April 2015

3. Research Center Project (in English)

Host institution	Kyushu University
Head of host institution	・ Name, position title Chiharu Kubo, President, Kyushu University
Research center	International Institute for Carbon-Neutral Energy Research (I^2CNER)
Center director	Prof. Petros Sofronis, University of Illinois at Urbana-Champaign, USA
Chief center-project officer(in December2010)	・ Name, affiliation, position title (in December 2010) Yukitaka Murakami (Trustee and Vice President, Kyushu University)
Project summary	・ Briefly describe the general plan of the project. <Center Project> ○ An international effort centered at Kyushu University has been mounted to contribute to the creation of a sustainable and environmentally-friendly society by conducting fundamental research for the advancement of low carbon emission and cost effective energy systems, and improvement of energy efficiency. The research is focused on the basic science underlying the technologies that hold promise for the implementation of a carbon-neutral society (CNS) in terms of a large reduction of greenhouse gas (GHG) emissions (70-80%) from 1990 levels by 2050. This grand challenge in science and engineering is addressed on the basis of two principles: efficiency increase (EI) in energy conversion and use, and lowering of carbon intensity (LCI) of fuel and electricity. There are many possible combinations of new EI and LCI technologies (scenarios) that can lead to the targeted GHG emissions reduction by 2050. The degree of development and deployment timing of these technology options creates the variability amongst scenarios. In close collaboration with the technical teams, the I^2CNER Energy Analysis team is generating scenarios utilizing the most promising new technology options. I^2CNER's research efforts are intimately tied to these scenarios because the short-, mid-, and long-term milestones of each of our research project roadmaps are established in consideration of the development and deployment timing of the various promising technology options in the scenarios. These scenarios and the I^2CNER Roadmaps, which are continuously evaluated and updated as I^2CNER and global energy research progress, help ensure the relevance of I^2CNER's research and roadmaps to CNS. By way of example, the array of technologies that I^2CNER's research aims to enable includes Solid Oxide Fuel Cells, Polymer Membrane based fuel cells, biomimetic and other novel catalyst concepts, and production, storage, and utilization of hydrogen as a fuel. Our research also explores the underlying science of CO_2 capture and storage technology, and the creation of a CO_2 conversion system for the production of value-added chemicals or the storage of renewable-based electricity. ○ There is no time more opportune for such an ongoing international research project, if one considers the international energy landscape. The joint centers/hubs for artificial photosynthesis (JCAP) and energy storage (JSESR) in the US, the ongoing research and industrial research efforts on advancing the science and implementation of geologic sequestration of carbon dioxide and photoelectrochemical hydrogen production funded by the US Department of Energy are key science and technology strategies for energy independence and sustainability. In fact, the I^2CNER research roadmap addresses

fundamental science issues underlying a large number of the technologies envisioned in the Fourth Strategic Energy Plan the government of Japan announced in April 2014, such as the development of next generation power generation technologies, energy conservation, distributed energy systems to raise efficiency, realization of the hydrogen economy, next generation of automobiles, etc. Thus, the fundamental science objectives of I^2CNER serve as a platform for coordinated research between Japanese and US institutions. We have established the "International Institute for Carbon-Neutral Energy Research (I^2CNER)" as a permanent center of excellence in which top-level researchers collaborate, cooperate, share knowledge and exchange ideas, and discuss and debate the science issues and their impact on society.

○ From a fundamental science viewpoint, a pervading theme in all areas of I^2CNER research is the lack of understanding of a range of phenomena occurring at the interface between materials/rocks and gasses such as hydrogen, oxygen, and CO_2. By way of example, we do not understand i) the mechanisms by which hydrogen is adsorbed in materials, making it difficult to design alloys resistant to hydrogen degradation of mechanical properties or to design a light-weight on-board storage medium with the desired hydrogenation/de-hydrogenation properties; ii) the properties and behavior of hydrogen and CO_2 under extreme pressures, iii) the triple-phase rocks/water/CO_2 interactions and the stability of geological traps, and iv) the optimum combination of photocatalyst stability in solution under illumination and the efficient utilization of solar radiation for hydrogen production. From this abbreviated list, it can readily be surmised that the phenomena we are addressing involve disparate length and time scales, ranging from nanometers to thousands of kilometers, and from nanoseconds to centuries. The proposed research addresses the issues as they pertain to all time and length scales, from atomic to the global scale, i.e., from the atom and molecule, to meso/macro-scale crystalline materials, to devices, up to geological formations. The phenomena, although occurring at different media and on disparate time and length scales, often evolve on the basis of the same processes (e.g., species adsorption, absorption, dissolution, diffusion, reaction, conduction) and are characterized by similar scientific principles. Thus, the Kyushu approach cross-cuts disciplinary boundaries through a judicious integration of information from atomistic/microscopic/macroscopic time and length scales for phenomena occurring at the interface of chemistry, physics, materials science, mechanics, geo-science, and biomimetics.

○ The administration and management of our project involves a constant peer evaluation and review of the research activities and outcomes in terms of efficiency and feasibility of each individual research project area, as well as their progress toward attaining the overall project objectives, that is, the realization of a carbon-neutral energy Japan. We have adopted a rigorous approach as we assess our research progress that is predicated on how our science advances technology development and how we impact the removal of roadblocks to a carbon-neutral energy society, such as the lack of a mechanism-based understanding of fatigue of materials or the lack of understanding and control over pore-scale processes and upscaling in CO_2 storage. Lastly, the I^2CNER project pays serious attention to the dissemination of its research results and its scientific culture in the society on several fronts. Tapping into the Illinois academic expertise, we may institute societal educational outreach programs. We leverage the expertise we gained during the last four years in organizing international symposia to engage the scientific community of the industry and government through specialized workshops. Strategies are in place for I^2CNER to inform the society at large about the benefits of a carbon-neutral society as our research begins impacting technology. These strategies pave the way for enriching public understanding of scientific achievements and at the same time, teaching our scientists necessary communication skills.

- In summary, the I^2CNER effort carries out research on fundamental science issues underscoring the removal of roadblocks toward a carbon-neutral energy Japan.

<Research Organization>

- The research effort is organized around high profile research teams of faculty of Kyushu University and partnering institutions worldwide. The Institute relies on top level domestic and internationally recognized researchers in the fields of chemistry, physics, materials science, mechanics, geo-science, and biomimetics. An important component of the organization is the Satellite Institute at the University of Illinois, which promulgates and administers the research activities in the US.

<Project Management>

One of the main goals of the Institute is the restructuring of research management at Kyushu University. This new approach to research administration relies heavily on the management style, academic experience, and scientific achievements of the Institute Director, Professor Sofronis.

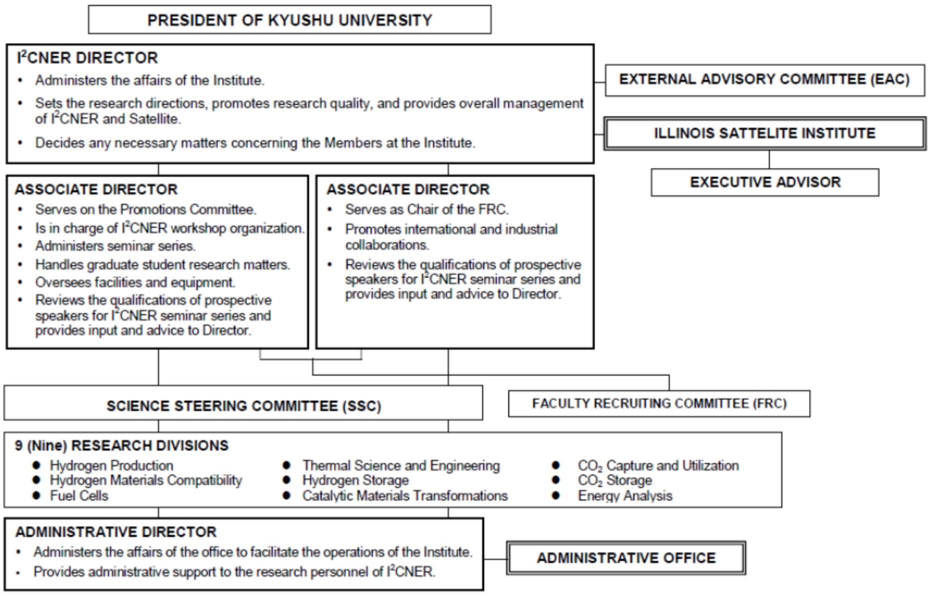
- The Institute has been established as an organization under the direct management of the President of Kyushu University. The Institute Director has direct access to the Office of the President and the Office of the Executive Vice President for Research. The Director is solely responsible for making decisions regarding the planning and conduct of 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. On all these matters, the Director consults the Science Steering Committee (SSC), which is headed by the Director and whose members (science advisors) include the division Lead Principal Investigators and any other additional members that the Director may deem appropriate.
- A vital component of the Institute is the External Advisory Committee (EAC), which is composed of national and international leaders in the field. This Committee is convened annually or, if deemed necessary by the Director, more frequently. The Committee reviews all aspects of the Institute, including its leadership and management, the research progress being made in each activity, and its plans for any initiatives. The Committee provides the Director with a written report on their findings and recommendations. The final decision regarding Institute activities is the responsibility of the Director.
- Another important standing committee of the Institute is the Internal Programs Review Committee (IPRC), 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.
- The Director is assisted by two Associate Directors: Prof. Ishihara, who is responsible for workshop organization, seminar series administration, and management of facilities and equipment, and Prof.

Takata, who is in charge of faculty recruitment, international and industrial collaborations, and graduate student research matters.

○ The role of the Science Steering Committee and the two Associate Directors is strictly advisory. The Director is solely responsible for making the final decisions.

○ The official language of the Institute is English.

I^2CNER ORGANIZATIONAL STRUCTURE



<Collaborations with other institutions and researchers>

○ To carry out its mission, the Institute established collaborations with internationally recognized research centers, universities, and national and international laboratories. These collaborations involve and promote research interactions and exchanges, and visits between the institutions and researchers.

a) Satellite Institute (University of Illinois at Urbana-Champaign, USA)
The Director of the WPI Institute, Professor P. Sofronis, is a faculty member at the University of Illinois at Urbana-Champaign, and is an internationally recognized expert on the effects of hydrogen on the mechanical properties of materials. The Illinois Satellite faculty members are all internationally recognized researchers in their respective areas of expertise. They were specifically invited to complement the I^2CNER research activities at Kyushu. Therefore, a Satellite Office has been established at Illinois to facilitate 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. Director Sofronis also serves as the Director of the Satellite Institute. In this latter capacity, he reports directly to the Dean of the College of Engineering at the University of Illinois. An agreement for undergraduate student exchange and a memorandum of understanding between Kyushu and Illinois are in place.

b) Collaborating Institutions and researchers
We are engaged in collaborative research with distinguished

	scientists from internationally recognized institutions, such as the National Fuel Cell Research Center (NFCRC) at the University of California, Irvine, the California Air Resources Board (CARB), SINTEF/NTNU of Norway, and the Helmholtz Zentrum Geesthacht (HZG) in Germany. In addition, researchers individually collaborate with their distinguished counterparts from institutions such as MIT, Max-Planck, Imperial College London, the University of Oxford, etc. These partnerships and collaborations include site visits to facilitate research by leveraging research capabilities. The set of these institutions is constantly changing, depending upon how I^2CNER's research objectives are attained and how research efforts are redirected or terminated.
	Major changes from initial project plan: ○ The Energy Analysis Division (EAD) was established to continuously review and revise the Institute's vision and roadmap toward a carbon-neutral society over time scales of short, middle, and long ranges. The idea is that the Institute addresses the roadblocks for a carbon-neutral energy society which are caused by the constraint of primary energy resources and availability on the basis of CO_2 emissions, efficiency, cost, national security, and resilience. The EAD's goals are to: i) assess the relevance of the Institute's research activities vis-à-vis I^2CNER's roadmap for a carbon-neutral society and ii) ensure that I^2CNER's research is informed of all relevant current and future energy options of Japan. ○ Whereas the original program was centered on Hydrogen and CO_2, as time progressed, and with the introduction of the Energy Analysis Division, we found that we can achieve a carbon-neutral energy society by pursuing the current mission statement, which is listed below. ○ As part of the transition of I^2CNER into a permanent unit within the Kyushu University system, a Faculty Council was established on April 1 2013. The establishment of the Faculty Council helped to facilitate the transfer of 9 PIs from the Faculty of Engineering.
Mission statement and/or center's identity	・ Briefly and clearly describe the mission statement and/or the project's identity as WPI center. I^2CNER is a collaboration between Japan and the international community, based at Kyushu University, with a Satellite Institute at the University of Illinois at Urbana-Champaign. At I^2CNER, our mission is to contribute to the creation of a sustainable and environmentally-friendly society by conducting fundamental research for the advancement of low carbon emission and cost effective energy systems, and improvement of energy efficiency. The array of technologies that I^2CNER's research aims to enable includes Solid Oxide Fuel Cells, Polymer Membrane based fuel cells, biomimetic and other novel catalyst concepts, and production, storage, and utilization of hydrogen as a fuel. Our research also explores the underlying science of CO_2 capture and storage technology, and the creation of a CO_2 conversion system for the production of value-added chemicals or the storage of renewable-based electricity. Additionally, it is our mission to establish an international academic environment that fosters innovation through collaboration and interdisciplinary research (fusion).

(1) Research fields

・ Specifying the inter-disciplinary field(s) to which the project may be closely related.

・ Describe the importance of the proposed research, including domestic and international R&D trends in the field and Japan's advantages.

・ If centers in similar fields already exist in Japan or overseas, please list them.

Research fields:
Fundamental science for an economy based on carbon neutral energy.
Multi/inter-disciplinary science, integrating Chemistry, Physics, Materials Science, Mechanics, Geoscience, and Biomimetics. We also plan to include additional disciplines in our research portfolio, such as mathematics, computational science, economics, technology forecasting, and life sciences.

