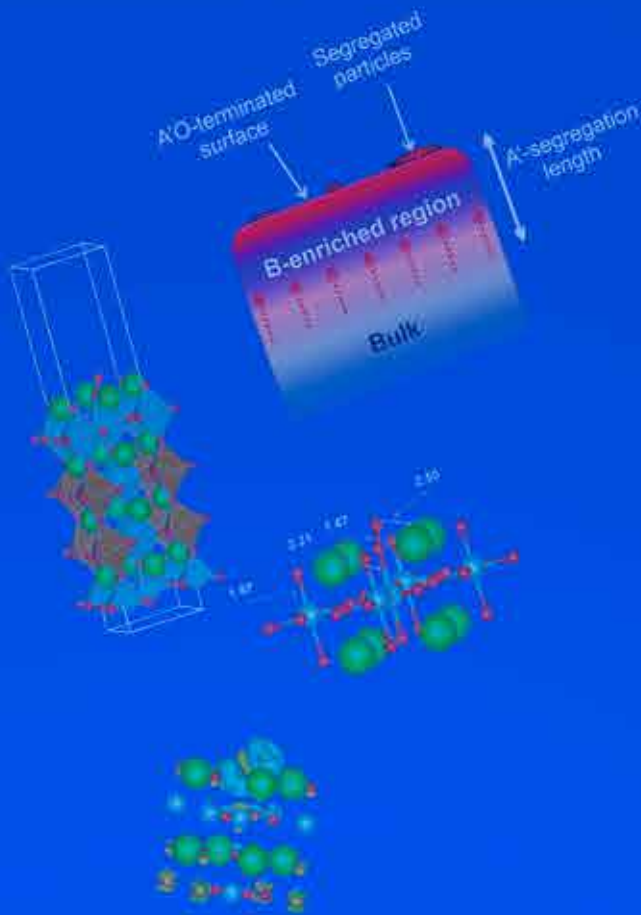


# I<sup>2</sup>CNER

International Institute for Carbon-Neutral Energy Research

## 2018 Annual Report



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# World Premier International Research Center Initiative (WPI)



## Background

An intensifying global demand for talented researchers is accelerating the need to develop the best scientific minds among the world's nations. This trend has prompted Japan to establish new research centers that attract top-notch researchers from around the world so as to place itself within the "circle" of excellent human resources.

## Program Summary

The World Premier International Research Center Initiative (WPI) has four basic objectives: advancing leading-edge research, creating interdisciplinary domains, establishing international research environments, and reforming research organizations. To achieve these four objectives, WPI research centers tackle the following challenges:

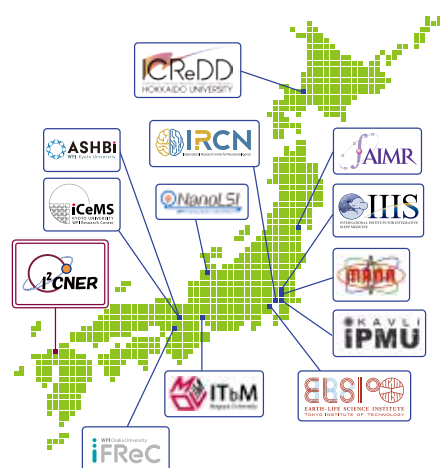
### A Critical Mass of Outstanding Researchers

- Bringing together top-level researchers within a host research institution
- Inviting top-notch researchers from around the world

### Attractive Research and Living Environment of Top International Standards

- Strong leadership by center director
- English as the primary language
- Rigorous system for evaluating research and system of merit-based compensation
- Strong support functions for researchers
- Facilities and equipment appropriate to a top world-level research center
- Housing and support for daily living and education of dependent children

To assist the WPI research centers in carrying out this mandate, the Japanese government provides them with long-term, large-scale financial support.



For more information:

MEXT Website [http://www.mext.go.jp/english/research\\_promotion/1303822.htm](http://www.mext.go.jp/english/research_promotion/1303822.htm)

