub> capture in the EFE thrust, he is also collaborating with Prof. Sugimura on the environmental effects on tribofilms in the AEM thrust. In addition, the platform for international collaborations and partnership will help advance the fusion of activities among the thrusts. Namely, the expertise of the following PIs and their corresponding Thrust: PI Kilner from Imperial College, London covers research themes in both AEM and AES Thrusts; PI Tuller from MIT covers the AEM and AES; PI Zhang from Tsinghua University covers the AEM and AES; PI Gewirth from UIUC covers the AEM and AES; and PI Lippert from ETH covers the AEM and AES.

Capitalizing on talent and resources across KU, new members (WPI Professors) will be invited to diversify I<sup>2</sup>CNER's expertise and research portfolio of the EFE thrust to include the integration of renewable energy with the grid, the interaction of the energy networks with the environment, and social and economic dynamics. These members have already interacted with I<sup>2</sup>CNER through the Applied Math and Economics Initiative. New WPI Professor Murata of the Dept. of Electrical Engineering will apply optimization theory to model residential energy consumption, accounting for customer behavior. New WPI Professor Managi of the Dept. of Urban and Environmental Engineering will investigate "welfare" models of energy, work, leisure, health, and finances to rank social and economic systems. From the Institute of Mathematics for Industry, new WPI Professor Shirai will use Persistent Homology to understand porous materials for CO<sub>2</sub> storage and new WPI Professor Hirose will use machine learning to analyze data and discover customer behaviors that affect the power grid.

*I<sup>2</sup>CNER's Platform for Societal and Industrial Implementation* will be tasked to accelerate impactful technology development and transfer to industry, and foster the advancement of interactions with national and international agencies. This platform will focus on the goals currently pursued by the Industrial Research Division, augmented with a societal dimension and with adequate resources to advance the engagement of I<sup>2</sup>CNER with industry and society at a broader institutional level. Resources will be sought to staff the platform with an expert that can bring the I<sup>2</sup>CNER research accomplishments to the attention of national and international corporations and help I<sup>2</sup>CNER execute its mission as a resource to national agencies such as METI on the current state-of-the-art in energy research. With regard to the social implementation, I<sup>2</sup>CNER's research will seek to deal with critical policy issues in Japan such as the aging, shrinking population with regard to low-carbon energy transition and will consider the impact of behavior, specifically the environmental and social equity impacts of household consumption and participation in the energy system. The Industrial Advisory Board will continue on with its role in advising on research relevance and counseling on technology transfer. Lastly, this platform will be working with the PIs and faculty of the three thrusts to pursue joint research funding among national agencies of the government of Japan, e.g. JSPS, and counterpart international agencies, e.g. US NSF.

I<sup>2</sup>CNER will continue to operate under the strong leadership of Director Sofronis, who will report to EVP Inoue in monthly face-to-face meetings (c.f. Section 6.1 of the Extension Progress Report).

New faculty expertise will be incorporated into I<sup>2</sup>CNER's Faculty Recruiting Committee to better recruit faculty in computational materials, informatics, or at the intersection of engineering and the disciplines of applied-math/economic/social/political sciences. In addition, I<sup>2</sup>CNER will seek resources (e.g. proposal submission) for hiring tenured international faculty and postdoctoral fellows that will catalyze interactions amongst the thrusts.

## **2-2. Initiatives and Plans that will Impel System Reforms**

Describe the Center's action plan that embodies the basic policies of the University Reform Plan, and the Center's plan and strategies that lead to host institution reforms either directly or via ripple effects (also to other institutions, if applicable). Describe also the Center's strategies for fostering and securing the next generation of researchers (e.g., introduction of tenure tracks), and the system reform for enhancing the Center's organizational management, such as the implementation/verification PDCA system.

### **I<sup>2</sup>CNER is spearheading KU Reforms**

I<sup>2</sup>CNER is spearheading KU Reforms through globalization and internationalization of its research and education within the University Reform Revitalization Program (URRP). I<sup>2</sup>CNER is at the center of KU's mid-term plan to "promote leading-edge research related to the carbon-neutral energy research domain in collaboration with the University of Illinois..." By having hired faculty in social sciences and mathematics and partnering with other KU units (e.g. IMI, Depts. of Electrical Engineering, Urban and Environmental Engineering, and Economics, I<sup>2</sup>CNER helps KU to collaborate in "diverse fields/domains, such as natural science (especially theory), mathematics, humanities, social sciences, etc..." The Institute will leverage the experience of the KU Administration, which is also part of the URRP. Lastly, under the third-period mid-term goal, I<sup>2</sup>CNER and KU developed Q-PIT, which encompasses the activities throughout the entire university that are relevant to research and education on energy (see section 3.1).