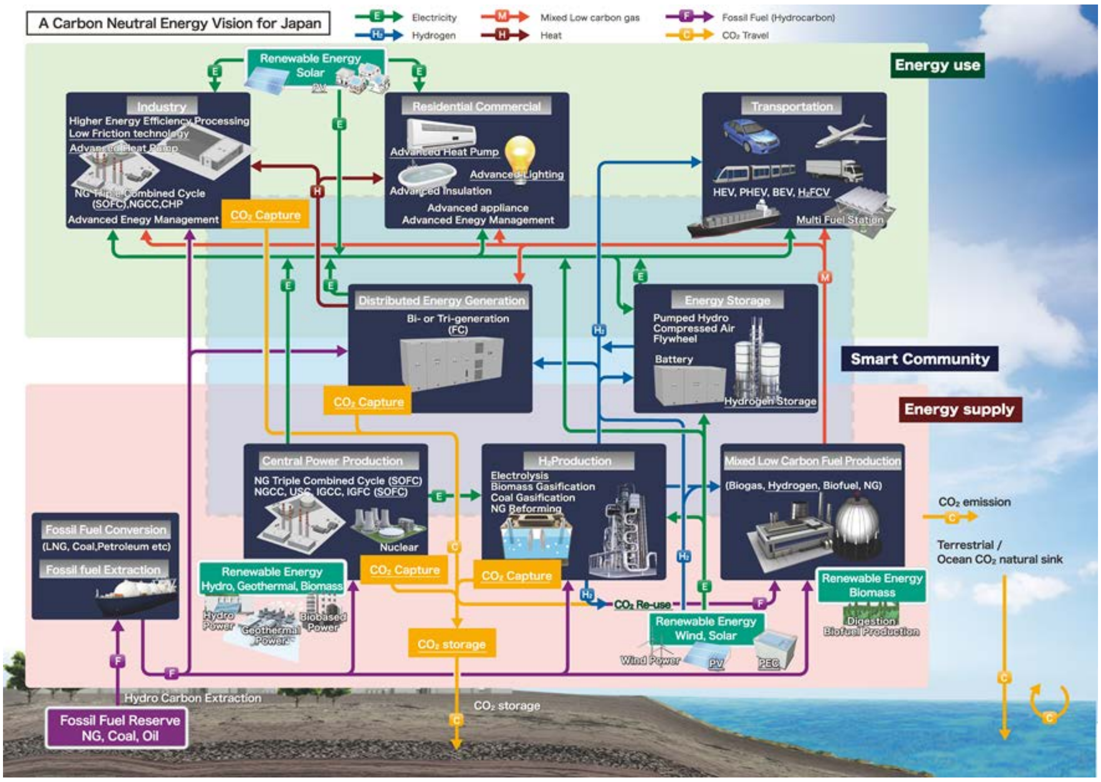
Importance of the proposed research:

○ The disasters caused by the Tohoku Region Pacific Coast Earthquake, tsunami, and Fukushima nuclear accident have brought to the fore serious issues related to the energy infrastructure and future of Japan. There is a vital need to develop sustainable sources of energy without CO_2 emissions, and to establish safe and reliable carbon capture and storage (CCS) systems for the realization of a carbon-neutral energy society.

○ From the viewpoint of limited fossil fuel resources, energy security, capital outflow, and the economic instability due to fluctuating and unpredictable oil prices, there is an urgent need for the establishment of a flexible energy system which integrates a diverse range of energy sources.

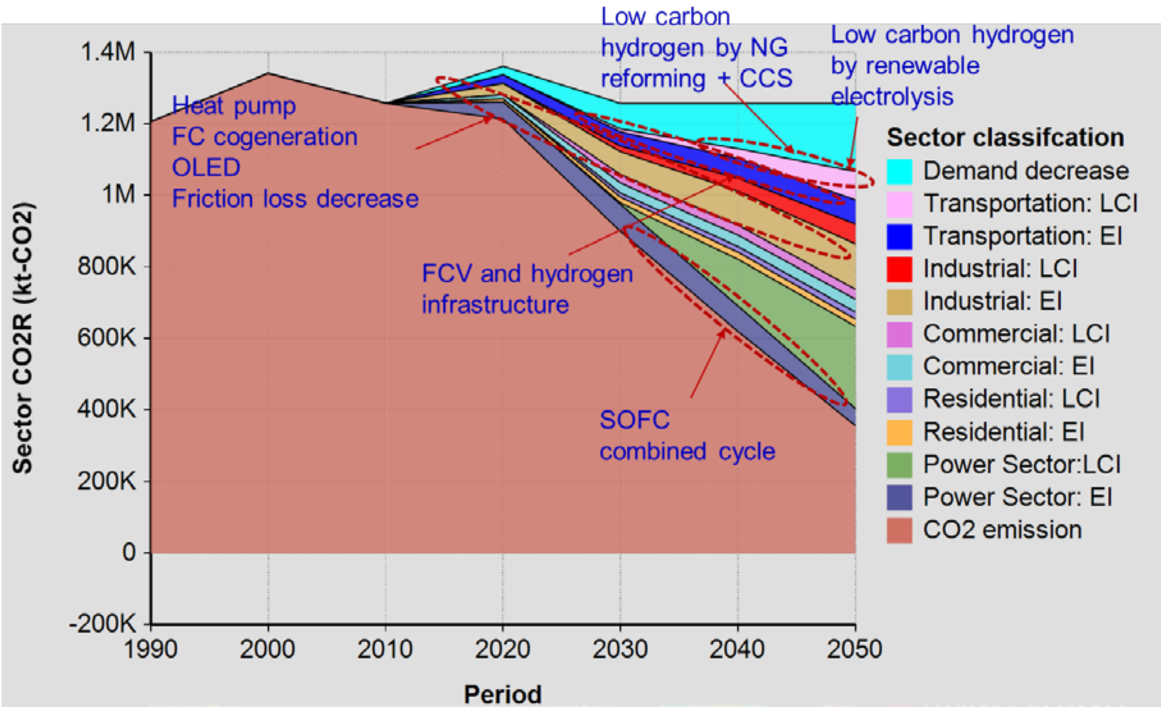
○ In 2009, the G8 announced the commitment of an 80% GHG reduction in 2050 relative to the 1990 level. The I^{2}CNER Vision for a low carbon society for Japan is based on setting a long-term target of a large reduction (70-80%) of greenhouse gas emissions by 2050. This target is primarily relevant to environmental concerns (climate mitigation), but is also relevant to energy security concerns caused by Japan's heavy reliance on imported fossil fuels. To help achieve the target through the development of new energy technologies, we also consider economic efficiency and safety issues. As a whole, we consider 3E+S (Environment, Energy Security, Economy and Safety) as basic view points for our approach.

○ The figure below shows the image and relationship between energy conversion and utilization sectors, which are connected by energy pathways that are represented by secondary energy (electricity, hydrogen, and mixed low carbon fuels using bio fuel) in a low carbon society. Some fossil fuel will still be provided to energy conversion sectors and industry with CO_2 capture and storage (CCS). Some captured CO_2 can be re-used as an energy carrier.



Energy Vision for Japan: Parameter Space of Technology Options

○ I^{2}CNER's research program is based on two major principles: efficiency increase (EI) in energy conversion and energy use, and lowering of carbon intensity (LCI) of fuel and electricity to adopt and develop future technologies. EI is pursued in energy transformation systems as well as end use systems and industrial processes. EI can be applied to existing systems, but is also achieved by replacing existing systems with new technology. LCI in electricity and fuel supply-use pathways is achieved using either renewables or CCS. LCI tends to need new facilities or new infrastructure or both. There are many possible combinations of new EI and LCI technologies and deployment timing (scenarios) that can lead to the targeted GHG emissions reduction by 2050. I²CNER's research efforts are intimately tied to these scenarios because the short-, mid-, and long-term milestones of each of our research project roadmaps are established in consideration of the development and deployment timing of the various promising technology options in the scenarios. Overall, our scenario analyses show that a large deployment of renewables along with CCS can achieve low carbon intensity in the power and transportation sectors, which, coupled with a large penetration of EI technologies across the sectors, results in as much as about 70% GHG emission reduction. The figure below shows a base scenario in which the development of important EI technologies with balanced deployment of LCI technologies and CCS can achieve a 71% reduction of CO_2 emissions from their 1990 level by 2050.



CO_2 reduction relative to 1990 levels by sector in a scenario which relies on development of important EI technologies and balanced deployment of LCI technologies and CCS

○ In addition, I²CNER is advancing green innovation, as demonstrated by the 18 submitted applications for patents and the large number of industries, such as the automotive (TOYOTA, Nissan, and HONDA), Kyocera, Mitsubishi Hitachi Power Systems, JX Nippon Oil and Energy, Air Liquide, and the JFE Steel Corporation, that are benefiting from ongoing joint research projects with I²CNER researchers. A technology transfer event has already taken place through TOKi engineering on a new type of metal packing for high-pressure hydrogen.

○ Japan has been one of the world's pioneers in the field of renewable/clean energy technologies, such as fuel cells for residential application, fuel cell vehicles, and hydrogen stations, and , Kyushu University has a strong research record and cutting-edge research facilities in these fields. For example, Kyushu University is internationally recognized for its research activities related to hydrogen energy, from fundamental science issues to the assessment and evaluation of actual fuel cells and hydrogen stations. Thus, the existing research foundations and accomplishments of Kyushu University have provided a valuable and advantageous setting for our international effort. Although the research on carbon capture and storage has been intensively undertaken worldwide, there are still a number of critical issues to be addressed, such as understanding the role of pore-scale flow processes on the large-scale migration of CO_2 before accurate predictions of CO_2 migration can be made. At I²CNER, i) we have performed the largest numerical simulation of liquid/supercritical CO_2 drainage and imbibition processes, including precipitation, which is central to accounting for the "dynamic" nature of the pore space as CO_2 is injected, and ii) we were the first to quantify the flow processes associated with liquid/supercritical CO_2 drainage and imbibition in laboratory experiments and quantified dynamic processes that drive CO_2 migration and trapping, termed Haines jumps. Pore-scale models do not account for such dynamics, yet we find that these intermittent events can greatly perturb trapped CO_2.

○ There are a number of energy centers worldwide, like the corresponding energy hubs in the U.S., that are targeting specific energy areas, such as storage or hydrogen production. However, I^2CNER is a highly unique center, in that its mission is holistic—it targets the energy problem from generation to utilization and aims to reduce emissions based on economy, efficiency, and security. In this regard, there is no other center like I^2CNER in the world.

(2) Research objectives

・ Describe in a clear and easy-to-understand manner the research objectives that the project seeks to achieve by the end of the grant period. In describing the objectives, the following should be articulated in an easily understandable manner: What kind of research do you plan to implement by fusing various fields within the environmental domain? In the process, what world-level scientific issues are sought to be resolved? What is the expected impact of the scientific advances to be achieved on society in the future?

・ Describe concretely the research plan to achieve these objectives.

○ We are conducting fundamental research for the advancement of low carbon emission and cost effective energy systems and improvement of energy efficiency. Our research efforts address project objectives within thematic research clusters (divisions). Within each project, research is carried out along a roadmap with short-, mid-, and long-term milestones and ultimate targets. The roadmaps, which are continuously updated as our research progresses, are compatible with the mission of I^2CNER, as actualized by the energy scenarios developed by the EAD, in collaboration with the technical divisions. To reach the roadmap targets, our approach involves multiple disciplines, such as chemistry, physics, materials science, mechanics, geoscience, and biomimetics, in order to investigate phenomena such as species diffusion taking place at the interface of interactions between materials and hydrogen, oxygen, and CO_2 at all scales, from the atomic to those for geological systems, and from nanoseconds to decades. We also aspire to contribute to the societal debate by informing the public about the benefits of transitioning to a carbon-neutral energy society and providing sound scientific data on geological sequestration of CO_2. Below, an outline of the research objectives for each individual division is presented, followed by a detailed description of the related research plans:

- Production of Hydrogen without forming CO_2. Use of solar energy to produce hydrogen through two pathways: high temperature electrolysis driven by organic photovoltaics (PV) and photoelectrochemical water splitting; Development of energy conservation devices: organic light emitting diode and low friction bearings.
- Develop predictive performance models for materials subjected to hydrogen-affected fatigue, fracture, wear, and seizure that revolutionize design and materials selection of components in hydrogen service.
- Development of more durable, efficient, and lower cost fuel cells, including polymer electrolyte fuel cells (PEFCs) and solid oxide fuel cells (SOFCs), to significantly reduce CO_2 emissions in the production of electricity and heat.
- Expand material thermophysical property information and thermal science and engineering to help enable the most effective use of materials in carbon-neutral energy technologies and to improve the energy efficiency of thermal processes.Research and develop new carrier materials for enhanced hydrogen mobile and stationary storage, as well as for hydrogen delivery.
- Develop breakthrough novel biomimetic based catalysts and pathways for the carbon neutral production of power (fuel cells), hydrogen, and hydrocarbon fuels based on solar energy resources. Develop new catalysis for fuel oxidation and regeneration, and novel materials to enable new carbon neutral fuel and energy cycles for electricity storage and energy distribution.
- Development of highly efficient materials for CO_2 separation in power generation and industrial processes, and creation of an energy efficient and cost effective CO_2 conversion

system for (i) production of value-added chemicals, such as a liquid fuel or their intermediates or (ii) storage as renewable energy.

- Identify and investigate key pore-scale processes that drive effective residual, solubility, and mineral CO_2 trapping in geologic formations typical of Japan; Translate this understanding to the development of methods for accurate reservoir characterization to ensure safe and enhanced CO_2 storage; Develop new effective methods for monitoring injected/leaked CO_2 in sub-seabed geologic formations, and identify field-scale CO_2 behavior; Propose and realize innovative CCS concepts suitable for geological formations typical of Japan.
- Provide carbon emission, energy efficiency, and cost analysis of current and emerging I^2CNER and other energy processes, technology, and infrastructure to help ensure I^2CNER and global energy related research is well-targeted towards a carbon neutral society. Continuously review and revise the Institute's vision and roadmap toward a carbon-neutral society based on I^2CNER and other energy system analyses.

Research Plan to achieve these objectives

In the following, the terms short-, mid-, and long-term refer to the corresponding timescales that are applied to the milestones in the division roadmaps.