JSPS Website <http://www.jsps.go.jp/english/e-toplevel/index.html>

<b>International Institute for Carbon-Neutral Energy Research (i<sup>2</sup>CNER) Kyushu University</b> Toward the realization of a low-carbon society, i <sup>2</sup> CNER aims to resolve the challenges of the use of hydrogen energy and CO <sub>2</sub> capture and sequestration by fusing together sciences from atomic level to global scale.	
<b>Kavli Institute for the Physics and Mathematics of the Universe (Kavli IP MU)</b> The University of Tokyo Institutes for Advanced Study, The University of Tokyo With accumulated research on mathematics, physics and astronomy, this research core works to bring light to the mysteries of the universe, such as its origin, and to provide an analysis of evolution.	<b>Advanced Institute for Materials Research (AIMR), Tohoku University</b> Integrating physics, chemistry, materials science, bioengineering, electronics and mechanical engineering, AIMR is striving to create innovative functional materials. A mathematical unit joined the team in 2011 to help establish a unified theory of materials science, aiming at the realization of a global materials research hub.
<b>Immunology Frontier Research Center (iFReC) Osaka University</b> An innovative research center, which pursues the goal of comprehensive understanding of immune reactions through the fusion of immunology, various imaging technologies, and Bioinformatics.	<b>International Center for Materials Nanoarchitectonics (MANA) National Institute for Materials Science</b> A major focus of our activities is the development of innovative materials on the basis of a new paradigm "nanoarchitectonics," ground-breaking innovation in nanotechnology.
<b>Institute for Integrated Cell-Material Sciences (iCeMS) Kyoto University</b> Established to integrate the cell and material sciences, the iCeMS combines the potential power of stem cells (e.g., ES/iPS cells) and of mesoscopic sciences to benefit medicine, pharmaceutical studies, the environment, and industry.	<b>Institute of Transformative Bio-Molecules (ITbM) Nagoya University</b> The goal of ITbM is to develop innovative functional molecules that make a marked change in the form and nature of biological science and technology (transformative bio-molecules). ITbM will connect molecules, create value, and change the world, one molecule at a time.
<b>International Institute for Integrative Sleep Medicine (IHS) University of Tsukuba</b> IHS aims to elucidate the function of sleep and the fundamental mechanisms of sleep/wake regulation and also aims to develop new strategies for diagnosis, prevention, and treatment of sleep disorders. Our goal is to contribute to promote human health through our sleep research.	<b>EARTH - LIFE SCIENCE INSTITUTE (ELSI) Tokyo Institute of Technology</b> ELSI focuses the origins of Earth and life. Both studies are inseparable because life should have originated in unique environment on the early Earth. To accomplish our challenge, we establish a world-leading interdisciplinary research hub by gathering excellent researchers in Earth and planetary sciences, life science, and related fields.
<b>Institute for the Advanced Study of Human Biology (ASHBi) Kyoto University</b> ASHBi investigates the core concepts of human biology with a particular focus on genome regulation and disease modeling, creating a foundation of knowledge for developing innovative and unique human-centric therapies.	<b>International Research Center for Neurointelligence (iRCN) The University of Tokyo</b> iRCN combines life sciences and information sciences to establish the new field of "neurointelligence". By clarifying the essence of human intelligence, overcoming neural disorders, and developing new AI technologies, we will contribute to a better future society.
<b>Institute for Chemical Reaction Design and Discovery (iCReDD) Hokkaido University</b> iCReDD integrates computational, information, and experimental sciences in order to obtain in-depth understanding of chemical reactions, which enables rational design and rapid development of new chemical reactions.	<b>Nano Life Science Institute (NanoLSI) Kanazawa University</b> Cells are the basic units of almost all life forms. We are developing nanoprobe technologies that allow direct imaging, analysis, and manipulation of the behavior and dynamics of important macromolecules in living organisms, such as proteins and nucleic acids, at the surface and interior of cells. We aim at acquiring a fundamental understanding of the various life phenomena at the nanoscale.

## Message from the Director



It is a tremendously exciting time to be a part of the efforts that are ongoing at I<sup>2</sup>CNER. As it enters its 10th year, the institute's momentum and scientific impact continue to increase rapidly. Many metrics support this claim: the number of scientific discoveries and breakthroughs has increased dramatically as have the technology transfers to industry; the number of industrial partnerships has increased as have the number of international universities seeking partnerships with I<sup>2</sup>CNER. With I<sup>2</sup>CNER's many missions and goals, this Annual Report is a sample of our best results since inception that have impacted and will impact society.

I<sup>2</sup>CNER's grand challenge is to develop the foundations for the engineering of energy systems that will address Japan's future energy needs and contribute to the reduction of the nation's CO<sub>2</sub> emissions by 70% from the 1990 levels by 2050. The impact of I<sup>2</sup>CNER's research on CO<sub>2</sub> emission reductions is summarized in an I<sup>2</sup>CNER Report, entitled "Toward 2050: Contributing to a Low Carbon Energy Society," which outlines both the direct CO<sub>2</sub> reductions enabled by I<sup>2</sup>CNER research thrusts and the industry contributions, which are underpinned by these innovations.