### **I<sup>2</sup>CNER Tenured Faculty Positions**

The Institute competes annually for tenured positions through the URRP. For specific details about tenured positions for the next generation of researchers, please see Section 3-2 below.

### **Cross-Appointment Employment System for International Faculty**

In view of the successful model of Director Sofronis' cross-appointment case, which was the first ever at KU, KU institutionalized a cross-appointment employment system in March 2015. The KU Administration is working to promote/encourage new appointments through this system, which may include researchers from the private sector (industry) within and outside Japan, and other universities and institutes, both foreign and domestic. By way of example, Prof. Y. Baryshnikov of the University of Illinois will be employed by IMI during the summers of 2019 and 2020. He will be helping I<sup>2</sup>CNER on issues related to the mathematical aspects of control-theoretic methods and data-analytic tools relevant to deployment and functionality of smart grid. As of April 1, 2019, Prof. Andrew Chapman of the EAD has been cross-appointed with the Department of Economics (60% at I<sup>2</sup>CNER and 40% at the Department of Economics) to advance interdisciplinary research between I<sup>2</sup>CNER and Economics. For specific details on the Cross-Appointment employment system, please see Section 6-3 of the Progress Report.

Beginning in FY17, KU has made a major academic change by implementing the Academic Quarter (4-

term) System, which makes it possible for cross-appointed faculty from overseas to teach courses at KU (e.g. the case of Prof. Y. Barysnikov). Reforming the KU academic calendar also enables KU faculty to participate more easily in research/teaching activities as cross-appointed faculty at overseas partner institutions.

### **Intra-University Faculty Transfer System**

KU's "Intra-University Faculty Transfer System" was triggered by the presence of I<sup>2</sup>CNER and was designed to enable flexibility in allocating faculty within the University for the purpose of improving the standards of education and research conducted at KU. I<sup>2</sup>CNER will use this system to have 6 PIs transferred (Ishihara, Takata, Ogo, Sugimura, Sasaki, and Tsuji). For full details, please see Section 6-3 of the Progress Report.

### **Young Faculty Involvement with Teaching**

I<sup>2</sup>CNER faculty have already been involved with teaching in three "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. KU 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.

KU seeks I<sup>2</sup>CNER's involvement in the establishment of the new School of Interdisciplinary Science and Innovation called "Kyo-so Gakubu" in Japanese, which opened in April 2018. The concept for the School is to facilitate "cultivating individuals with a global mindset, capable of coordinating different knowledge and perspectives, and collaborating with others to create solutions/innovations in the global society which has grown more complex and diversified." A new international energy course will be developed that will contribute to the international education of Japanese students and help meet the goal of the "Kyo-So" concept for the new School.

In addition, I<sup>2</sup>CNER will play a crucial role in the new "Excellent" Graduate School program(s) to be established at KU, if the proposals submitted are successful. About 30 students will take courses in this new program, 5-10 of whom will be advised/supervised by I<sup>2</sup>CNER faculty. KU envisions that I<sup>2</sup>CNER's faculty involvement in this graduate education program(s) will advance the research/educational capabilities of KU and foster the international graduate education culture throughout KU. Moreover, students will be very likely to seek graduate degrees with I<sup>2</sup>CNER faculty after taking courses from them in the School of Interdisciplinary Science and Innovation.