1) Hydrogen Production (Lead Principal Investigator: Prof. Ishihara)

The research in this division falls under the themes of energy production, conservation, and storage. Energy production is based on the conversion of solar to electric energy, storage is achieved through hydrogen fuel, and conservation is achieved through enhanced lighting efficiency based on high efficiency solid state lighting. Unique aspects are techniques for the analysis of the interface structure of organic dye and inorganic semiconductors, experimental materials synthesis, device fabrication and testing, and theory-based materials development. Projects encompass novel inorganic and organic photocatalysts and electrodes, synthesis of novel molecules for organic light emitters and photoelectrochemical and photovoltaic cells, and materials for electrochemical and electrolytic water reduction. As a complement, organic light emitting devices are being developed for high efficiency lighting for energy conservation. Selected results are:

Photocatalytic water splitting

Artificial photosynthesis, specifically photocatalytic water splitting**,** is a promising approach for innovative hydrogen production without CO_2 generation. Current solar photocatalysts suffer from two critical problems: either their band gaps are too large for efficient utilization of solar radiation, or they are unstable under illumination. We are pioneering a fresh approach to a new class of extremely light-absorbent, stable materials. Our approach is based on a highly-interdisciplinary coupling of 'correlated metal oxides' (playground materials for the condensed matter physics community), with titanium dioxide (TiO_2), the workhorse for photocatalytic water splitting. Correlated metal oxides such as $SrRuO_3$ are unique: they display semiconductor-like optical absorption and metal-like conductivity. The coupling of these two materials (Fig. 1a) offers large optical absorption in the correlated metal oxide, efficient charge transport of hot carriers from the oxide to the TiO_2, and the desirable surface chemistry of TiO_2 for catalyzing chemical reactions [1]. We have demonstrated the generality of this approach by showing that several correlated metal oxide – TiO_2 systems ($SrRuO_3$, $LiNiO_3$, $SrVO_3$, $LaSrMnO_3$, $LaSrCoO_3$) exhibit dramatically enhanced photocatalytic activity [2]. This work addresses the Project 2 (photocatalytic water splitting) short-term milestone of achieving energy conversion efficiency larger than 1%, as specified in Reference 2-1.

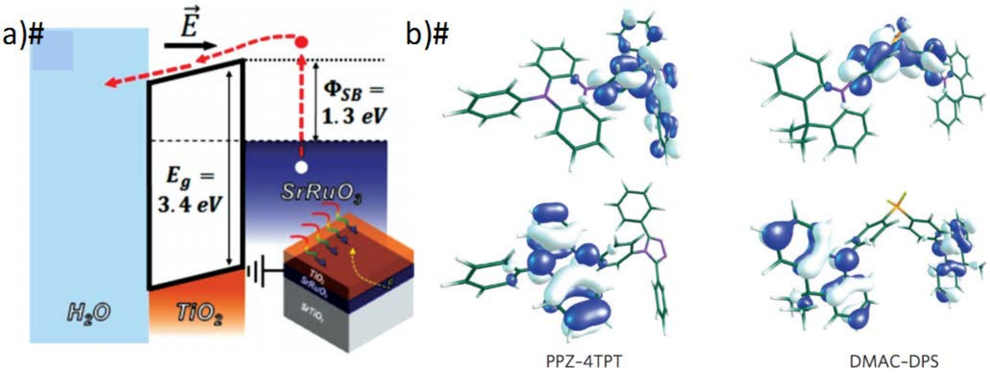


Fig. 1: a) Hot carrier injection enables the photoexcited carriers in $SrRuO_3$ to quickly transfer to the TiO_2 [1,2]. b) Molecular complexes designed with first-principles for thermally-activated delayed fluorescence for high efficiency blue OLEDs [3,4].

Organic Light-emitting Diodes (OLEDs)

Organic light-emitting diodes (OLEDs) have been considered to be a promising approach to solid-state, low power lighting. However, efficiencies remain low, while costs can be prohibitively high. The most common fluoresence scheme, light generation, is limited because only 25% of the excited carriers (the singlets) can produce light. While the newer phosphorescence schemes eliminate this limitation, allowing for nearly 100% luminescence, widespread usage is constrained by the need to use expensive noble metals. In this accomplishment, we have demonstrated blue OLEDs that enable light generation from all excited carriers, without the need for noble metals [3]. The approach is based on thermally-activated delayed fluorescence (TADF), a third-generation scheme developed by the Adachi group [4]. It relies on thermally-activated charge-transfer: a thermally accessible gap between the lowest singlet and the triplet excited states enables the harvesting of both singlets and triplets. Quantum mechanical simulation was used to assess several candidate molecules and identify those exhibiting the desired low energy difference between the singlet-triplet state (Fig 1b). The system demonstrates an external quantum efficiency of 19.5%, comparable to the best phosphorescent OLEDs commonly used today. The accomplishments described above address the Project 3-1 (OLEDs) short-term milestone of achieving energy conversion efficiency larger than 100lm/W, as specified in Reference 2-1.

Future Directions

At present, complete water splitting has not been achieved due to several limitations, including efficient light absorption, efficient charge carrier lifetimes and separation, and favorable reaction chemistry. Our future directions target key critical improvements, such as:

- *Molecular switching schemes.* To date, our division developed the double excitation Z-scheme mechanism, which combines a structure-controlled oxide semiconductor and an organic semiconductor to produce hydrogen and oxygen efficiently. Targeting our long-term objectives, we will expand on this by introducing the *molecular switch* concept, which allows carrier flow in only one direction. We have also developed the methodology for very fast charge transfer to an organic compound using novel oxynitrides in tandem with new organic semiconductors. In the proposed research, we will investigate generation of hydrogen through complete water splitting and newly proposed combinations, such as enzymes like hydrogenase with an inorganic photocatalyst system.
- *Solar cell/Steam Electrolysis.* Since our short-term objectives are aimed at achieving higher efficiency H_2 production via combined solar cells and steam electrolysis, we will focus on organic perovskite compounds as organic semiconductors, and the application of stable double perovskites as the electrodes for steam electrolyzers. Additionally, oxide cathodes will be studied for CO_2-H_2O co-electrolysis for conversion to useful compounds like CH_4.
- *Enabling Fundamental Studies.* We will carry out research on the biomimetic synthesis of new inorganic-organic semiconductors; the control of dye at material interfaces; the charge transfer process; the structure of the electrodes in solar and electrolytic cells at the atomic level; and the separation efficiency of photo-excited charges. Ultimately, our research will contribute to the development of a hydrogen production technology without CO_2 emission. This work will target the development of a new type of photocatalyst using active centers for the enzyme, through the integration of molecular chemistry, biomimetics, biomaterials, green

chemistry, and surface chemistry. (short- to long-term)

- *Energy conservation.* Energy conservation devices are also covered in this division, since lighting is a large source of energy consumption. We will focus on designing new light emitting molecules based on thermal activated delayed fluorescence (TADF) exhibiting larger sizes and increased stability. (short- to long-term)

References:

1. Lee, S., Apgar, B. A. and Martin, L. W. (2013), Strong visible-light absorption and hot-carrier injection in TiO2/SrRuO3 heterostructures, Advanced Energy Materials, 3 (8), 1084-1090.
2. Apgar, B. A., Lee, S., Schroeder, L.E. and Martin, L. W. (2013), Enhanced photoelectrochemical activity in All-oxide heterojunction devices based on correlated “metallic” oxides, *Advanced Materials*, 25 (43), 6201-6206.
3. Zhang, Q., Li, B., Huang, S., Nomura, H., Tanaka, H., and Adachi, C. (2014), Efficient blue organic light-emitting diodes employing thermally activated delayed fluorescence, *Nature Photonics*, 8 (4), 326-332.
4. Uoyama, H., Goushi, K., Shizu, K., Nomura, H. and Adachi, C. (2012), Highly efficient organic light-emitting diodes from delayed fluorescence, *Nature*, 492 (7428), 234-238.

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

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

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

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

Fatigue crack growth rate experiments were performed on the pipeline steel X52 in hydrogen gas with controlled oxygen concentrations. The approach in these experiments represented a radical departure from previous studies, since key variables, e.g., oxygen concentration, load-cycle frequency, and mean stress, were identified and systematically varied. As a result, unequivocal trends for the effects of oxygen on hydrogen-accelerated crack growth were revealed for the first time. The quality of these data enabled postulation of the physics governing oxygen inhibition of hydrogen-accelerated crack growth [1]. Based on these proposed physics, an analytical model was developed to predict inhibition as a function of inert-environment crack growth rate, oxygen concentration, load-cycle frequency, and mean stress. The model accurately quantifies how these variables affect the onset of accelerated crack growth for X52 steel in hydrogen gas containing trace oxygen concentrations (Fig. 2). In summary, this model is the only predictive capability for quantifying the effects of oxygen on hydrogen-accelerated fatigue crack growth.

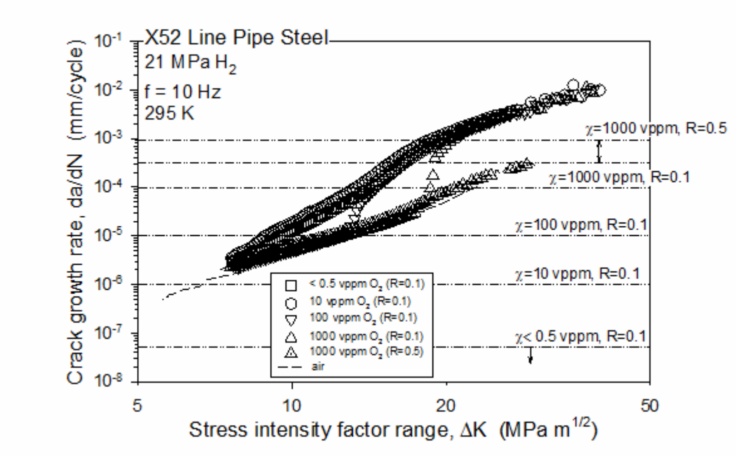


Fig. 2: The measured onset of hydrogen-accelerated crack growth (symbols) is reliably predicted (dashed lines) as a function of oxygen concentration (□) and mean stress (R) [1].

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

Future Directions

- Define the physics-informed fatigue limit and its relationship to environmental conditions and material characteristics for structural metals in hydrogen gas, emphasizing high strength alloys. (short- to long-term)
- Identify mechanisms for hydrogen-induced fracture mode transitions in ferritic and austenitic alloys, considering the role of hydrogen-induced microstructure evolution. Transform this evidence into physical descriptions of H_2-assisted crack propagation in low-strength steels, for the first time including the role of microstructure-scale stresses. (short- to mid-term)
- Formulate and validate a predictive model of hydrogen-assisted fatigue crack growth for low-strength steels. (mid-term)
- Develop and apply advanced materials testing methods to define relationships between material characteristics (e.g., alloy composition) and hydrogen-affected deformation mode in austenitic alloys. Apply these experimental data to inform and validate theoretical constitutive descriptions of material behavior based on the crystallinity of slip. (short-term)
- Develop hydrogen-compatible, lower-cost austenitic stainless steels having 800 MPa yield strength and quantify their fatigue limit in hydrogen gas. (long-term)
- Evaluate and improve sensitivity of material damage sensors for stationary hydrogen pressure vessels. Integrate predictive hydrogen-assisted fatigue crack growth model and material damage sensors in functioning structural health monitoring system for pressure vessels. (short- to long-term)
- Discover effects of environment on tribo-film formation with low friction materials including coatings and polymers. (short-term)
- Define salient factors in surface processes, hydrogen uptake, structural changes, and resulting tribo-failures for rolling and sliding in various environments. (short-term)
- Develop models of mechanical and chemical processes relevant to tribo-failures and tribo-film formation. (short-term)

References:

1. Somerday, B. P., Sofronis, P., Nibur, K.A., San Marchi, C. and Kirchheim, R. (2013), Elucidating the Variables Affecting Accelerated Fatigue Crack Growth of Steels in Hydrogen Gas with Low Oxygen Concentrations, *Acta Materialia*, 61 (16), 6153-6170.
2. Staykov, A., Yamabe, J. and Somerday, B. P. (2014), Effect of Hydrogen Gas Impurities on the Hydrogen Dissociation on Iron Surface, *International Journal of Quantum Chemistry*, 114 (10), 626-635

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

The objective of this division is to develop more durable and efficient, lower cost fuel cells, such as polymer electrolyte fuel cells (PEFCs) and solid oxide fuel cells (SOFCs). In PEFCs, efforts are directed at a) the development of higher temperature (> 100˚C) hydrogen PEM fuel cells with durable catalyst support, b) finding and evaluating high temperature electrolytes with emphasis on a polybenzimidazole (PBI)-based ionomer in combination with carbon nanotubes, including additional materials, such as graphene. In SOFCs, efforts are directed at exploring degradation mechanisms of pressurized SOFCs and understanding fundamental surface/interfacial catalytic processes on metal oxides for fuel-flexible stationary and power-plant applications, especially the Integrated Gasification Fuel Cell Combined Cycle (IGFC) and the Natural Gas Triple Combined Cycle. Selected representative results are:

Alternative Electrocatalysts

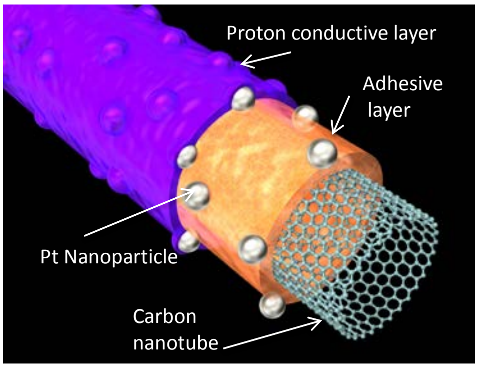


Fig. 3: Carbon nanotube-based fuel cell electrocatalyst without any defect sites that shows ~100 times higher durability than a conventional carbon black fuel cell catalyst [10]. The catalyst was fabricated using a bottom-up nano-assembly method.

A novel polymer electrolyte fuel cell (PEFC) exhibiting remarkably high durability (single cell test: >400,000 cycles using the common standard protocol set by Japanese car makers to check this voltage cycle durability) and high power density operating at 120 ˚C under non-humidified conditions has been developed (Fig. 3). These results are at least a factor of five better than that presently available from the current state-of-the-art high-temperature operation PEFCs. The dramatic improvement in durability was achieved using a polybenzimidazole (PBI) membrane developed by the group of PI Nakashima [1-7]. This durable PEFC for high-temperature operation will accelerate the technological shift from Nafion-based low-temperature PEFCs to a PBI-based high-temperature PEFC. By realizing the high-temperature PEFC, PEFCs will achieve a higher efficiency and lower Pt poisoning than Nafion-based PEFCs. In addition, since high purity of H_2 is not necessary for a high-temperature PEFC, a large reduction in poisoning can be expected. Along with recent catalyst developments, [8] these results solve three major problems attendant new PEFCs: durability, humidification, and high temperature operation, as described in the NEDO roadmap.