As a result of our current accomplishments, approximately 0.43% of the total required CO<sub>2</sub> reductions, and as a result of our projected future achievements, approximately 5.26% of the total required reductions can be realized by I<sup>2</sup>CNER technologies and innovations if they are applied to appropriate energy systems. Significantly, in addition to I<sup>2</sup>CNER's direct contributions, development and implementation of I<sup>2</sup>CNER's relevant technology efforts will account for a further 35.1% of the 2050 target, which demonstrates that I<sup>2</sup>CNER's research efforts underpin impactful energy technologies. The relevance of the I<sup>2</sup>CNER research efforts and objectives in enabling the government of Japan's green innovation initiative is demonstrated by the 53 projects that have resulted in technology transfer. These events are summarized in I<sup>2</sup>CNER's report: "Technology Transfer Summary: I<sup>2</sup>CNER's Interaction with and Impact on Industry." In addition, since inception, I<sup>2</sup>CNER has had a total of 122 collaborative projects with industry.

I<sup>2</sup>CNER has established itself as a worldwide brand by making international, collaboration-driven transformational scientific advances, which will lead to a carbon-neutral energy society. The high-impact transformational reforms being instituted by the Kyushu University Administration with I<sup>2</sup>CNER's help, as well as I<sup>2</sup>CNER's strategy for furthering technology-driven research, are also positioning Kyushu University on the map of academic and energy technology leaders.

In addition to collaborations in engineering and the physical sciences, I<sup>2</sup>CNER has developed international collaborative programs that enable new cultural exchanges between Japan and the United States. Undergraduate and graduate students, faculty, and staff from both Kyushu University and University of Illinois have worked in a wide variety of ways with colleagues and shared cultural experiences such as city and museum experiences to working in laboratories resulting in published co-authored research articles. The future successful goals of I<sup>2</sup>CNER research for 2050 fall on our younger researchers and their ability to collaborate in a collegial, communicative, and independent environment where all are welcome without traditional barriers. I look forward to the continued building of the scientific and cultural bridges between Japan, the United States, and the world.

A handwritten signature in black ink, appearing to read 'Petros Sofronis'. The signature is stylized and fluid, with a long horizontal stroke at the end.

Professor Petros Sofronis, Ph.D.  
Director, International Institute for Carbon-Neutral Energy Research  
(I<sup>2</sup>CNER)



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

### Mission

At I<sup>2</sup>CNER, 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<sup>2</sup>CNER'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<sub>2</sub> capture and storage technology or the conversion of CO<sub>2</sub> to a useful product. Additionally, it is our mission to establish an international academic environment that fosters innovation through collaboration and interdisciplinary research (fusion).

### Science Organization

The Institute is organized in thematic research clusters (divisions) which address specific research objectives. Each research division is led by a designated WPI Principal Investigator (Lead PI) of the Institute. Typically, there are several research groups within each division which focus on individual aspects of the primary division objectives. The divisions are:

- Molecular Photoconversion Devices
- Hydrogen Materials Compatibility
- Electrochemical Energy Conversion
- Thermal Science and Engineering
- Catalytic Materials Transformations

- CO<sub>2</sub> Capture and Utilization
- CO<sub>2</sub> Storage
- Energy Analysis (Applied Math for Energy)

Not only are I<sup>2</sup>CNER's researchers tasked with crossing the boundaries of various scientific disciplines, but they also must work hard to bridge the Pacific Ocean. The I<sup>2</sup>CNER project is highly unique, in that it has its main facility at Kyushu University (KU) in Japan and a Satellite facility at the University of Illinois at Urbana-Champaign (UIUC) in the United States. The research projects at UIUC are complementary to and integrated with those at KU. In addition, the Satellite Institute is a hub for identifying and engaging state of the art research programs and faculty at universities and other research institutions in the U.S. and internationally with which I<sup>2</sup>CNER can collaborate. These collaborations with first class international research centers, universities, and national laboratories help I<sup>2</sup>CNER to ensure that its mission has maximum impact in Japan and throughout the world. In order to sustain its fruitful international relationships, the I<sup>2</sup>CNER Administration encourages the Institute's researchers to engage in exchange visits with all its international partners, especially the Satellite Institute. The symbiotic relationship between KU and UIUC is exemplary of I<sup>2</sup>CNER's vision for the international collaborations necessary to achieve breakthroughs in fundamental science.