### **Promotion and Tenure of Young Faculty**

I<sup>2</sup>CNER is impacting the traditional Japanese research structure and faculty model because its academic structure and processes of promotion, tenure, and merit-based compensation of its faculty and postdocs follow the highest standards for top-tier universities in the world. The Institute follows a process for promoting faculty and postdocs which breaks away from the Japanese tradition and instead applies the same standards as top US universities. The process involves a confidential assessment by world-leading scientists from the international community in the candidate's area of expertise. The process is carried out by a promotions committee that is interdisciplinary and which involves senior faculty from both KU and Illinois. The importance of interdisciplinary research is emphasized and is a requirement for promotion and tenure within the Institute. In consultation with the Associate Directors and the Division Lead PIs, the Director considers initiating the process of granting tenure when outstanding young researchers of the Institute are identified as deserving of consideration for tenure and tenured positions are available within the KU system. The tenure process follows exactly the same protocol as the promotion process. In summary, the promotion and tenure system of I<sup>2</sup>CNER will continue to offer its young faculty and postdocs the opportunity to advance their careers in a way that is internationally visible, and which has obvious implications for their career development beyond I<sup>2</sup>CNER.

### **Opportunities for young faculty and postdocs at the University of Illinois**

Young faculty have had the opportunity to take long-term sabbaticals based on the Agreement on Academic Cooperation between KU and Illinois (signed in FY14). The process has already been carried out with our newly hired applied math faculty, Profs. Matsue and Nguyen-Dinh, who had their sabbatical at Illinois respectively from Sept. 23, 2018 to Mar. 29, 2019 and Oct. 30, 2017 to Mar. 30, 2018. The same opportunities will be sought through the revised agreement between the two universities which is currently being negotiated for extension and renewal.

### 3. Center's Position within Host Institution and Measures to Provide It with Resources

Describe the Center's future plans with regard to the following points after the funding period ends.

#### 3-1. From a Mid- to Long-term Perspective, the Position of the Center within the Organization of the Host Institution

Describe where the Center will be placed within the host institution's overall organizational strategy under the leadership of the institution's head.

- In Appendix 3, diagram the Center's position within the organization of the host institution, and describe that positioning using excerpts from the institution's mid- to long-term plan. If the plan has not been established yet, describe the consideration being given to the Center's positioning.

I<sup>2</sup>CNER is a permanent Research Institute of Kyushu University.

#### Kyushu University's Mid-term Plan

I<sup>2</sup>CNER is at the center of the KU mid-term plan to "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<sup>2</sup>CNER)." In its third-period mid-term goal and plans, KU developed an energy-related plan centered on I<sup>2</sup>CNER. In addition, KU will "proactively advance collaboration and cooperation between I<sup>2</sup>CNER and other diverse fields/domains, such as natural science (especially theory), mathematics, humanities, and social sciences, etc., and will further improve its research system by leveraging the experience of the Kyushu University Administration."

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

The Q-PIT was inaugurated on October 1, 2016 to bring together green-energy engineers with unexpected partners such as mathematicians, political scientists, social scientists, and economists, to "solve the global challenges necessary to achieve a balance between emissions caused by humans and the removal of greenhouse gasses in the second half of this century," as President Kubo announced. Drawing from its international research experiences and approaches, I<sup>2</sup>CNER will play a central role in this new organization by helping to promote and advance a wide range of collaborations on energy research with other KU units. This will allow the Institute to capitalize on opportunities to broaden and enrich its energy portfolio while also helping Q-PIT advance its mission to catalyze interactions between diverse and disparate disciplines and units. I<sup>2</sup>CNER's Director Sofronis is member of the strategic committee of Q-PIT.

#### Plans after the funding period ends

The Director's vision is that I<sup>2</sup>CNER will remain strong and agile by developing a core of embedded centers that will operate beyond the WPI funding period by leveraging the ongoing and new initiatives of major sponsors. Such successful center is the Research Center for Next Generation Refrigerant Properties (NEXT-RP) which was established in FY16 and will continue beyond 2020. I<sup>2</sup>CNER will interact with, and assist with the mission of the Platform for Inter/Transdisciplinary Energy Research (Q-PIT), on future faculty resources. Through its new *Platform for Societal and Industrial Implementation*, I<sup>2</sup>CNER will expand its outreach to promote the deployment of its technology to industries that will fund I<sup>2</sup>CNER projects (e.g. recent partnership with Mazda Motor Corp. and future partnerships with Toshiba and Air-Liquide). Lastly I<sup>2</sup>CNER plans to submit a "Gaisan-Yokyu" proposal to MEXT seeking support for the implementation of the "Three Thrust, Two Platform" restructuring plans. Thus, I<sup>2</sup>CNER will sustain itself and evolve to accommodate breakthroughs in carbon-neutral energy technology and/or shifting priorities.