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

Understanding the origin of chemical expansion in SOFCs and developing new materials with reduced chemical expansion.

In many advanced electrodes for low temperature SOFCs, non-stoichiometry induced dilation (chemical expansion) can lead to large strains and stresses during operation, ultimately resulting in mechanical failure. The group of PI Tuller, et al. showed the critical role of both cations and oxygen vacancies in this dilation. [9]. Along with PI Kilner, they found that cation substitution could be used to manipulate the chemical expansion coefficient [10]. Experimental realization of this concept came through studies of isovalent Zr substitution in cerium oxide, where chemical expansion was derived experimentally and computationally with density functional theory (DFT) calculations on $Zr_{0.5}Ce_{0.5}O_{2-\delta}$ [11]. Zr substitution was found to decrease the chemical expansion coefficient relative to that observed in ceria alone. The origin of the reduced chemical expansion coefficient is associated with a larger contraction of the lattice around oxygen vacancies. Recent work by the group demonstrated that charge localization on reduced cations can also play a significant role in chemical expansion reduction[12].This discovery has strong implications for reducing chemical expansion in SOFCs, thus increasing their durability.

Future Directions

- Develop an improved, lower cost, higher temperature (> 100˚C) PEFC (HT-PEFC) with higher efficiency and better durability for fuel cell vehicles by developing alternative materials. HT-PEFCs exhibit significant advantages in fuel efficiency improvement and CO poisoning suppression. (mid- to long-term)
- Develop high-temperature membrane-electrode assembly (MEA). (short-term)
- Develop durable catalyst support for HT operation, with a specific focus on graphene, carbon nanotubes, mesoporous carbons, and SnO_2. (mid-term)
- Develop Pt-free catalysts optimized for HT operation. (mid-term)
- Understand the interplay of protons and electrons in HT catalysis relevant to fuel cells.
- Develop high temperature electrolyte based on polybenzimidazole (PBI), and charge-transfer complex hybrid films. (short-term)
- Understand degradation mechanism in SOFCs and fundamental surface/interfacial catalytic processes on metal oxides for SOFCs to realize the long-term chemically durable SOFCs for ambient operation. (mid- to long-term)
- Achieve 10-year cell durability, with all major degradation mechanisms understood. (mid-term)
- Develop advanced electrodes for higher activity (cathode) and higher fuel utilization. (anode) (mid- to long-term)
- Achieve long-term durability for higher system efficiency of 60%LHV (total efficiency of 90%). (long-term)

References:

1. Fujigaya, T. and Nakashima, N. (2013), Fuel Cell Electrocatalyst Using Polybenzimidazole-Modified Carbon Nanotubes As Support Materials, *Advanced Materials*, 25 (12), 1666-1681.
2. Fujigaya, T., Okamoto, M., Matsumoto, K., Kaneko, K. and Nakashima, N. (2013), Interfacial engineering of platinum catalyst for fuel cells: Methanol oxidation is dramatically improved by polymer coating on a platinum catalyst, *ChemCatChem*, 5 (7), 1701-1704.
3. Berber, M. R., Fujigaya, T. and Nakashima, N. (2014), High-Temperature Polymer Electrolyte Fuel Cell Using Poly(vinylphosphonic acid) as an Electrolyte Shows a Remarkable Durability, *ChemCatChem*, 6 (2), 567-571.
4. Fujigaya, T., Hirata, S. and Nakashima, N. (2014), A Highly-Durable Fuel Cell Electrocatalyst Based on Polybenzimidazole-coated Stacked Graphene, *Journal of Materials Chemistry A*, 2 (11), 3888-3893.
5. Fujigaya, T., Kim, C., Matsumoto, K. and Nakashima, N. (2014), Palladium-based Anion-exchange Membrane Fuel Cell using KOH-doped Polybenzimidazole as the Electrolyte, *ChemPlusChem*, 79 (3), 400-405.
6. Berber, M. R., Fujigaya, T., Sasaki, K. and Nakashima, N. (2013), Remarkably Durable High Temperature Polymer Electrolyte Fuel Cell Based on Poly(vinylphosphonic acid)-doped Polybenzimidazole, *Scientific Reports*, 3, 1764.
7. Fujigaya, T., Kim, C., Matsumoto, K. and Nakashima, N. (2013), Effective Anchoring of Pt-Nanoparticles onto Sulfonated Polyelectrolyte-Wrapped Carbon Nanotubes for Use as a Fuel Cell Electrocatalyst, *Polymer Journal*, 45 (3), 326-330.
8. Liu, J., Takeshi, D., Orejon, D., Sasaki, K. and Lyth, S. M. (2014), Defective Nitrogen-Doped Graphene Foam: A Metal-Free, Non-Precious Electrocatalyst for the Oxygen Reduction Reaction in Acid, *Journal of the Electrochemical Society*, 161 (4), F544-F550.
9. Marrocchelli, D., Bishop, S. R., Tuller, H. L. and Yildiz, B. (2012), Understanding chemical expansion in non-stoichiometric oxides: ceria and zirconia case studies, *Advanced Functional Materials*, 22 (9), 1958-1965.
10. Marrocchelli, D., Bishop, S. R. and Kilner J. A. (2013), Chemical expansion and its dependence on the host cation radius, *Journal of Materials Chemistry A*, 1 (26), 7673-7680.
11. Bishop, S. R., Marrocchelli, D., Fang, W., Amezawa, K., Yashiro, K. and Watson, G. W. (2013), Reducing the chemical expansion coefficient in ceria by addition of zirconia, *Energy and Environmental Science*, 6 (4), 1142-1146.
12. Bishop, S. R., Marrocchelli, D., Chatzichristodoulou, C., Perry, N. H., Mogensen, M. B., Tuller, H. L. and Wachsman, E. D. (2014), Chemical Expansion: Implications for Electrochemical Energy Storage and Conversion Devices, *Annual Review of Materials Research*, 44, 205-239.

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

The objective of this division is to enable the most effective use of materials in carbon-neutral energy technologies and to improve the energy efficiency of thermal processes by expanding our knowledge of material thermophysical properties and thermal science and engineering. More specifically, research in the division aims at: expanding our knowledge-base of thermophysical properties of hydrogen and alternative refrigerants to enable their most efficient use to reduce CO_2 emissions; improving our understanding of the basic science of heat and mass transfer to enable the development of more efficient energy systems; and researching new thermal energy heat pump and refrigeration systems focused on the use of waste heat and new refrigerants for improved overall energy efficiency and reduced CO_2 emissions.
Selected representative results are:

Vacuum generation by hydrogen permeation: hydrogen purity gas analyzer

Thermophysical properties of hydrogen are of practical importance in a variety of hydrogen energy systems, such as hydrogen refueling applications and on-board high pressure hydrogen tanks of FCVs. In such hydrogen systems, a high level of airtightness is required for safe hydrogen storage. However, hydrogen leaks easily from the vessel wall, especially at high temperatures. Hence, the permeability of hydrogen is a key parameter for vessel design and prediction of the leak rate of hydrogen through material walls. PI Takata and coworkers [1] have developed a simple apparatus for the measurement of permeability of hydrogen by monitoring pressure inside tubular vessels made of SUS316L and Inconel 625 (Fig. 4, top). They found that by heating the vessel up to 300-500°C, the inside pressure decreases and finally reaches the vacuum condition (Fig. 4, bottom) after heating for 5 hours at 500°C for the case of Inconel 625.

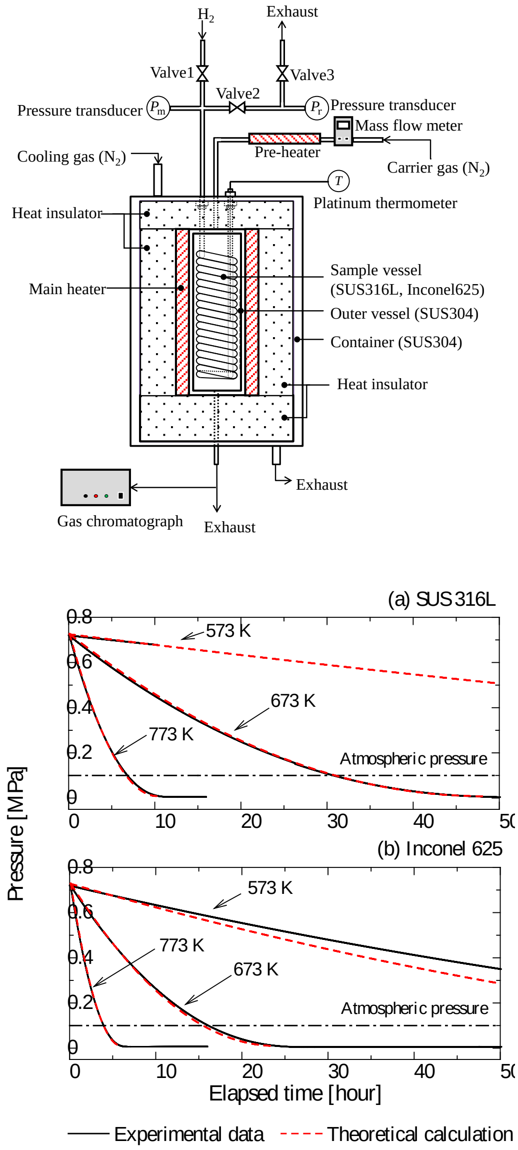


Fig. 4. (top) A simple apparatus for the measurement of permeability of hydrogen.

(bottom) (a) Pressure change with heating time for SUS316L. (b) Pressure change with heating time for Inconel 625.

It is known that hydrogen leaks through metal vessel walls with an attendant decrease of pressure. However, the present work is the first demonstration of an inside vessel nearly reaching vacuum conditions. This phenomenon is explained by the fact that the driving force for permeation is proportional to the difference of the square root of hydrogen partial pressures inside and outside the vessel. Since the partial pressure of hydrogen in the air is very small, the partial pressure inside the vessel can decrease to an almost zero value (exactly, the partial pressure of impurities). The ratio of the final internal pressure to the initial pressure is equal to the mole fraction of impurities. The present method can be used to evaluate and design hydrogen purity gas analyzers.

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

Future directions

- Development of boiling surface with onset of boiling at less than 2K in superheating and with critical heat flux (CHF) by 2.5 times higher than copper surface. Clear understanding of wettability effects in liquid-vapor phase change. Apply this technology to a high-performance device cooling. (short-term)
- Measurement of heat transfer characteristics of micro liquid layer in boiling and evaporation process by making use of thermoreflectance method. (mid-term)
- Clear understanding of multiscale thermal transport in liquid-vapor phase change. (short- to long-term)
- Accumulation of adsorption isotherm and kinetics data of natural or low global warming potential (GWP) refrigerant onto activated carbon for the clear understanding of adsorption/desorption process of activated carbon. (short-term)
- Development of heat and mass transfer (HMT) enhancement technique for adsorption heat exchanger. Apply this technique to develop a waste heat-driven air-conditioning and refrigeration system. (long-term)
- Measurement of hydrogen properties, such as PVT, viscosity and permeability at high pressures. The data measured are used to develop a hydrogen thermophysical property database. (short-term)
- Measurement of thermophysical properties for new refrigerants and development of its database. Apply this to optimum design of air-conditioning and refrigeration system using low-GWP refrigerants. (short- to mid-term)
- Atomic scale understanding of adsorption phenomena for carbon-based adsorbents and establishment of adsorption kinetic enhancement technique. (mid-term)
- Development of rapid adsorption/desorption heat exchanger using activated carbon based composite adsorbent for waste heat-driven heat pump and refrigeration systems. (mid- to long-term)

5) Hydrogen Storage (Lead Principal Investigator: Prof. Akiba)

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

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

V-Ti-based BCC structure alloys are one of the most promising candidates for on board applications. The research in the division focuses on removing the two major roadblocks: low gravimetric capacity and short cycle life. The gravimetric capacity roadblock derives from microstructure evolution and lattice defect generation with hydrogenation cycles. With the use of transmission electron microscopy (TEM) the division's work elucidated the effects of Ti/V ratio on the microstructure and hydrogenation/dehydrogenation properties of Ti-V binary BCC [1]. It was found that the effective hydrogen capacity decreases and the density of twin boundaries increases with increasing Ti content. This indicates that twin boundaries formed upon hydrogenation act as hydrogen traps, thus increasing the desorption resistance of these alloys which was also found to correlate with the increased enthalpy for hydride formation with increasing V content. Metal borohydrides, e.g. $M(BH_4)_n$, have hydrogen capacity of over 10 wt %, but reaction speed and hydrogen release temperature are serious roadblocks at present. To study and improve the thermodynamic and kinetic properties of this system, the division developed a novel solvent-free synthesis process [2] that can be applied to the synthesis of various kinds of dehydrogenation intermediates (e.g. $[B_3H_8]^-$, $[B_5H_9]^{2-}$), which are extremely important to the clarification of the de- and re-hydrogenation mechanisms of metal borohydrides.

TiFe is a low cost, ideal hydrogen storage material for stationary storage. It absorbs and desorbs hydrogen at room temperature under ambient hydrogen pressure in a more compact form than liquefied hydrogen. Although it has been reported as a storage system in late 1970s, it was abandoned for decades because activation (hydrogen absorption/desorption) requires heating at temperatures higher than 400°C under 30 bar (or higher) of hydrogen. In an ongoing collaboration, PIs Akiba and Horita targeted this issue of activation based on their complementary background, ideas, and techniques. Using high-pressure torsion (HPT) techniques, PI Horita and his co-workers introduced enormously large strains in TiFe samples and measured their hydrogen storage and cycle life properties. Surprisingly, TiFe after the HTP treatment readily absorbs hydrogen without activation at high temperature and high pressure as was required before (Fig. 5) [3]. In addition, even though Ti and Fe are easily oxidized, TiFe exposed to air for a few months after several cycles of hydrogenation/dehydrogenation still readily reacts with hydrogen without activation. Fe-rich islands forming by HPT are suggested to act as catalysts for hydrogen dissociation, the microcracks and nanograin boundaries act as pathways for hydrogen transport, and probably dislocations for the sites of hydride formation [9].