Figure 3. I<sup>2</sup>CNER Building 1

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

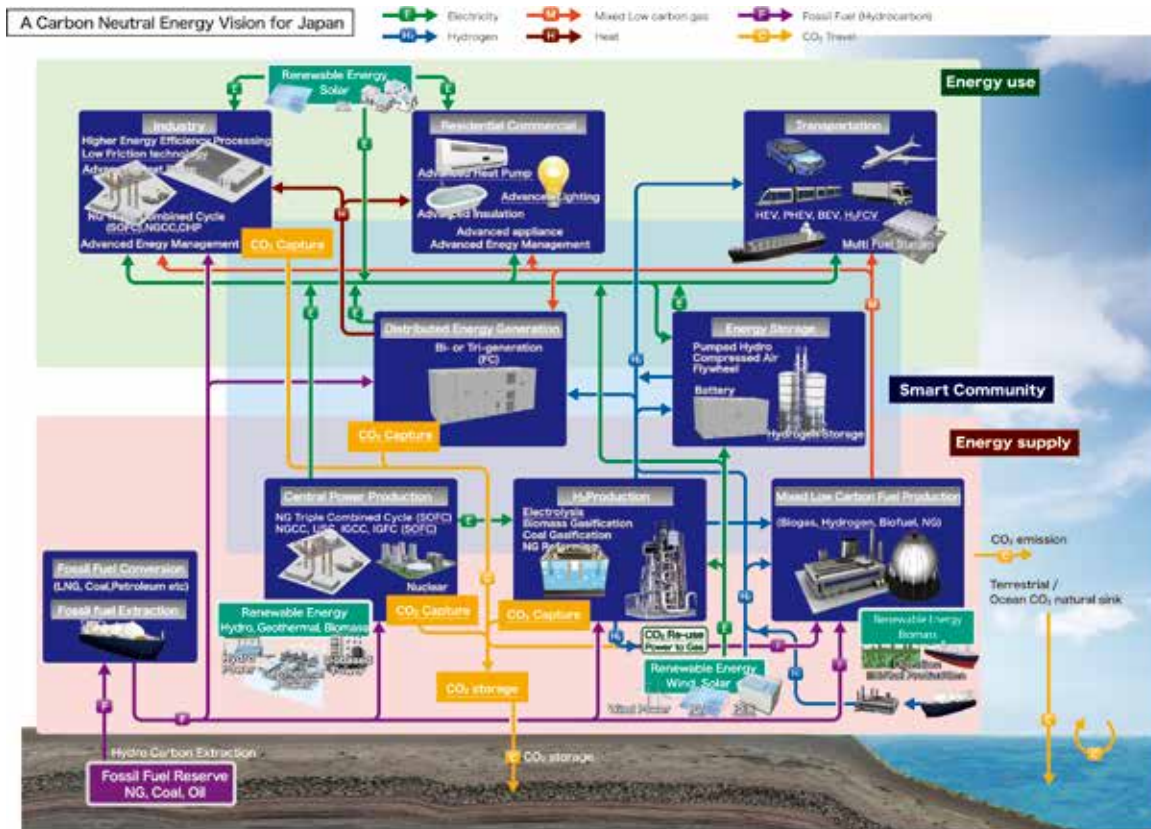


Figure 4.1. Parameter Space of Technology Options.

## Background

Our vision of a carbon-neutral energy society (CNS) is to help identify the future technology options for a CNS by sharing a common image of a future for Japan with people in and outside of I<sup>2</sup>CNER. In 2009, the G8 announced the commitment of an 80% greenhouse gas (GHG) emissions reduction in 2050 relative to the 1990 level. The I<sup>2</sup>CNER vision for a low carbon society for Japan is based on setting a long-term target of a large reduction (70-80%) of GHG by 2050. This target is particularly relevant to energy security concerns caused by Japan's current heavy reliance on imported fossil fuels, which are depletable and scarce resources. To achieve the target by developing new technology, 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 the vision.

In drawing our vision, we consider two major principles, efficiency increase (we call it "EI" hereafter) in energy conversion and energy use, and lowering of

carbon intensity (we call it "LCI" hereafter) of fuel and electricity to adopt and develop future technologies. EI should be pursued in energy transformation systems as well as end use systems, including home appliances. This idea will also be pursued in 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, nuclear, or CCS. LCI tends to need new facilities or new infrastructure or both.

Fig.4.1 shows the image and relation of energy conversion sectors and energy use sectors which are connected by energy pathways represented by secondary energy (electricity, hydrogen, and mixed low carbon fuels using biofuel) in a low carbon society. Some fossil fuel extracted from underground will still be provided to energy conversion sectors and industry with CO<sub>2</sub> capture and sequestration (CCS). Some captured CO<sub>2</sub> can be reused as an energy carrier.

## I<sup>2</sup>CNER Scenarios for Carbon-Neutral Energy Society

There are many possible scenarios to achieve our 3E+S energy vision. EI technology developments are important. Therefore, they are included across the scenarios. LCI technologies can have the greatest impact on GHG emissions and thus enable achieving the challenging GHG emissions reduction target. As mentioned in Annual Progress Reports of previous years, we explored and developed multiple scenarios by prioritizing different LCI technologies, renewables, and CCS outlined in Fig.4.1 Nuclear is not prioritized in the scenarios at this point because of public concerns about safety. The variability of development and deployment of these technologies causes the differences among the scenarios.