#### 3-2. Host Institution's Action Plan for Sustaining and Advancing the Center as a World Premier International Research Center (e.g., Positioning, Financial Resources)

- In Appendix 4, describe the host institution's resource allocation plans for the Center, including the allocation of posts (in both its research and administrative divisions).

#### Securing and Filling I<sup>2</sup>CNER Tenured Faculty Positions

KU implements the URRP to encourage its units to actively review and reform their structure to revitalize the University. The President's Vision for tenured PIs in I<sup>2</sup>CNER is that the units compete for tenured positions through annual proposal submissions. I<sup>2</sup>CNER has been successful at winning and filling positions, and KU will make efforts to secure additional positions for the Institute. By the end of FY18, I<sup>2</sup>CNER filled a total of 6 Associate and 4 Full Professor positions, and 2 tenure-track assistant professors on applied math for energy jointly with IMI. I<sup>2</sup>CNER has a remaining point balance of 0.791 that will be

used to hire another tenured Associate Professor in FY19.

### **I<sup>2</sup>CNER's Place in Kyushu University Infrastructure**

The university will grant I<sup>2</sup>CNER Building II (a total floor space of 5,014 m<sup>2</sup>) free of charge to provide the I<sup>2</sup>CNER researchers with the requisite environment to continue their cutting-edge research. The space provided by this support significantly exceeds the space allotment per researcher under the university's regular policy.

### **Kyushu University Administration Support of I<sup>2</sup>CNER Administrative Office**

KU will support the salaries of the required staff members, thus securing the successful operation of the "*Three Thrust, Two Platform*" new I<sup>2</sup>CNER organization.

## Appendix 1 List of Principal Investigators (for Progress Plan)

\* If the number of principal investigators exceeds 10, add rows as appropriate.

\* Give age as of 1 April 2020

\* For investigators who cannot participate in the center project from FY 2020, indicate the time that their participation will start in the "Notes" column.

	Name	Age	Current affiliation (position title, organization, department)	Academic degree and current specialties	Notes (Enter "new" or "ongoing")
1	Center Director Petros Sofronis	62	Prof., I <sup>2</sup> CNER, Kyushu University	Ph.D., Micromechanics of materials, Environmental degradation of materials	Ongoing
2	Tatsumi Ishihara	58	Prof., I <sup>2</sup> CNER, Kyushu University	Dr. of Engineering, Catalyst and solid state electrochemistry	Ongoing
3	Chihaya Adachi	56	Prof., Department of Applied Chemistry, Kyushu University	Dr. of Engineering, Materials science, device physics	Ongoing
4	Atsushi Takahara	64	Prof., I <sup>2</sup> CNER, Kyushu University	Dr. of Engineering, Surface and Interface Characterization	Ongoing (will retire from Kyushu University on March 31, 2021)
5	Seiji Ogo	56	Prof., I <sup>2</sup> CNER, Kyushu University	Dr. of Science, Green Chemistry	Ongoing
6	Kazunari Sasaki	55	Prof., I <sup>2</sup> CNER, Kyushu University	Dr. of Science and Technology, Fuel cell materials, Inorganic materials	Ongoing
7	Harry L. Tuller	74	Prof., Department of Materials Science and Engineering, Massachusetts Institute of Technology, USA	Dr. of Engineering Science, Functional electroceramic materials	Ongoing
8	John A. Kilner	73	Prof., Department of Materials, Imperial College, London, UK	Ph.D., Materials for solid oxide fuel cells and electrolysers	Ongoing
9	Joichi Sugimura	62	Prof., I <sup>2</sup> CNER, Kyushu University	Dr. of Engineering, Tribology and Machine Design	Ongoing
10	Yasuyuki Takata	63	Prof., I <sup>2</sup> CNER, Kyushu University	Dr. of Engineering, Thermal Engineering	Ongoing
11	Xing Zhang	58	Prof., Department of Engineering Mechanics, Tsinghua University, China	Ph.D., Thermal Science	Ongoing
12	Brian P. Somerday	51	Dr., South West Research Institute, USA	Ph.D., Materials Science and Engineering	Ongoing
13	Reiner Kirchheim	76	Prof., The Institut für Metallphysik, University of Göttingen, Germany	Ph.D., Hydrogen in Metals, Thermodynamics of alloys, Interstitial solution and diffusion in glasses	Ongoing