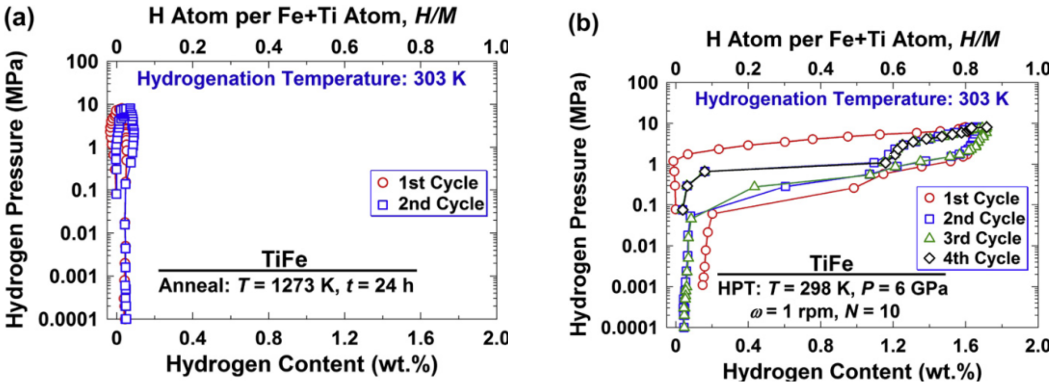


Fig. 5 : Pressure-composition isotherms for (a) annealed samples and (b) HPT-processed sample

Future directions

- By applying a diverse range of approaches of molecular chemistry, surface science, solid mechanics, solid-state physics, and materials science, we will investigate Ti-based and nitride-based materials for mobile application and Mg-based and inorganic hydrides (borohydrides) for stationary application.
- In the short term (2015-2020), effective hydrogen capacity and durability of Ti-based hydrogen storage alloys will be improved. For the nitride materials, composite material systems will be investigated and candidate systems will be downselected. For Mg-based hydrogen storage material development, in the short term, kinetics and cycle ability will be improved based on nanotechnology. For borohydride materials, reaction intermediates will be identified and pure intermediates will be synthesized. The milestone of the short-term research is development of a hydrogen storage system for mobile hydrogen storage with volume smaller than 178 L to store 5 kg hydrogen, weight density around 5 wt.%, and cost less than 500,000 Japanese Yen. The mid-term (2021-2030) targets for mobile application

are a system with smaller than 150 L and with cost less than 200,000 Yen. In the midterm, onboard application of these materials may be started as the large-scale production of FCVs starts. For the long term (2031-2050), the ultimate targets of our project are the development of hydrogen storage systems with flexible tank design, smaller than 100 L, more than 7.5 wt.% in weight density and less than 100,000 Yen in cost (not necessary for all these factors to be met).

- In the midterm, Mg-based materials with enhanced and optimized capacity, thermodynamics and thermal conductivity will be developed and optimum borohydride with promising thermodynamics will be downselected and materials having more than 10 wt% capacities under 100C° and 10 MPa may be developed. In the long term, Mg-based hydrogen storage materials with over 7 wt% capacity, cycling stability over 10000 times remaining more than 90% capacity, and other appropriate properties, including low cost, will be developed. Borohydrides developed will be applied for stationary application. The ultimate target is application of these developed materials for energy storage of intermittent renewable power.
- Research will also be directed to high-pressure torsion (HPT) techniques aiming to develop materials for onboard and stationary applications. In the short-term and mid-term, the HPT technique will be developed for TiFe based hydrogen storage alloys with enhanced kinetics as well as improved impurity effects, and for Mg-based hydrogen storage alloys with proper properties for low temperature onboard hydrogen storage. In the mid-term, scaling-up of the HPT process for fabrication of large quantity material will be tried. In the long-term, commercialization of HPT-processed TiFe based materials for stationary storage application and Mg-based alloys for onboard storage application will be started. Ultimate targets include safe utilization of HPT-processed TiFe and Mg-based hydrogen storage materials for stationary and onboard applications.

References:
1. Matsuda, J. and Akiba, E. (2013), Lattice defects in V-Ti BCC alloys before and after hydrogenation, Journal of Alloys and Compounds, 581, 369-372.
2. He, L., Li, H.-W., Hwang, S.-J. and Akiba, E. (2014), Facile Solvent-Free Synthesis of Anhydrous Alkali Metal Dodecaborate M2B12H12 (M = Li, Na, K), The Journal of Physical Chemistry C, 118 (12), 6084-6089.
3. Edalati, K., Matsuda, J., Iwaoka, H., Toh, S., Akiba, E. and Horita, Z. (2013), High-pressure torsion of TiFe intermetallics for activation of hydrogen storage at room temperature with heterogeneous nanostructure, International Journal of Hydrogen Energy, 38 (11), 4622-4627.
4. Edalati, K., Matsuda, J., Arita, M., Daio, T., Akiba, E. and Horita, Z. (2013), Mechanism of activation of TiFe intermetallics for hydrogen storage by severe plastic deformation using high-pressure torsion, Applied Physics Letters, 103 (14), 143902.

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

The objective of this division is to contribute to the creation of innovative carbon-neutral technologies by developing “Novel Catalysts,” underlining both aspects of basic science and engineering. The activities are focused on investigating catalysis-related “Solar Energy and Energy Conservation,” all of which have the potential to significantly increase energy efficiency and reduce CO_2 emissions in energy, power, or industrial production processes. Projects in the division address the development of: (i) novel biological and biomimetic catalysts for H_2, CO_2, and H_2O activation based on naturally occurring enzymes; (ii) materials development toward the realization of a carbon-neutral power generation cycle. Selected representative results based on biology’s ways with hydrogen are :

Hydrogenase from Citrobacter sp. S–77 Surpasses Platinum as an Electrode for H_2 Oxidation Reaction

An enzymatic fuel cell catalyst is a worthy goal in itself, but of particular interest was its surprising efficiency. Reported herein is an electrode for H_2 oxidation, and it is based on [NiFe]hydrogenase from *Citrobacter* sp. S-77 ([NiFe]S77) [1]. It has a 637 times higher mass activity than Pt (calculated

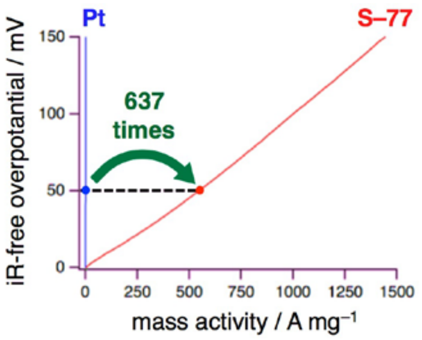


Fig. 6. Mass activity for H_2-oxidation of [NiFe]S77 in PEFC, as compared with that of Pt.

based on 1 mg of [NiFe]S77 or Pt) at 50 mV in a hydrogen half-cell (Fig. 6). The [NiFe]S77 electrode is also stable in air and, unlike Pt, can be recovered 100 % after poisoning by carbon monoxide. Following characterization of the [NiFe]S77 electrode, a fuel cell comprising a [NiFe]S77 anode and Pt cathode was constructed and shown to have a higher power density than that achievable by Pt.

The first synthetic analog of the active site of [NiFe]hydrogenase that oxidizes H_2

Chemists have long sought to mimic enzymatic hydrogen activation with structurally simpler compounds. The group of PI Ogo reported a functional [NiFe]-based model of [NiFe]hydrogenase enzymes (Fig. 7). 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 [3]. It was found that the hydrido ligand is predominantly associated with the Fe center. The ligand's hydridic character is manifested by the liberation of H_2 via reactions with strong acids.

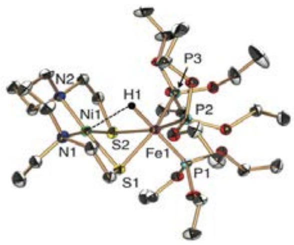


Fig. 7. A functional [NiFe]-based model of [NiFe]hydrogenase enzymes.

The results from biological and synthetic catalysts will help accelerate hydrogen fuel cell technology, and emphasize the dramatic progress of hydrogen activation using a non-precious metal catalyst, leading the way toward a low-cost hydrogen fuel cell [1-4]. These two breakthrough studies support the short-term milestone in the roadmap for the division's project focused on the development of novel biocatalysts and biomimetic catalysts for H_2-activation.

CO_2-free power generation on iron-group-nanoalloy catalyst via selective oxidation of ethylene glycol to oxalic acid in alkaline media

Management of CO_2 emissions requires development of alternative and sustainable energy cycle systems. We succeeded in power generation using a direct ethylene glycol alkaline fuel cell (AFC) employing an FeCoNi nanoalloy as an anode catalyst and a solid-oxide electrolyte that has oxygen reduction ability, i.e., a completely precious-metal-free system (Fig. 8). The FeCoNi catalyst exhibited a high selectivity for oxalic acid formation from EG without CO_2 formation [5].

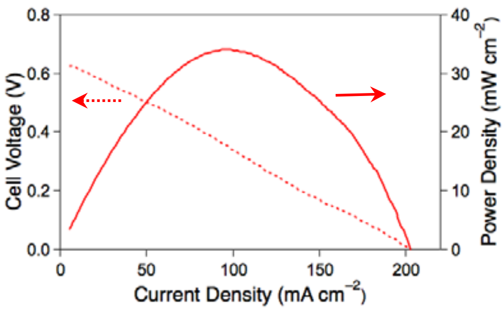


Fig. 8. Performance of direct ethylene glycol AFC employing FeCoNi/C.

Future Directions

- As a path to achieving the research objectives, Prof. Ogo group has examined and understood the aspect of biological systems, which are very important to the design and synthesis of bio-inspired model catalysts. This new fusion technology between Chemistry and Biochemistry holds high promise for the production of fuels (hydrogen, alcohols, formate, etc.) from CO_2 and solar energy. The approach can be tied to artificial photosynthesis processes, thus providing an effective utilization of the generated oxygen.
- In parallel, Prof. Rauchfuss group has completed related studies on a separately designed biomimetic catalyst, but with a focus on novel cofactors. While the fundamental work by the Ogo and Rauchfuss groups is intrinsically interesting, it is of specific and practical value with respect to the evolution of new catalysts as described in the division's roadmap. Between the efforts of these two research groups, I^{2}CNER is in position to lead the world in the elucidation of the mechanism for biomimetic hydrogen activation.
- Prof. Yamauchi's group is focused on developing "nanoalloy catalysts for a carbon neutral energy cycle."
- The specific future research directions are summarized as follows:

  Development of novel biomimetic catalysts for H_2, CO_2, and H_2O activation based on naturally occurring enzymes.

  - H_2-activation: Isolation of new hydrogenase and its model complex (short-term)
  - CO_2-Conversion: Isolation of formate dehydrogenase and its model complex (short-term)
  - Water-splitting reaction: Isolation of photosystem II and its model photosystem II (short-term)

- Practical H_2-catalyst and crystal structure of the hydrogenase (mid-term)
- Practical CO_2 catalyst and crystal structure of the formate dehydrogenase (mid-term)
- Artificial photosynthesis and structural analysis of the photosystem II (mid-term)
- H_2-catalyst: low cost and highly efficient practical application (long-term)
- CO_2 catalyst: low cost and highly efficient practical application (long-term)
- Artificial photosynthesis: low cost and highly efficient system (long-term)

Materials development toward realization of carbon-neutral power generation cycles

- Non-platinum catalysts: 50 mW cm^{-2} (short-term)
- Fuel regeneration by electroreduction: 1% (short-term)
- Solid alkaline electrolytes for high temperature: 120°C (mid-term)
- Solid alkaline electrolytes: 10^{-3} S cm^{-1} (mid-term)
- Power generation: 500 mW cm^{-2} (mid-term)
- Fuel regeneration by electroreduction: 80% (long-term)
- Air tolerant alkaline fuel cell: operation in the air (long-term)
- Power generation cycle without CO_2 emission (long-term)

References:
1. Matsumoto, T., Eguchi, S., Nakai, H., Hibino T., Yoon, K.-S. and Ogo, S. (2014), [NiFe]Hydrogenase from *Citrobacter* sp. S-77 Surpasses Platinum as an Electrode for H_2 Oxidation Reaction, *Angewandte Chemie - International Edition*, 53(34), 8895–8898.
2. Nguyen, N.T., Mori, Y., Matsumoto, T., Yatabe, T., Kabe, R., Nakai, H., Yoon, K.-S. and Ogo, S. (2014) A [NiFe]hydrogenase model that catalyses the release of hydrogen from formic acid, *Chem. Commum.* 50(87), 13385–13387.
3. Ogo, S., Ichikawa, K., Kishima, T., Matsumoto, T., Nakai, H., Kusaka, K. and Ohhara, T. (2013), A Functional [NiFe]Hydrogenase Mimic That Catalyzes Electron and Hydride Transfer from H_2, *Science, 339 (6120)*, 682-684.
4. Matsumoto, T., Kim, K. and Ogo, S. (2011), Molecular Catalysis in a Fuel Cell, *Angewandte Chemie - International Edition*, 50 (47), 11202-11205.
5. Matsumoto, T., Sadakiyo, M., Ooi, M.L., Kitano, S., Yamauchi, M., Yamamoto, T., Matsumura, S., Kato, K., and Takeguchi, T., (2014), CO_2-free power generation on an iron group nanoalloy catalyst via selective oxidation of ethylene glycol to oxalic acid in alkaline media, *Scientific reports*, 4 (5620), 1-6

7) CO_2 Capture and Utilization (Lead Principal Investigator: Prof. Fujikawa)

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

Free-standing and nanometer-thick membrane for gas separation and elucidation of the mechanism of preferential CO_2 permeation

The group of PI Fujikawa succeeded in preparing a nanometer-thick membrane by a conventional spin-coating process (patent submitted). A less than 200-nm thick membrane of an epoxy resin can be transferred and mounted on a porous support (Fig. 9a). CO_2 gas passes through preferentially in comparison to nitrogen gas under humid conditions. In this membrane, amine residues of the epoxy resin are necessary not only for making a membrane hydrophilic but also for good affinity with CO_2. This result is a first example of preferential CO_2 separation by a nanometer-thick membrane.

The group of Dr. Taniguchi applied photo-polymerization of poly (ethylene glycol) (PEG) dimethacrylate in the presence of dendrimers to create dendrimer-containing polymeric membranes, and found that Poly(amidoamine) (PAMAM) dendrimers exhibit excellent affinity to CO_2 [1]. The resulting membranes show excellent CO_2 separation performance over H_2, controlled by several parameters, most notably, PAMAM dendrimer fraction, dendrimer generation, PEG length, and humidity. Mechanistically, CO_2 turns to bicarbonate and carbamate (Fig. 9b), with the former being the major migrating species through the membrane while the latter suppresses H_2 permeation by the formation of quasi-crosslinks with PAMAM dendrimers [2].