A most likely future energy system is what we termed Scenario A in last year's Annual Progress Report, which in essence is a balanced scenario, involving a combination of renewable energy deployment and carbon capture and storage technologies. The second, Scenario D introduces hydrogen into the energy system, predominantly imported from overseas.

In terms of Scenario A, we are analyzing the inherent compromises which emerge between system cost, energy security, and overall feasibility of the deployment of renewables, CCS, and nuclear technologies, along with system EI over time. Renewables are prioritized because they improve energy security and reduce energy related emissions but intermittency is an issue which must be dealt with at the system level, especially considering the uncertainty surrounding the contribution from nuclear. In addition, the potential contribution of wind, which has not been deployed as quickly as solar PV under the Feed-in Tarrif (FIT), and implications on intermittency and storage approaches as well as their costs continue to be explored.

Scenario D also has the potential to emerge as a future scenario. It utilizes imported hydrogen sourced from coal gasification (in combination with CCS) underpinning carbon neutral transport as well as industry, residential, and power generation applications in Japan. Uncertainty surrounding CCS storage potential (domestic and international) and stakeholder acceptance (including industry) continue to guide our analysis and ongoing revision of our scenarios.

**Scenario A (Balanced):** Development of important EI technologies and balanced deployment of renewable and CCS. About 71% CO<sub>2</sub> emissions reduction relative to 1990 in 2050.

### Contribution to EI

Heat pump and FC cogeneration for residential & commercial from 2020. Low temperature heat utilization for industry from 2020. Fuel cell and hydrogen material & storage for transportation from 2020. SOFC (durability, generation efficiency, and coal gas application) for power industry in 2030-2050.

### Contribution to LCI through renewables

Hydrogen storage and new battery technology to adjust intermittent PV and wind power from 2030. Development of electrolysis (PEM and high temperature steam) using renewable electricity to provide low carbon hydrogen from 2030.

### Contribution to LCI through CCS

Low cost membrane CO<sub>2</sub> capture technology for IGCC and other fossil fuel based power generation from 2030. Development of simulation technology for CO<sub>2</sub> monitoring and storage site characterization from 2030 through seismic approaches.

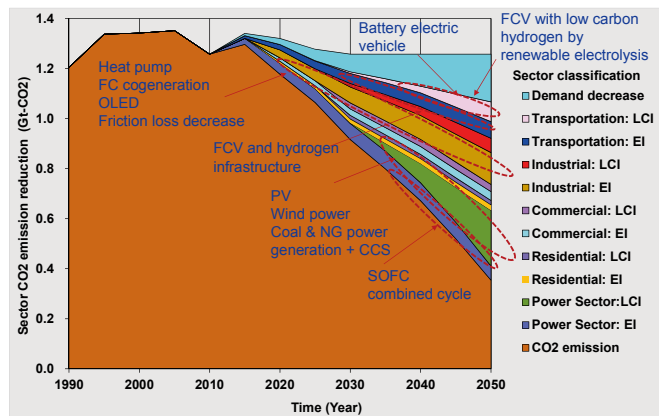


Figure 4.2. CO<sub>2</sub> reduction relative to 1990 by sector in Scenario A.

**Scenario D (Hydrogen Import):** Low carbon hydrogen import with balanced application of LCI technologies including nuclear power, assuming commercial hydrogen import will start from 2030 mainly for power generation. About 71% CO<sub>2</sub> reduction relative to 1990 in 2050 I<sup>2</sup>CNER's contribution to CCS.

*Contribution to EI and LCI technologies in addition to those in scenario A*

Through: (i) initiation of full-scale hydrogen economy, which I<sup>2</sup>CNER's hydrogen compatible material research and hydrogen physical property research underpin; (ii) mixing natural gas with hydrogen and generating pure hydrogen turbine power from 2030; (iii) supplementing the delay of nuclear generation restart by hydrogen power generation and CCS deployment; (iv) hydrogen infrastructure for fuel cell vehicles using imported hydrogen from 2030; (v) distributed power generation using SOFC and imported hydrogen from 2040.

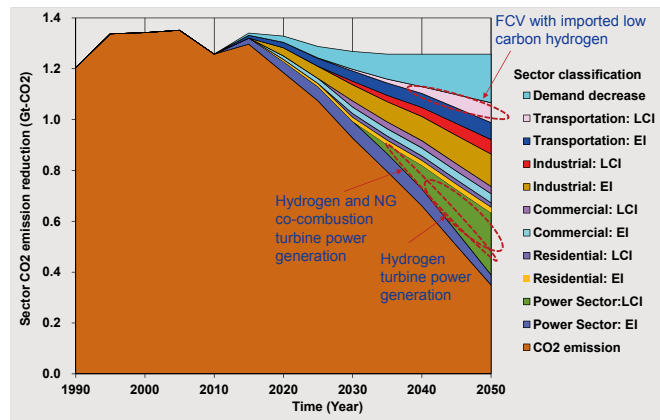


Figure 4.3. CO<sub>2</sub> reduction relative to 1990 by sector in Scenario D.