14	Miho Yamauchi	46	Prof., I <sup>2</sup> CNER, Kyushu University	Dr. of Science, Solid-state physical chemistry, Solid-state NMR, Nano materials, Catalysis, Hydrogen storage	Ongoing
15	Ken Sakai	58	Prof., Department of Chemistry Faculty of Sciences, Kyushu University	Ph.D., Inorganic Chemistry	Ongoing
16	Andrew A. Gewirth	60	Prof., Department of Chemistry, University of Illinois at Urbana Champaign, USA	Ph.D., Chemistry	Ongoing
17	Kenneth T. Christensen	46	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	Ongoing
18	Shigenori Fujikawa	49	Associate Prof., I <sup>2</sup> CNER, Kyushu University	Dr. of Engineering, Nanoscience and engineering	Ongoing
19	Takeshi Tsuji	40	Prof., I <sup>2</sup> CNER, Kyushu University	Dr. of Science, Earth and Planetary Science, Resource engineering, Space exploration	Ongoing
20	Hiroshige Matsumoto	53	Prof., I <sup>2</sup> CNER, Kyushu University	Dr. of Engineering, Solid electrochemistry and Solid state ionics	Ongoing
21	Bidyut B. Saha	54	Prof., I <sup>2</sup> CNER, Kyushu University	Dr. of Engineering, Thermal Engineering, Heat Transfer, Refrigeration and Air- conditioning Engineering, Adsorption Desalination	Ongoing
22	Thomas Lippert	57	Prof., Department of Chemistry and Applied Biosciences, Laboratory of Inorganic Chemistry, Swiss Federal Institute of Technology Zurich, and Paul Scherrer Institut, Thin Films & Interfaces Group, Villigen-PSI, Switzerland	Dr. of Science, Physical Chemistry	Ongoing
23	Tsuyohiko Fujigaya	43	Prof., Department of Applied Chemistry, Kyushu University	Ph.D. of Chemistry, Polymer Chemistry and Supramolecular Chemistry	Ongoing
24	Aleksandar T. Staykov	41	Associate Prof., I <sup>2</sup> CNER, Kyushu University	Dr. of Science, Physical and Theoretical Chemistry	Ongoing
25	Hiroaki Watanabe	47	Associate Prof., Department of Mechanical Engineering, Kyushu University	Ph.D. Engineering	Ongoing
26	Masanobu Kubota	50	Prof., I <sup>2</sup> CNER, Kyushu University	Dr. of Engineering, Strength of engineering materials, Metal fatigue, Fretting fatigue, Hydrogen structural materials	New (As of April 1, 2019)