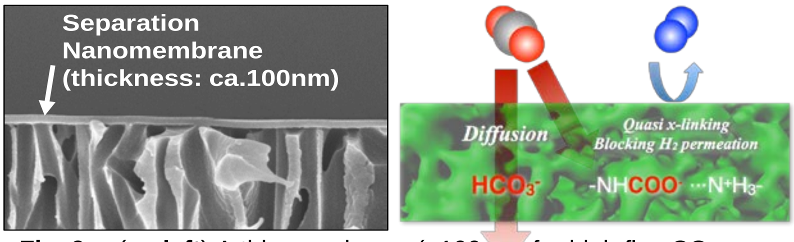


Fig. 9. (**a - left**) A thin membrane (<100nm) for high flux CO_2 separation, (**b - right**) Mechanism for preferential CO_2 permeation through the PAMAM dendrimer-based membranes; The formation of carbamates between dendrimers prevents H_2 permeation.

Electrochemical CO_2 Conversion

The group of Illinois Satellite faculty Prof. Kenis succeeded in developing a number of high performance catalysts and electrodes for the electroreduction of CO_2 to CO, a building block in synthesis of fuels and chemicals via the Fischer-Tropsch process. For example, an air-brush based catalyst deposition method was shown to lead to high quality electrodes with thin, crack-free catalyst layers and excellent electrochemical performance [3]. Also, several new catalysts have been studied, including titania supported Ag, which reduces the amount of silver needed for similar or better CO_2 reduction performance, due to high dispersity of the Ag nanoparticles and beneficial participation of the support material in the stabilization of a reaction intermediate [4]. An iridium-based anode catalyst (instead of Pt) was shown to exhibit excellent performance for the oxygen evolution reaction, enabling electrolyzer cell potentials as low as −1.55 V with a cathode overpotential of only 0.02 V, and providing a partial current density for reduction of CO_2 to CO as high as 250 mA cm^{-2} (compared to ~130 mA cm^{-2} with a Pt instead of a IrO_2 anode), and overall energy efficiencies as high as 70% [5]. In more recent work, a better cathode catalyst comprised of polymer-wrapped nanotubes covered with highly disperse Au nanoparticles was developed.

Future Directions

We have established the general fabrication process of nano-meter thick, free-standing membranes without defects. We are now focusing on material development to incorporate the CO_2 affinity into a membrane for preferential CO_2 permeation. We have already found that a membrane containing poly-amine dendrimer shows high CO_2 affinity over H_2. Based on this finding, the molecular design and development of membranes will be pursued for the next few years as a short term research milestone. Our target mixture gases are CO_2/N_2, CO_2/H_2 and CO_2/CH_4 since they are major gas sources in the process of pre- and post-combustion, and natural gas purification, respectively. Each of these gas sources requires a different type of separation mechanism based on the chemical and physical properties of the membrane. The elucidation of the molecular mechanisms for gas permeation is a key prerequisite for development of separation membranes; even in conventional separation membranes, knowledge of the separation mechanisms is still lacking. Our research efforts will be focused precisely on identifying the CO_2 separation mechanisms at the molecular level using a combined experimental and computation science approach. Improvement of membrane robustness and durability and the feasibility of CO_2 separation by our membranes will be pursued as mid- and long-term milestones.

- In the last few years, we have developed several highly active catalysts and electrodes for the conversion of CO_2 into CO, which, when mixed with H_2, can be turned into fuels. With these 10-20 x more active catalysts, the rate-limiting step for this process has become mass transport of reactants and products to the catalyst. In the short-term, we will replace commercial gas diffusion electrodes with home-made ones that incorporate nano-membranes to overcome mass transport limitations. Second, we also are pursuing catalysts that are based on Cu for the production of value-added products such as methanol, ethylene, and ethanol. Third, on the longer term, we will investigate (through experiment and through process analysis) the feasibility of electrochemical conversion of CO_2 as a method for large scale energy storage of otherwise wasted renewable energy. Current utilization of generated renewable power from sources such as solar and wind is only 30% because of the lack of large scale energy storage capacity. In this scenario, CO_2 conversion will increase the utilization of available renewable power, thus reducing CO_2 emissions.

References:

1. Taniguchi, I., Duan, S., Kai, T., Kazama, S. and Jinnai, H. (2013), Effect of phase-separated structure on CO_2 separation performance of poly(amidoamine) dendrimer immobilized in a poly(ethylene glycol) network, *Journal of Materials Chemistry A*, 1 (46), 14514-14523.
2. Taniguchi, I., Urai, H., Kai, T., Duan, S. and Kazama, S. (2013), A CO_2-selective molecular gate of Poly(amidoamine) dendrimer immobilized in a poly(ethylene glycol) network, *Journal of Membrane Science*, 444, 96-100.
3. Jhong, H.-R.M., Brushett, F.R., Kenis, P.J.A. (2013), The effects of catalyst deposition methodology on electrode performance, *Advanced Energy Materials*, 3(5), 589-599.
4. Ma, S., Lan, Y., Perez, G.M.J., Moniri, S., Kenis, P.J.A. (2014), Silver supported on titania as an active catalyst for electrochemical carbon dioxide reduction, *ChemSusChem*, 7(3), 866-874.
5. Ma, S., Luo, R., Moniri, S., Lan, Y., Kenis, P.J.A. (2014), Efficient electrochemical flow system with improved anode for the conversion of CO_2 to CO, *Journal of the Electrochemical Society*, 161(10), F1124-F1131.

8) CO_2 Storage (Lead Principal Investigator: Prof. Tsuji)

The objective of this division is to: develop methods of reservoir characterization and modeling, and new effective monitoring of injected/leaked CO_2 to help ensure safe and permanent CO_2 sequestration in sub-seabed geologic formations; and propose and realize new carbon storage concepts suitable for geological formations and rock types typical of Japan. The research projects and efforts have been established in such a way that they take into consideration the heterogeneity of the geological formations in Japan, the limited availability of geological data for CO_2 injection in aquifer formations, and the requirement for long term monitoring of pressure variations near seismogenic faults. Selected representative results include:

Simulation of injected and trapped CO_2 and estimation of CO_2 stored volume from seismic velocity

Accurate a priori evaluation of potential storage site fidelity and prediction of CO_2 fate following injection, both via reservoir-scale simulations, requires a fundamental understanding of the physical and chemical processes responsible for CO_2 trapping at the pore scale. PI Tsuji's group is performing ground-breaking modeling and simulation of multiphase reactive flow in heterogeneous rock using a digital rock model reconstructed from micro-CT images of reservoir rock (Fig. 10a) in concert with the lattice Boltzmann method (LBM; Fig. 10b). This study revealed a strong interfacial effect on the relative permeability – a key parameter in reservoir monitoring, characterization and prediction [1]. The influence of mineralization was then simulated, indicating that, for the relative permeability, pore space reduction due to mineral precipitation (Fig. 10d) has a greater influence on the non-wetting phase than on the wetting phase [2]. These LBM simulations are, to our knowledge, the largest of their kind for studying CO_2 trapping in reservoir rock. Complementary experiments are on-going in Prof. Kenneth Christensen's group at the Illinois I^{2}CNER Satellite Center.

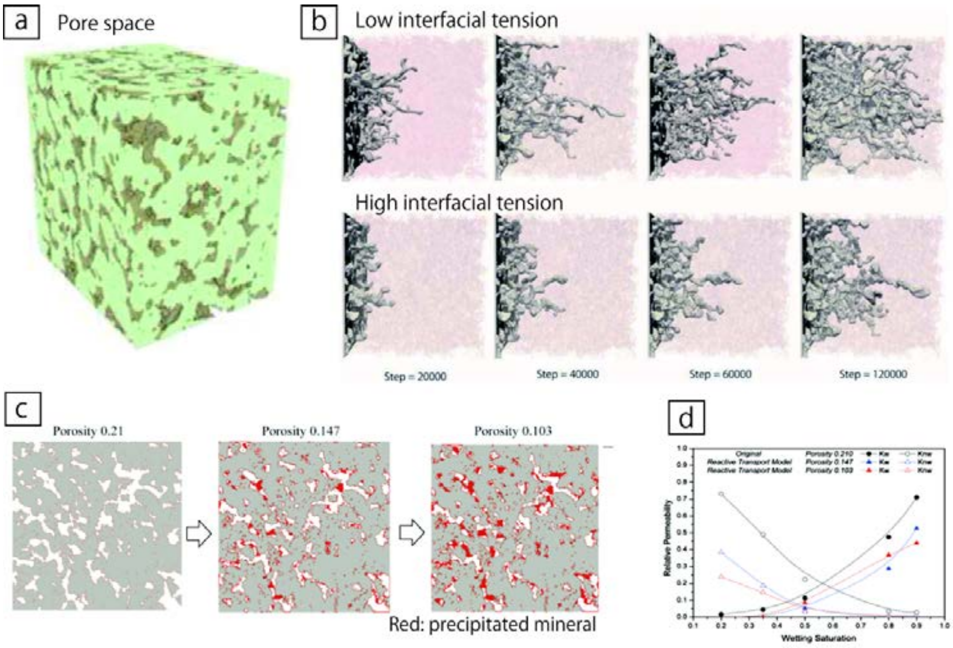


Fig. 10. a) Pore geometry of the Berea sandstone extracted from micro-X CT images, b) Supercritical CO_2 infiltration into rock as a function of interfacial tension [33], c) Mineral precipitation calculated from the CO_2 flow within the rock [34], d) Relative permeability as a function of mineral precipitation.

Dr. Kitamura, in collaboration with Prof. Tsuji and Illinois Satellite faculty Profs. Christensen and Valocchi, recently reported elastic wave velocities for heterogeneous two-phase flow through small-scale heterogeneity in porous sandstone, complemented by LBM simulations [3]. The results of this effort highlighted the impact of pore-scale heterogeneity on migration of CO_2, particularly around laminae in porous sandstone which are found to act as barriers for CO_2. In contrast, the flow of water was found to be unaffected by these laminae. The LBM simulations provided additional evidence of this phenomenon. Thus, this effort suggests that pore-scale heterogeneity can act as a gate for CO_2, and thus strongly controls its migration behavior in porous sandstone.

Future directions

Reveal CO_2 trapping mechanisms and CO_2 interaction in order to predict CO_2 fate and enhance trapping

- Model the migration behavior of injected CO_2 within the pore space, particularly trapping mechanisms (residual, solubility, and mineral trapping), both from laboratory experiments and numerical simulation. In the numerical simulation, we couple hydrological and geomechanical modeling in order to better understand CO_2 injection induced earthquakes. (short-term)
- Upscale porous flow phenomena in order to predict field-scale CO_2 behavior. The scale dependence of the injected CO_2 is mainly derived from heterogeneity of the geological formations, thus we must reveal the influence of heterogeneity on the CO_2 behavior. In the long-term, we will develop a predictive framework for accurate reservoir characterization (in pre-injection) and long-term CO_2 fate (in post-injection) for geological structures typical of Japan. (mid- to long-term)
- Explore ideas for increasing CO_2 storage capacity and security by enhanced residual and solubility trapping. In the long-term, we hope to increase storage capacity and security by enhanced mineral trapping. (mid-to long-term)

Develop a long-term, reliable monitoring system for injected CO_2 and identify field-scale CO_2 behavior

- Develop a method to detect heterogeneous geological structures, including fractures, with high resolution. (short-term)
- Develop an effective monitoring system to detect injected CO_2 in the rock. To quantitatively estimate hydrological properties from the monitoring data, we are conducting laboratory and theoretical studies. In the mid-term, we plan to “establish” a reliable monitoring system to investigate field-scale CO_2 behavior. (short- to mid-term)

- Clarify the scale-dependence of CO_2 behavior by comparing the monitoring-derived field-scale behavior with our pore-scale modeling results. (mid-term)

Develop reliable monitoring system for leaked CO_2

- Develop a detection/monitoring system for the leaked CO_2. (short-term)
- Deploy this monitoring system in the field for leaked CO_2. (mid-term)

References:
1. Jiang, F., Tsuji, T. and Hu, C. (2014), Elucidating the role of interfacial tension for hydrological properties of two-phase flow in natural sandstone by an improved lattice Boltzmann method, *Transport in Porous Media*, 104, 205-229.
2. Jiang, F. and Tsuji, T. (2014), Changes in pore geometry and relative permeability caused by carbonate precipitation in porous media, *Physical Review E*, 90, 053306 (10 pp).
3. Kitamura, K., Jiang, F., Valocchi, A. J. , Chiyonobu, S., Tsuji, T., and Christensen K. T. (2014), The Study of Heterogeneous Two-Phase Flow around Small-Scale Heterogeneity in Porous Sandstone by Measured Elastic Wave Velocities and LBM Simulation, *Journal of Geophysical Research–Solid Earth*, 119, 7564-7577.

9) Energy Analysis (Acting Division Leader, Prof. Itaoka)

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

Energy Vision for Japan

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

Future Directions

Analyses that are in progress or planned include:

- A quantitative vision for a low carbon emission energy infrastructure for Japan in 2050.
- Analysis of the potential for Japan to import low carbon fuel or energy. This could include a variety of biofuels or other options.
- Detailed analysis of the Japan electricity grid and infrastructure and how to dramatically reduce carbon emissions through the use of renewable resources and energy storage while meeting Japan's future power needs.
- Analysis of the needs and deployment of a hydrogen infrastructure for Japan for fuel cell vehicles.
- Energy, exergy, carbon emission, and cost analyses of specific I^{2}CNER research projects and other new emerging technologies to quantify the benefits and help provide research directions for I^{2}CNER.

(3) Management

i) Center director

・ Provide the name of the center director, his/her age (as of 1 April 2015), , specialties, and brief career profile(within 5 lines).

・ If there is a plan to change the center director, how does the new center director intend to construct the center and what is his/her vision of objectives to be achieved? Provide a synopsis written by the new center director (free format).

Name：Petros Sofronis (57)
Affiliation, position title： Professor, University of Illinois, USA
Specialties: Solid mechanics, finite element methods, micromechanics of materials, elastic-plastic fracture mechanics, hydrogen embrittlement.