I<sup>2</sup>CNER's research efforts are intimately tied to these scenarios because the short-, mid-, and long-term milestones of each of our division roadmaps were established in consideration of our intent to remove the roadblocks for the development and deployment timing of the various promising technology options in the scenarios. The updating of the I<sup>2</sup>CNER roadmap and research portfolio for the removal of roadblocks toward CNS is carried out by the continuous interaction among the technical divisions and the Energy Analysis Division.



## I<sup>2</sup>CNER's Contribution to the 2050 CO<sub>2</sub> Reduction Target

Based on our analysis of current and future achievements, approximately 0.43% of the total required CO<sub>2</sub> reductions via current achievements and approximately 5.26% of the total required reductions through our future achievements can be realized by I<sup>2</sup>CNER technologies and innovations if they are applied to appropriate energy systems (limiting the contribution of any one technology to 50% of the resultant market). In addition to I<sup>2</sup>CNER's direct contributions, all I<sup>2</sup>CNER activities also contribute to the overall relevant industry efforts (a further 35.1% of the 2050 target, shown in dark grey in Fig. 5.b) through the provision of underpinning technologies and analyses.

As shown in Fig.5.b, the leading contributors to I<sup>2</sup>CNER's 2050 CO<sub>2</sub> reduction efforts include energy storage and carriers, encompassing electrolysis and the reversible fuel cell; CO<sub>2</sub> capture and storage, through novel CO<sub>2</sub> separation membranes and monitoring technologies; and energy efficiency, utilizing energy saving heat loop-tube technologies and friction reducing coatings. EAD continues to analyze each technology thrust within I<sup>2</sup>CNER in line with our energy system scenarios to ensure that our contribution toward CO<sub>2</sub> reduction and to underpinning industry efforts is maximized.

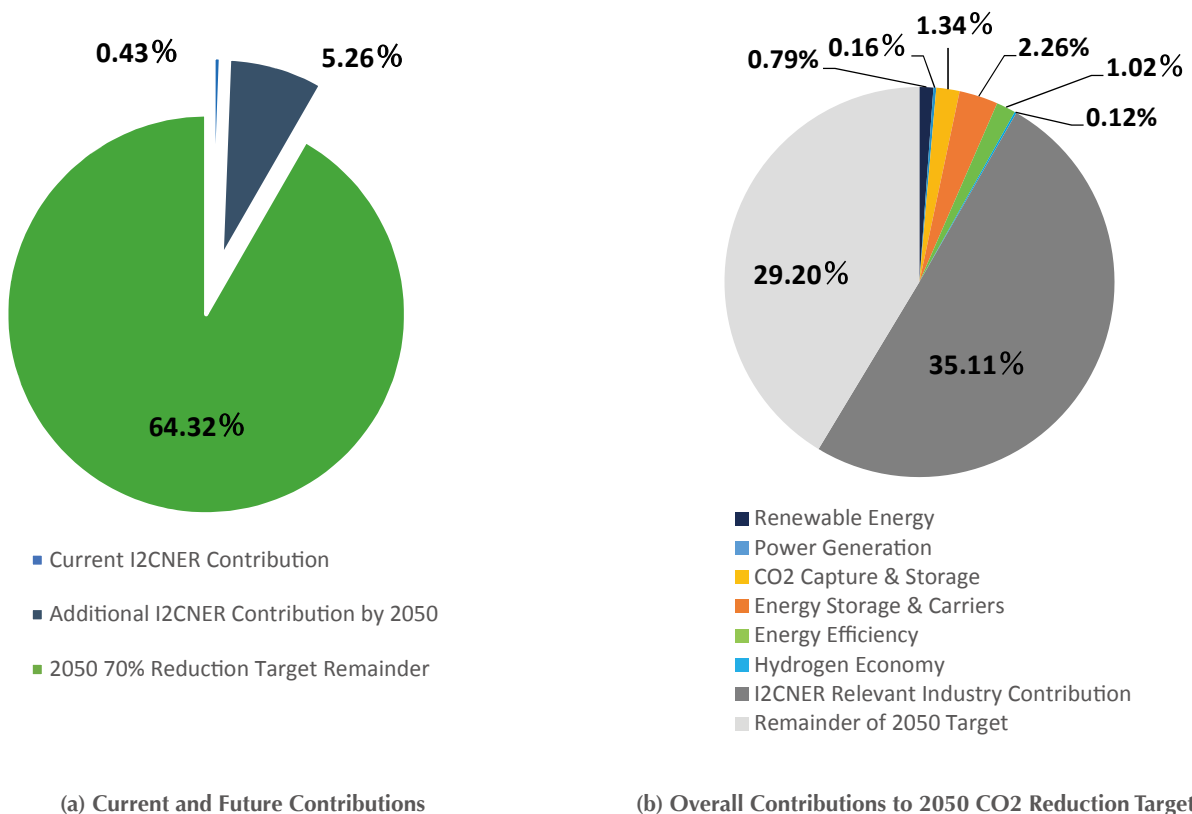


Figure 5. I<sup>2</sup>CNER's current and future contributions to CO<sub>2</sub> reduction in Japan.