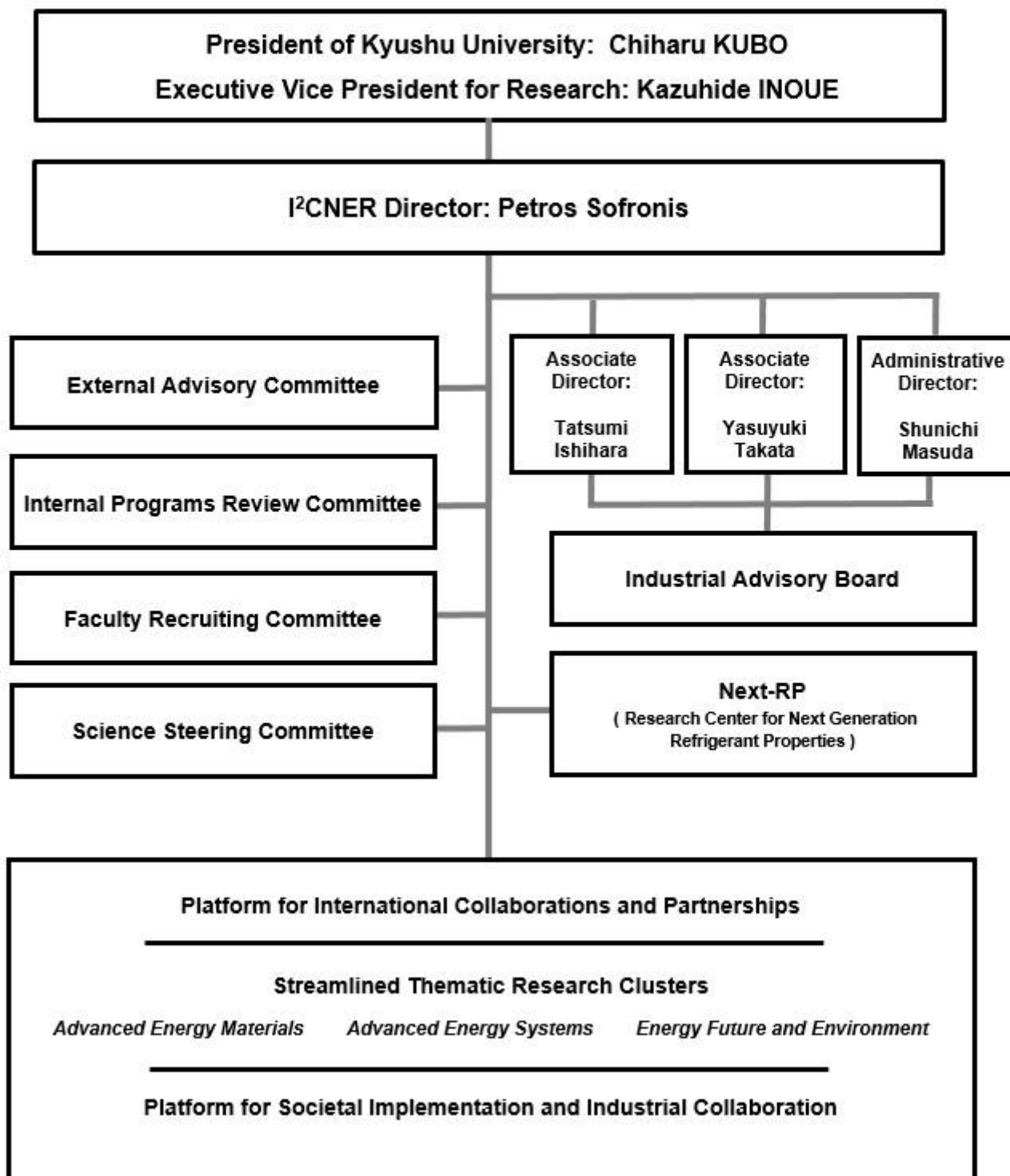
27	James Stubbins	71	Prof., Department of Nuclear, Plasma, and Radiological Engineering, University of Illinois at Urbana- Champaign	Ph.D. Materials Science, Development and assessment of materials for energy systems	New (Proposed for FY 2020)
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## World Premier International Research Center Initiative (WPI) Appendix 2 Diagram of Management System

Diagram management system in an easily understood manner.

- If any changes will be made in the management system from that in the latest "center project," describe them. Especially describe any important changes being planned in such as the center director, administrative director, head of host institution, and officer(s) in charge at the host institution (e.g., executive vice president for research).