Suitability as the Institute Director:
Prof. Sofronis' education and research orientation are in the area of mechanics of materials, which includes the disciplines of elasticity, viscoelasticity, plasticity, fracture mechanics, and micromechanics of defect interactions. He received his PhD in Theoretical and Applied Mechanics from the University of Illinois at Urbana-Champaign (UIUC) in 1987. He has been a faculty member at UIUC since 1991. Beginning in 2007 to date, Prof. Sofronis has served as the Mechanical Science and Engineering Department Associate Head for Mechanics Programs. He is also a fellow of the American Society of Mechanical Engineers (ASME) and the Japan Society for the Promotion of Science (JSPS).

Professor Sofronis has been active in the field of environmental degradation of materials for nearly 30 years. Since 1991, Sofronis has been a principal investigator in the interdisciplinary environment of the Materials Research Laboratory at the University of Illinois at Urbana-Champaign. Sofronis has investigated phenomena of hydrogen embrittlement of materials by coupling mechanics of materials with experimental observations at the atomistic scale. His theory on the hydrogen-induced shielding of defect interactions to explain the mechanism of hydrogen enhanced localized plasticity for embrittlement is the first proposed rational explanation of the hydrogen-induced fracture given worldwide. Recently, Sofronis is working on materials for the new hydrogen economy in collaboration. His research aims at developing and verifying a lifetime prediction methodology for failure of materials used in hydrogen gaseous environments. Development and validation of such predictive capability and strategies to avoid material degradation is of paramount importance to the rapid assessment of the suitability of using the current natural gas pipeline distribution system for hydrogen transport in the new hydrogen economy and of the susceptibility of new alloys tailored for use in hydrogen related applications.

Professor Sofronis' expertise on the interaction of materials with severe chemomechanical environments is extremely relevant to the fields that constitute the main theme of I^2CNER: gas interactions (H, O, CO_2) with matter. These internationally recognized scientific credentials will enable him to administer the Institute's research activities by applying and requiring the highest standards for high quality research.

ii) Administrative director

・ Provide the name of the administrative director, his/her age (as of 1 April 2015), and his/her brief career profile(within 5 lines).

Yukio Fujiki (66)
Distinguished Professor, Kyushu University

Prof Fujiki's work focuses on the homeostasis of peroxisome, an intracellular organelle, and human fatal genetic disease termed peroxisome biogenesis disorders including Zellweger syndrome, all of which are linked to a failure of peroxisome assembly. Prof Fujiki and his colleagues identified 15 pathogenic *PEX* genes responsible for PBDs. Prof Fujiki's lab tackles the problems involving membrane assembly, matrix protein import, morphogenesis, and homeostasis of peroxisomes. Prof. Fujiki has been a Professor in the Department of Biology in the Faculty of Science at Kyushu University since 1994. In 2009, he was named a Distinguished Professor. Prof Fujiki served as an

Executive Vice President of Kyushu University from 2010 to 2014.
The administrative director's primary function is to develop and execute the financial, managerial, and administrative functions of I^2CNER so that the Director can focus on administering and executing the overall research mission of the institute.

iii) Composition of administrative staff

・ Concretely describe how the administrative staff is organized.

○ In order to efficiently respond to the requests from the Institute Director and researchers, and also to provide an ideal research environment, there is an Administrative Office (AO) specially set up for I^2CNER. The AO consists of 1) a general affairs and human recourses section; 2) an accounting and contracting group; 3) a research support and international affairs section; and 4) a public relations group.

○ The administrative officers in the AO of the Institute get support from other administrative officers in Kyushu University who also have competent English language skills. Personnel outside Kyushu University with competent technical knowledge, experience, and English language skills are employed in the AO. The official language in the AO is English.

○ The Institute offers support to international researchers for their research activities, as well as other services both within and outside the University, in close cooperation with the existing International Student and Researcher Support Center of Kyushu University. The Institute offers full-time support including visa applications, accommodations, airport pickups, administrative procedures at the University, alien registrations, paper work and processes required for banking, school attendance, etc., and the purchasing of essential items, such as mobile phones, and related payments.

Below are the main tasks allocated to each of the departments of the AO:

1) General affairs and human recourses
General management of the Institute, preparation of meetings, management of the Institute policy, human resource management, such as employment, salary and business trips, safety management, and support services for international researchers.

2) Accounting and contracting
Compiling of budget, resourcing of Institute facilities, equipment and other goods, payments for goods, salary, business trips, etc., and general accounting.

3) Research support and international affairs
Preparation of grant application documents, presentation of research findings, project designs and agreement for collaborative research work, application for and management of patents (in conjunction with the office for Intellectual Property), etc.

4) Public relations
Public relations, advertisement, management of the homepage, support of international visitors, organization of international conferences, etc.

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

iv) Decision-making system

・ Concretely describe the center's decision-making system.

○ The Institute has been established as an organization under the direct management of the President of Kyushu University. The Institute Director has direct access to the Office of the President through the Office of the Executive Vice President for Research. 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 review 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. On all these matters, the Director consults the Science Steering Committee (SSC), which is headed by the Director and whose members (science advisors) include the division Lead Principal Investigators and any other additional members that the Director may deem appropriate.

○ A vital component of the Institute is the External Advisory Committee (EAC), which is composed of national and international leaders in the field. This Committee is convened annually or, if deemed necessary by the Director, more frequently. The Committee reviews all aspects of the Institute, including its leadership and management, the research progress being made in each activity, and its plans for any initiatives. The Committee provides the Director with a written report on their findings and recommendations. The final decision regarding Institute activities is the responsibility of the Director.

○ Another important standing committee of the Institute is the Internal Programs Review Committee (IPRC), 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.

○ The Director is assisted by two Associate Directors; Prof. Ishihara, who is responsible for workshop organization, seminar series administration, and management of facilities and equipment, and Prof. Takata, who is in charge of faculty recruitment, international and industrial collaborations, and graduate student research matters.

○ The role of the Science Steering Committee and the two Associate Directors is strictly advisory. The Director is solely responsible for making the final decisions.

○ In the Director's absence (while he is in the US), the administration of the Institute is governed by document "22. Management and Administration."

v) Allocation of authority between the center director and the host institution's side

・ Concretely describe how authority is allocated between the center director and the host institution's side.

○ The appointment/dismissal of the Institute Director and authorization for employment of the Principal Investigators is authorized by the President of Kyushu University. The Institute Director has the authority for the other administrative operations, as listed above.

(4) Researchers and other center staffs, satellites, partner institutions

i) The "core" to be established within the host institution

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

	numbers		
	At beginning	At end of FY 2014	Final goal (Date: month, year)
Researchers from within the host institution	16	13	14
Foreign researchers invited from abroad	11	9	10
Researchers invited from other Japanese institutions	3	2	1
Total principal investigators	30	24	25

・ Describe the concrete plan to achieve final staffing goal, including steps and timetables.
・ Attach a list of principal investigators using the Appendix. Place an asterisk (*) by names of the investigators considered to be ranked among the world's top researchers. Describe the policy and strategy for inviting the PIs who are to be included after 1 April 2015.

All chief researchers are to participate in the program from the commencement of the project.

b) Total members

	Numbers		
	At beginning	At end of FY 2014	Final goal (Date: month, year)
Researchers	71 < 21, 30%>	165 <74, 45%> [17, 10%]	172 < 78, 45%> [29, 17%]
Principal investigators	30 < 11, 37%>	24 <9, 38%> [1, 4%]	25 < 9, 36%> [1, 4%]
Other researchers	41 < 10, 24%>	141 <65, 46%> [16, 11%]	147 <69, 47%> [28, 19%]
Research support staff	32	60	70
Administrative staff	23	18	21
Total number of people who form the "core" of the research center	126	243	263

・ Enter the total number of people in the columns above. In the "Researchers" column, put the number and percentage of overseas researchers in the < > brackets and the number and percentage of female researchers in the [ ] brackets.

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

ii) Collaboration with other institutions

・ If the "core" forms linkages with other institutions, domestic and/or foreign, by establishing satellite functions, Provide the name of the partner institution(s), and describe the role of the satellite functions, personnel composition and structure, and collaborative framework between the host institution and the said partner institutions (e.g., contracts to be concluded, scheme for resource transfer).

・ If some of the principal investigators will be stationed at satellites, attach a list of these principal investigators and the name of their satellite organizations using the Appendix.

・ If the "core" forms organic linkages with other institutions, domestic and/or foreign, without establishing satellite functions, provide the names of the partner institutions and describe their roles and linkages within the center project.

○ To achieve success, collaborative and coordinated research efforts central to the mission of the Institute are conducted in partnership with faculty and staff at other national and international institutions. This activity involves not only research collaboration, but also exchange of personnel. Broadening the research base from Kyushu University further promotes the Institute activities and helps establish it as center of excellence.

- o Satellite Institute: University of Illinois at Urbana-Champaign, USA
  - The University of Illinois at Urbana-Champaign is a top-world institution in a number of areas, such as the field of hydrogen energy and materials research, etc. The Illinois Satellite faculty members are all internationally recognized researchers in their respective areas of expertise. They were specifically invited to complement the I^{2}CNER research activities at Kyushu. In addition to conducting Institute related research, the Satellite Institution serves as the base for identifying and engaging key research programs and faculty at national and international universities and institutions. Director Sofronis also serves as the Director of the Satellite Institute. In this latter capacity, he reports directly to the Dean of the College of Engineering at the University of Illinois. A Memorandum of Understanding (MoU) for interaction between Kyushu and Illinois and an agreement for undergraduate student exchange are in place. Appropriate additional agreements between Kyushu University and the University of Illinois, e.g. on joint degree programs, will be negotiated. The Satellite has been allocated a spacious office suite housed within the Department of Mechanical Science and Engineering. Office space is available

for Japanese researchers during their visits to the Illinois campus. Satellite faculty laboratories are available for use by collaborators/counterparts from Kyushu. In addition, campus-level shared-use facilities and laboratories at Illinois are available to all researchers for a usage fee.

- o Partner Institutions
  - MoUs for research interaction and collaboration have been signed between I^{2}CNER and the National Fuel Cell Research Center (NFCRC) at the University of California, Irvine and NTNU/SINTEF of Norway. A letter of understanding has been signed with the California Air Resources Board (CARB). In addition, there are about 20 ongoing collaborative research activities between I^{2}CNER PIs, full time faculty, and postdocs, and faculty and researchers from premier institutions worldwide. The list of these institutions includes MIT, UC Berkeley, Max-Planck, the University of Oxford, the Helmholtz-Zentrum Geesthacht (HZG) in Germany, the Dalian Institute of Chemical Physics, and the Swiss Federal Institute of Technology Zurich (ETH), among others.

(5) Research Environment

・ Concretely describe measures to be taken to satisfy each of the requirements outlined below, including steps and timetables.

○ Provide an environment in which researchers can devote themselves exclusively to their research, by exempting them from other duties and providing them with adequate staff support to handle paperwork and other administrative functions.

- In order for the Institute researchers to focus exclusively on their research, we employ an efficient and competent Administrative Office (AO) to execute all required administrative work needed for a world-class Institute. This involves planning of the Institute's budget, purchasing of equipment and goods, procurement procedures, business trips procedures and preparation support, grant application preparation and submission processes, support for presentations, assistance for joint research projects and launching of new initiatives, handling of contracts, patent applications, publications processes, and facilitating visitors. We provide a strong support infrastructure so that the researchers of the Institute can pursue I^{2}CNER's mission with no hindrances whatsoever. In particular, we plan for administrative personnel visits between Kyushu and the Illinois Satellite in order for the staff to gain international perspectives.
- In addition, we constantly work toward improving the skills of the technical staff employed in the support of research operations and maintenance of facilities and equipment.
- Furthermore, we plan to decrease the academic teaching load for the Institute researchers.

○ Provide startup research funding as necessary to ensure that top-caliber researchers invited to the center do not upon arrival lose momentum in vigorously pursuing their work out of concern over the need to apply immediately for competitive grants.

- In order to facilitate the ability of Institute researchers and invited researchers from external institutions to focus on their research—with no need for immediate engagement on grant application preparation for research funding—we provide the necessary research facilities and equipment whenever possible so that the researchers can start and/or continue their research. Also, funds won by young faculty through I^{2}CNER's Competitive Funding Program, which primarily supports interdisciplinary research, can be used to support research in the Institute in collaboration with their visitors.

○ As a rule, fill postdoctoral positions through open international solicitations.

- To recruit well qualified post-doctoral research associates, advertisements for the positions are placed on the web site of Kyushu University, Kyushu University Offices overseas in Great Britain, California, Washington D.C., Munich, Korea, Beijing, etc., at the Satellite Institute's web site at Illinois, and major international academic magazines and related magazines in Japan. The recruitment process is supervised by the Institute Director and administered by the Faculty Recruiting Committee (FRC), which includes key members of the Institute and any other faculty who can provide input for cases of targeted hiring. The corresponding recruitment practices at the University of Illinois are used in the hiring of all Institute research personnel. In addition, I^{2}CNER principal investigators are proactive in suggesting highly qualified international and Japanese candidates.

○ Establish English as the primary language for work-related communication, and appoint administrative personnel who can facilitate the use of English in the work process.

- English is the primary language for work-related communications.
- To foster an English speaking environment in the Institute, we employ personnel from Kyushu University who are fluent in English in the AO.

○ Adopt a rigorous system for evaluating research and a system of merit-based compensation. (For example, institute a merit-based annual salary system primarily for researchers from outside the host institution. As a basic rule, the salaries of researchers who were already employed at the host institution prior to the centers' establishment are to be paid by the host institution.)

- Compensation considerations are based upon a special agreement between I^2CNER and Kyushu University entitled "Regulations on Special Measures on the Hiring of National University Corporation Kyushu University International Institute for Carbon-Neutral Energy Research Employees." As a result of this special agreement, the Institute follows a special merit-based salary system which deviates from the established salary ranges. Evaluation of individual faculty and researcher performance is carried out annually by the Director and the two Associate Directors, or more frequently, if deemed necessary by the Director. The evaluation criteria are those listed in the Institute's governing document on Faculty Promotion and include interdisciplinary research publications, invited presentations in international conferences, and development of an independently funded research program, and more generally, contributions to the interests and mission of the Institute. The Director communicates the outcome of the evaluation to the faculty and researchers annually via a letter in which the importance of interdisciplinary research is emphasized consistently. Individual faculty and researcher salaries are determined based on this evaluation, as decided by the Director, in consultation with the two Associate Directors.

○ Provide equipment and facilities, including laboratory space, appropriate to a top world-level research center.