## Energy Analysis (Acting Division Leader: Prof. Itaoka)

### Overview

This division plays a critical role in I<sup>2</sup>CNER. It is responsible for providing analyses of carbon emissions, energy efficiency, and cost of current and emerging I<sup>2</sup>CNER and other energy processes, technology, and infrastructure. These analyses help ensure that I<sup>2</sup>CNER's and global energy-related research are well targeted toward a carbon neutral society for Japan and the world as a whole. Additionally, 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<sup>2</sup>CNER and other energy system analyses.

### Hydrogen station deployment for fuel cell vehicles

The objective of this study was to develop an effective model for domestic hydrogen station deployment and identify prospective areas for hydrogen stations locations to meet future refueling demands of fuel cell vehicles (FCV). A deployment model employing location allocation theory using GIS (geographic information system) was used to consider user convenience and FCV penetration phases.

The model assumed that current high-priced luxury car (over 5 million yen) owners were the potential initial FCV customers and medium class car (over 3 million yen) owners were the potential FCV customers of the future. Based on our model results, we concluded that the most effective approach was to locate the hydrogen stations in a way that minimizes average distance between potential customers and nearest hydrogen stations (Fig. 6.1). The study also identified gaps between existing and planned stations, and the suggested station sites. This gap analysis identified certain cities, particularly prefectural capital cities, in need of coverage. The results were directly reported to the Ministry of Economy, Trade and Industry and shared with hydrogen station stakeholders to support hydrogen deployment policy and planning in Japan. Also, the model results of follow-up analyses are currently used by JHyM (the Japan Hydrogen Station Network Joint Company), created by major car companies and energy companies to develop hydrogen refueling infrastructure.

### Energy Transitions: The People, Technology, and Systems Nexus

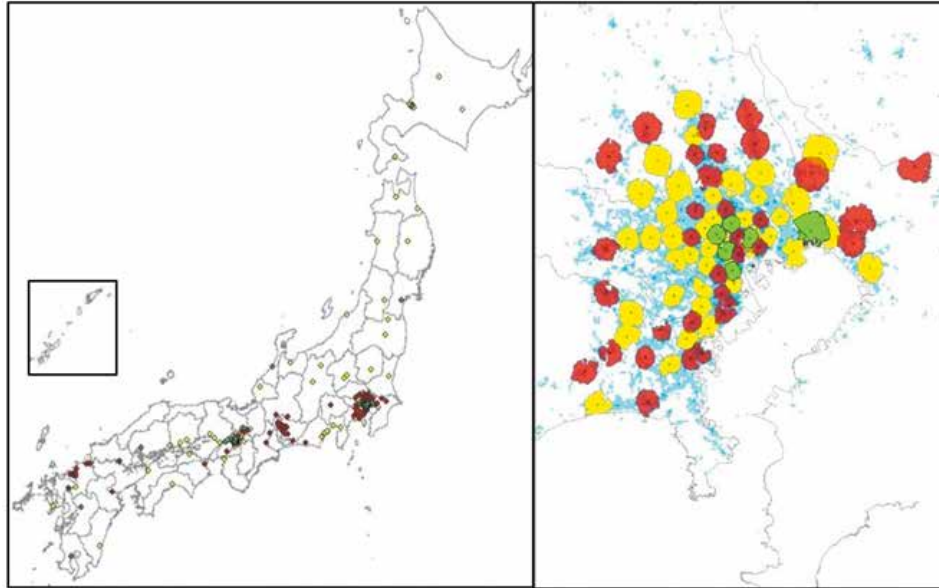
The Japanese energy system is undergoing an energy transition from a system traditionally highly reliant on nuclear and fossil fuel energy sources toward a low-carbon energy system which includes renewable energy and complementary technologies including hydrogen and battery storage, and carbon capture and storage. Our research focuses on a number of aspects

including the influence of exogenous shocks and liberalization on the transition progress, and the role of the socio-technical regime on further influencing the nature of the market and technologies which will enable a successful low-carbon energy transition. In the 'people-technology-systems' nexus, we consider a broad range of issues underpinning the transition in a systemic manner, identifying policy implications and priority I<sup>2</sup>CNER technologies which may contribute to the transition in Japan and internationally.