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



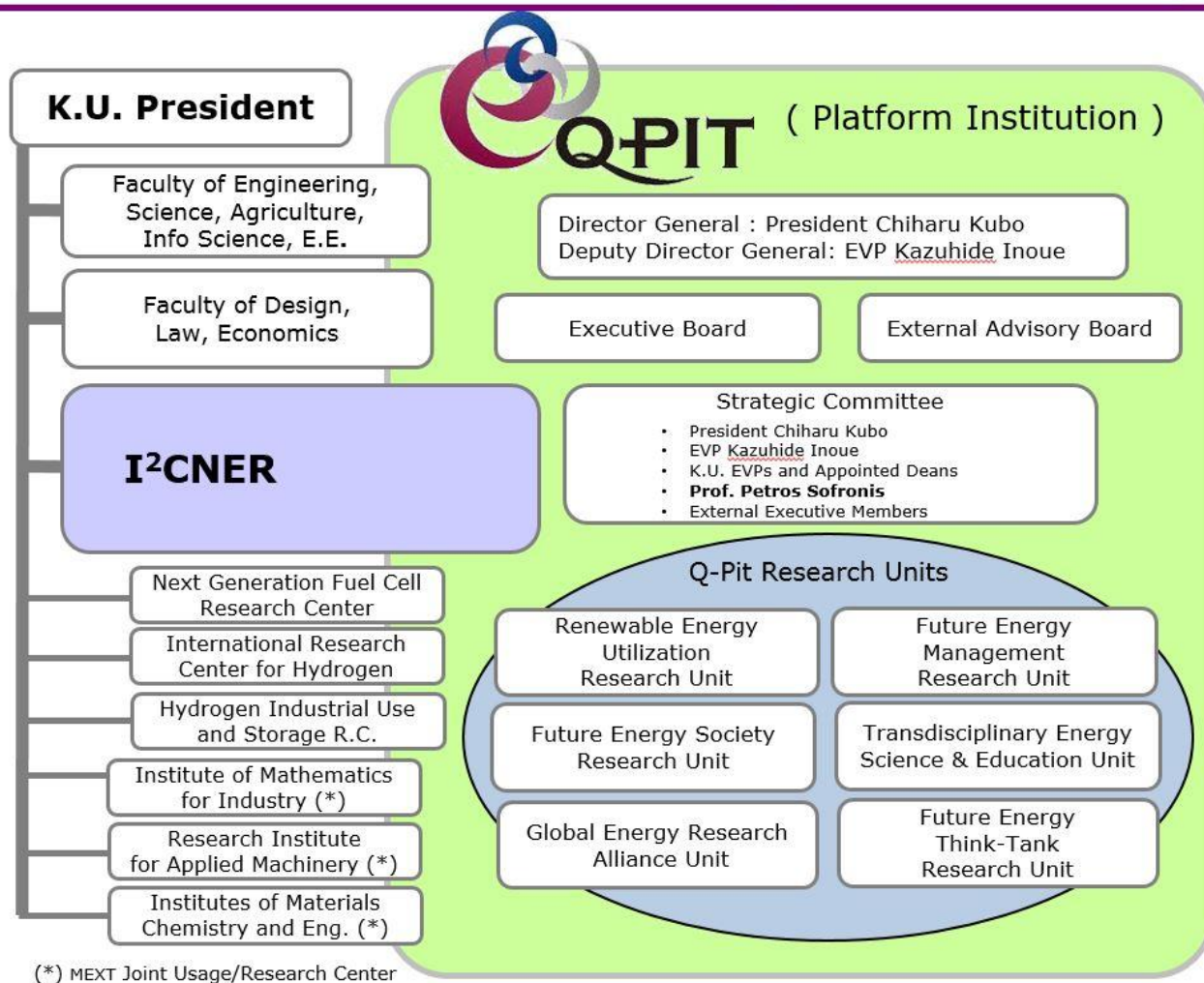
Beginning April 1, 2019, Professor Kazuhide Inoue is the Executive Vice President for Research and Finance of Kyushu University. Continuing the tradition of regular interactions with the KU administration, Director Sofronis has already begun meeting with EVP Inoue on a monthly basis.

Due to the reduced level of financial resources beyond 2020, I<sup>2</sup>CNER's research operations, international engagement, brain circulation, technology transfer, and socioeconomic outreach will be executed and advanced through the "*Three Thrust, Two Platform*" approach as indicated in the previous page and fully described in Section 1, subsection "A Vision for Future Impact." This consolidation will result in i) strengthening of the international character of the research activities as it shall be easier for the international PIs to engage in more than one Thrust, ii) accentuating the interactions that were taking place across former division boundaries on projects involving multiple research efforts such as CO<sub>2</sub> reduction for value added products, co-electrolysis of CO<sub>2</sub>, the conversion of excess renewable electricity into electrofuels, iii) more effective coordination of efforts toward technology transfer, and iv) more accurate analysis of the societal and economic impact of each individual research project, as the energy analysis team will be able to more effectively collect, compare, and process data from the consolidated research efforts.

### Appendix 3 Position of the Center within Host Institution

\* Diagram the Center's position within the organization of the host institution, and describe that positioning using excerpts from the institution's mid- to long-term plan. If the plan has not been established yet, describe the consideration being given to the Center's positioning.