- In order to continue developing a research environment befitting a top world-level research institute, and to promote collaboration and fusion research, I^2CNER building 1 (approximately 4,873 m^2) was completed at the end of November 2012. All the Institute's members moved "under one roof" into I^2CNER 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^2CNER researcher. The first floor lobby features a spacious lounge with a high ceiling and electronic black boards in order to encourage impromptu meetings and exchange of scientific views among I^2CNER members. Facility equipment, such as fume foods and pneumatic piping, has been installed in I^2CNER Building 1. I^2CNER Building 2 has been designed similarly.
- A second I^2CNER building, which has 4 stories and a total floor space of 5,000 m^2, is currently being built. Floor plans for the building include 8 large-scale labs, 2 open offices, and 1 administrative office, with the majority of rooms being designed as open, common experimental spaces in order to promote interdisciplinary research. Completion of I^2CNER Building 2 is planned for the end of February 2015.
- In January 2013, an additional 7 labs, 15 researcher offices, and a server room were secured for I^2CNER's Fuel Cell researchers out of the space allocated to the Next-Generation Fuel Cell Research Center within the I^2CNER building. We have also secured labs for researchers of MIT and Imperial College London in order to promote exchange of researchers between KU and these renowned foreign institutions.
- I^2CNER's laboratories are equipped with state of the art equipment. By way of example, the list includes Complex Fatigue Testing System combined with a scanning electron microscope for mechanical behavior testing; RF Plasma Sputtering Apparatus (Thin Film Deposition Methods) for deposition of multi composition films using simultaneous sputtering of multiple targets; Low Energy Ion Scattering (LEIS); Secondary Ion Mass Spectrometry (TOF-SIMS) for surface and interface analysis.; Ar Cluster Ion Beam X-Ray Photoelectron Spectroscopy (XPS) for elemental analysis; Nuclear Magnetic Resonance Spectroscopy System for the non-destructive and quantitative study of molecules in a solution and in a solid state.
- A challenge for the Institute is to develop our bottom-up model of energy systems based on our current analytical tool. To accelerate data collection and improve reliability of our

analyses, the EAD will be provided with all necessary resources, such purchasing of rights to access large databases of energy facilities and market movement created by outside entities (e.g. Bloomberg New Energy Finance). Such resources will enable the EAD to study the extension of the future directions of our research to include analysis of the contribution of Japanese technologies or I^2CNER's enabling technologies to international CO_2 emission reductions.

○ Hold international research conferences or symposiums regularly (at least once a year) to bring the world's leading researchers together at the center.

- I^2CNER holds annually a symposium addressing the current scientific state-of-the-art in its thematic research areas. The objective of this series of international symposia is to identify what I^2CNER researchers see as the major roadblocks, challenges, and opportunities in those fields, to demonstrate how the Institute's efforts are addressing these, and to show where the Institute's research activities lie in terms of excellence, successful fusion, and interdisciplinary impact relative to the spectrum of research being carried out today in the scientific world globally. The symposia are followed by more specific workshops organized by each research division. These workshops are brainstorming fora and opportunities to identify strengths and weaknesses in our research portfolio and explore how we might best accomplish critical growth in scientific breadth of the divisions.
- I^2CNER researchers are establishing a tradition of participating, organizing, and hosting international conferences and specialized workshops with active participation from world famous researchers and institutions on a regular basis and on all aspects of the research activities of the Institute. Examples of conference and symposia themes are hydrogen energy and fuel cells, the HYDROGENIUS & I^2CNER Joint Research Symposium on hydrogen economy, hydrogen production by photocatalytic water splitting, sustainable material conversion systems, innovative CO_2 capture, and CO_2 geological storage.
- Another tradition I^2CNER is establishing is the hosting of the Tokyo Symposium, which is sponsored by the U.S. Embassy in order to bring I^2CNER research activities to the attention of the energy stakeholders in the capital of Japan and the international community. So far, two symposia were hosted in 2012 and 2014, both with the presence of the US Ambassador to Japan, and high-ranking government officials from MEXT, DOE, and the White House.
- The I^2CNER Satellite is also hosting targeted area symposia in order to strengthen the interaction of I^2CNER's researchers at Kyushu and Illinois with the international community.

○ Other measures to ensure that top-caliber researchers from around the world can comfortably devote themselves to their research in a competitive international environment, if any.

- The Administrative Office offers full-time support to international researchers in the area of invitation procedures, including visa application processing and accommodations on campus. Additionally, the I^2CNER Administrative Office provides extensive living support and assistance with medical checkups, private accommodations, family support, travel arrangements, and introduction to the Japanese social insurance system, including medical, just to name a few.
- We have university facilities to accommodate international researchers such as "Ito Guest House," which is on Ito campus, where I^2CNER is located. We also make arrangements for fully-furnished private apartments with easy-access to Kyushu University for long-term stays.
- In order to help international researchers adjust to life on campus, there are bilingual displays (Japanese and English) on the bus timetables at campus bus stops and destination signs on busses running between campus and the nearest train station. In addition, there is a campus loop bus stop in front of I^2CNER Building 1 and a campus shuttle bus stop in front of Shiiki Hall, which is adjacent to I^2CNER Building 1. The Kyushu University cafeterias also offer menus written in English.

(6) Indicators for evaluating a center's global standing

・ Describe concretely the following points.

i) Criteria and methods to be used for evaluating the center's global standing in the subject field

I^2CNER is a mission-driven (Green Innovation) research center, but it is focused on basic science. As such, it can be evaluated on the basis of the following metrics:

1) Relevance of the I^2CNER research efforts and objectives to enable the green innovation initiative of the government of Japan; 2) Approach to carrying out research. This can be evaluated by the quality of the publications in high impact, discipline-oriented journals. By publishing in such journals, a stringent review process addresses whether the research advances what is considered state-of-the-art by a community of experts is ensured; 3) International awards and number of article citations the Institute's work receives, which are an indicator of overall standing and visibility; 4) Degree of realization of milestones and targets in research roadmaps; 5) Level of collaboration with international research centers and efforts and degree of research interdisciplinarity; 6) Number and quality of participating industrial partners; 7) Filing for patents; 8) Technology transfer events. It is our understanding that Technology transfer events are more important than number of patents pending.

The overriding metric is that quality needs to pervade all I^2CNER operations.

ii) Results of current assessment made using said criteria and methods

I^2CNER has established objectives and roadmaps for each research division in support of its mission for a carbon neutral energy Japan; generated world-class results whose impact is recognized worldwide; the productivity of its researchers is similar to and even exceeds that of other thematically focused centers in the world; its researchers garnered national and international awards; enabled research collaborations between Japan, the US, and Europe; its researchers submitted a large number of patent applications; and a large number of industries are benefiting from ongoing joint research projects with I^2CNER researchers.

iii) Goals to be achieved through the project (at time of final evaluation)

The primary goal by the time of the 10-year evaluation of the Institute from its inception is that the Institute will have established its reputation and brand as an international center of excellence for fundamental research toward meeting its mission for a carbon-neutral energy Japan. Indicators for meeting this goal shall be well-recognized breakthroughs in fundamental research (e.g., discovery of how hydrogen promotes fatigue of materials or discovery of new catalysts for biomimetic CO_2 activation or efficient photocatalytic water splitting). Such breakthroughs on fundamental science will allow the Institute to expand its mission for its second term to include directions addressing technology development, such as the design of a new alloy for hydrogen resistant materials, new alloys for on-board hydrogen storage, technologically viable production of hydrogen through artificial photosynthesis, new low-cost catalysts for fuel cells, and demonstration projects for geo-sequestration of carbon.

(7) Securing research funding

Future prospects

・ Describe the concrete prospects for securing resources that match or exceed the project grant.

I^2CNER researchers will leverage the established infrastructure and research culture of the Institute to aggressively pursue more funding in the coming years. By way of example, efforts currently under way are through the Core-to-Core international program of the JSPS and the PIRE program of NSF. In addition, I^2CNER PIs are pursuing large funding of their research efforts in the form of research centers. As an Institute, I^2CNER will leverage the initiatives of the Government of Japan for globalization of the national universities. Due to its linkage with the University of Illinois, I^2CNER, along with KU, is in a unique position to compete for these government initiatives for resources and future expansion on strategically important university-wide programs. Additional resources are expected to come from technology transfer or patent sales and Corporation-supported non-tenured faculty members, whose research is impactful to the corporation's operations.

・ Calculate the total amount of research funding (e.g., competitive funding) based on the percentage of time the researchers devote to research activities at the center vis-à-vis the total time they spend conducting research activities. Be sure the prospects are realistically based on the past record.

The total amount of research funding acquired by I^2CNER members including main Japanese Principal Investigators in the past five years (FY2009-2013, JPY/USD=120), is over 19.5 million dollars per annum on average. In the coming years, the goal is to continue securing external research funds at an even higher rate by aggressively pursuing external sources as stated above.

Others

・ Describe activities and initiatives to be taken after project funding ends.

President Kubo's vision for the future of I^2CNER, as announced in the WPI Program Committee Meeting on Nov. 18, 2014 in Tokyo is that I^2CNER is a permanent unit of Kyushu University. With the revision of the Regulations of Kyushu University effective April 1, 2013, I^2CNER's position is clearly defined as a permanent research institute of Kyushu University without regard to the length of the WPI Program.

・ Describe expected ripple effects（e.g., how the research center project will have trailblazing components that can be referred to by other departments in the host institution and/or other research institutions when attempting to build their own top world-level research centers）.

It is expected that other units and organizations of the Kyushu University will benefit from the academic administration system of this Institute, which is being morphed according to the academic stature of the Institute Director. We expect that the Institute mode of operation will serve as a role model for the entire Kyushu University system in the areas of recruiting, mentoring, and promoting researchers, establishing and promoting international collaborations with top-class research institutions, vigorous peer evaluation of research and faculty productivity, allocation of research resources and personnel financial compensation according to academic qualifications, scientific visibility, and established research record, etc. Examples of ripple effects already in place and continuously expanding are:

・ Describe other important measures to be taken in creating a world premier international research center, if any.
・ Describe activities and initiatives to be taken after project funding ends.
・ Describe expected ripple effects (e.g., how the research center project will have trailblazing components that can be referred to by other departments in the host institution and/or other research institutions when attempting to build their own top world-level research centers).

○ *New Merit-based Annual Salary System*

Kyushu University's new merit-based annual salary system for faculty members is intended to promote revitalization by securing diverse, international, and competent personnel. KU aims to continuously review and improve this system to make KU an attractive place for young scientists to initiate their career and for senior scientists to expand their research programs.

○ *I^2CNER Research Hub*

Following the completion of I^2CNER Building 1, which was built at the heart of the Center Zone on Ito campus, Kyushu University approved the development of I^2CNER Building 2, as well as a Center of Innovation (COI), "the Center for Co-Evolutional Social Systems (CESS)," in the same vicinity. The area surrounding I^2CNER Building 1 is being developed rapidly for the transformation of the Center Zone into Kyushu University's new research hub/industry-academia zone. In April 2014, the university's administration moved into the newly-built Shiiki Hall, which is adjacent to I^2CNER Building 1.

○ *Cross-Appointment*

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

○ *Travel Expenses for Inviting Researchers from Overseas*

When inviting renowned researchers from overseas, I^2CNER has a unique practice of flexibly handling their travel expenses where appropriate. This is already making positive ripple effects, and becoming an approved/common practice across all units of Kyushu University.

○ *Intra-University Faculty Transfer System*

Kyushu University's "Intra-University Faculty Transfer System" enables flexibility in allocating faculty within the University for the purpose of improving the standards of education and research conducted at KU. Utilizing this personnel-system reform, 9 senior-level Kyushu faculty have been transferred to I^2CNER and serve as the core Kyushu-based PIs of I^2CNER. Another unit of KU, the "Institute of Mathematics for Industry," has already started personnel transfers using the Intra-University Faculty Transfer System.

・ Describe other important measures to be taken in creating a world premier international research center, if any.

To address the issues of tenure appointments in I^2CNER and teaching load for I^2CNER faculty, which were raised at the WPI Program Committee Meeting on Nov. 18, 2014, the following represents the new vision for I^2CNER, as formulated by President Kubo:

○ *Tenured PIs in I^2CNER*

I^2CNER embarks upon its second term as a permanent unit of KU. According to President Kubo's vision, there are going to be (10) tenured PIs organically in I^2CNER. The rest of the 10-15 PI positions in I^2CNER (out of the 20-25) will come from either: a) other units of KU through the Intra-University Transfer System (this means that those tenured faculty can return to their original departments after they have spent a reasonable amount of time in I^2CNER), b) through cross-appointments between I^2CNER and other units of KU, e.g. economics, sciences, mathematics, life sciences, etc., or c) through cross-appointments between I^2CNER and its international partner institutes and industry. In addition, the vision is that 3 to 4 PIs amongst the 10 tenured faculty will be non-Japanese. In order to support the recruitment of such distinguished researchers as tenured I^2CNER PIs from abroad, Kyushu University has recently introduced in its Education and Research Council the new Annual Salary Scheme, which allows for these foreign faculty to be compensated with a competitive salary, according to international standards. Lastly, apart from the PI categories (a), (b), and (c) above, I^2CNER will have Visiting Fellows (PI level). As of April 1, 2015, I^2CNER will have a total of 2 full professor and 7 associate professor tenured positions.

○ *Teaching load for I^2CNER faculty*

I^2CNER faculty will be involved with teaching. In fact, KU values this involvement and views it as essential to the revitalization of its programs by bringing into the classroom faculty with international experiences with cutting-edge research. The load will be flexible in order to help maintain the highest possible standards of performance, both for their research and teaching obligations. I^2CNER's young faculty have already begun teaching joint courses on energy. These courses are part of the globalization program of KU, such as the former GLOBAL 30 and the recent Top Global University (TGU) Program of MEXT. As such, the average teaching load for I^2CNER's young faculty is low (co-teaching of a single course per academic term). In addition, KU is planning to establish an International Liberal Arts and Sciences College (this is a tentative name and it is a new undergraduate school) within the coming 4 years in the framework of the TGU program. This college will encompass both physical and social sciences. We envision that I^2CNER's young faculty will help the educational mission of the new college by offering science and technology courses in their relevant fields, again, in a way that balances research and teaching obligations. Also, since the PIs in categories (a), (b), and (c) reported in the previous paragraph will bring their graduate students from their home departments in I^2CNER, it is our vision that the tenured PIs in I^2CNER will supervise these students jointly.

○ Kyushu University will help the Director to diversify the population of I^2CNER PIs and expertise in areas such as mathematics, economics, social and life sciences, and computational science.