## Position of the Center within Kyushu University



- Kyushu University (KU) has used the successful I<sup>2</sup>CNER model in establishing Kyushu Univ. Platform for Interdisciplinary/Transdisciplinary Research (Q-PIT).
- KU has strategically involved the entire university in Q-PIT by introducing new systems and applying the "I<sup>2</sup>CNER approach" to both research and education.
- At the same time, Q-PIT facilitates the mission of I<sup>2</sup>CNER in bringing about system reform.
- The campus-wide strategy leads to an action framework that enables I<sup>2</sup>CNER to carry out its research, education, technology transfer, and societal outreach and engagement:
  - i) I<sup>2</sup>CNER will help develop the application for the M.S. and Ph.D. programs of Excellence/Superiority of MEXT that KU will submit next year;
  - ii) I<sup>2</sup>CNER will further integrate with Q-PIT by providing office/lab space to additional faculty from the humanities, social sciences, and economic sciences;
  - iii) I<sup>2</sup>CNER will assist KU in the establishment of a strategic partnership with the University of Illinois.

## Appendix 4. Resource Allocation Plan for Sustaining and Advancing the WPI Center

Annual Plans (FY 2020 –FY 2024)					
<Fund >	(million yen)				
Fiscal Year	2020	2021	2022	2023	2024
- WPI grant	-(*)	-(*)	-(*)	-(*)	-(*)
- Funding from host institution (detail)	616	616	616	616	616
Personnel	385	385	385	385	385
Project activities	97	97	97	97	97
Travel	25	25	25	25	25
Equipment	0	0	0	0	0
Other research projects	109	109	109	109	109
Costs of Satellites	0	0	0	0	0
- Funding from external sources	1,260	1,309	1,358	1,407	1,455
Total	1,876	1,925	1,974	2,023	2,071
<Personnel>	(Person)				
Fiscal Year	2020	2021	2022	2023	2024
- Personnel resources from host institution	130 (102)	130 (102)	130 (102)	130 (102)	130 (102)
- Faculty members (including researchers)	95 (87)	95 (87)	95 (87)	95 (87)	95 (87)
Full-time	21 (21)	21 (21)	21 (21)	21 (21)	21 (21)
Concurrent	74 (66)	74 (66)	74 (66)	74 (66)	74 (66)
- Postdocs	10	10	10	10	10
- RA etc.					
- Research support staffs	10	10	10	10	10
- Administrative staffs	15 (15)	15 (15)	15 (15)	15 (15)	15 (15)

(\*) Do not include expected grant.

- When entering amounts, round down numbers to the first decimal.

- When funding is stated in a range between two amounts, explain the reason for the lower and upper amounts and fluctuations between them.

### < Measures to be implemented from FY 2020 >

- Strategy and action plan for allocating personnel (posts) , space, and others measures required for the Centers' progress.

After the termination of the WPI fund on March 31, 2020, Kyushu University will continue to support I<sup>2</sup>CNER (through strategic allocation of personnel and financial resources) and ensure its success as a world leading research center. The University views the continuation of I<sup>2</sup>CNER's activities beyond the WPI Program period as imperative. In fact, effective April 1, 2013, with the revision of the Regulations of KU, I<sup>2</sup>CNER's position was clearly defined as a permanent Research Institute without regard to the length of the WPI Program.

#### 1. Action plan for allocating personnel resources (posts)

The university will fully support employment expenses for 22 of I<sup>2</sup>CNER's core faculty (10 tenured, 6 transferred PIs, and 4 additional PIs and 2 tenure-track assistant professors hired jointly with IMI). The percentage of foreign researchers (over 50%) and the number of PIs (27 as of April 1, 2020) in the institute will be maintained at the same level as in FY2019.

## 2. Action plan for allocating space

The university will grant I<sup>2</sup>CNER Building II (a total floor space of 5,014m<sup>2</sup>) free of charge to provide an environment for I<sup>2</sup>CNER researchers to continue cutting-edge research. The space provided by this support significantly exceeds the space allotment per researcher under the university's regular policy.

## 3. Other measures for the Center's progress

The university plans to endorse the two platforms in the new organization of I<sup>2</sup>CNER: "Platform for International Collaborations and Partnerships" and "Platform for Societal and Industrial Implementation." These two platforms will advance I<sup>2</sup>CNER's and KU's international collaborations on basic research and accelerate societal impact through effective communication of I<sup>2</sup>CNER's scientific accomplishments and impactful technology development and transfer.

## 4. Kyushu University Administration Support of I<sup>2</sup>CNER Administrative Office

KU will support the salaries of the required staff members, thus securing the successful operation of the "*Three Thrust, Two Platform*" new I<sup>2</sup>CNER organization.