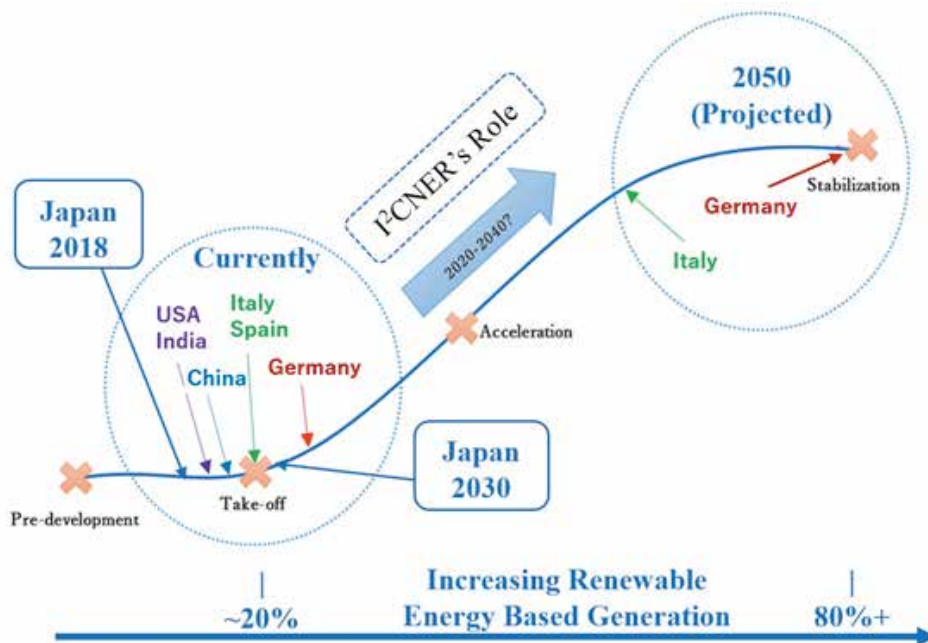
The EAD carried out: i) a comparative review of Japan and transition leaders' progress and policies supporting the transition, drawing learnings to improve future progress, and, ii) a national survey to establish stakeholder activeness. As shown in Fig. 6.2, Japan's progress toward a successful transition lags behind that of international leaders, however Japan may have a future competitive advantage in being a late enactor of energy market liberalization. Further, through an investigation of householder knowledge, usage and preferences toward energy and energy policies, we were able to deduce three distinct tiers of stakeholder activeness and motivation. Approximately 14.6% of Japanese consumers are likely to actively seek economic and environmental benefits through market products and services, 41% of consumers act, depending on the level of perceived benefit, while a further 44.4% of people remain indifferent to new market products and services.

Additional analysis was undertaken on potential impacts on the future transition, by incorporating householder preferences in a bottom-up/strategic policy hybrid approach. It was identified that an additional quantum of renewable energy and a reduction in nuclear power could be achieved in Japan by involving householders in the energy system through initiatives including demand response, network storage, and self-sufficiency.

## Selected Research Accomplishments



**Figure 6.1.** Red dots and red areas show existing/planned station sites and their 10 minute driving radii. The additional stations that will be created, bringing the total of initial stations to 100, are indicated by green dots (10 minute driving radii indicated by green areas). The additional stations (initial 100 to 200 stations) and their 10 minute driving radii are indicated by yellow dots and yellow areas. The initial 5,000 customers are represented by blue areas. The additional 15,000 customers, which will bring the total to 20,000 early customers, are represented by light blue areas. Lastly, the additional 30,000 customers, which will bring the total to 50,000 early customers, are represented by pale blue areas.



**Figure 6.2.** Leading countries' current position and projection toward a successful energy transition.

## Molecular Photoconversion Devices (Lead PI: Prof. Ishihara)

### Overview

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

### Photovoltaic conversion efficiency and stability in hybrid perovskite based devices

Achievement of both high photovoltaic conversion efficiency and stability in hybrid perovskite based devices remains a key challenge to the technology. The Adachi group, working with international collaborators, has achieved globally-recognized successes in hybrid perovskite photovoltaics as well as demonstrated key mechanisms for degradation. Some of the most important contributions include the following: (i) The group was one of the first to identify degradation of the lead-iodide in lead-containing perovskites, resulting in formation of metallic lead. This was shown to be connected to moisture and oxygen in the device layers. The group showed that changing the processing conditions for the device to avoid exposure to these, they could dramatically improve lifetime (by a factor of 2.5). The formation of metallic lead was also connected directly to carrier recombination states in the materials, which is a primary cause of efficiency loss. (ii) The group has also demonstrated an entirely new method for stabilizing perovskite photovoltaics by including additives in the deposition precursor solutions. As one example of this process they showed that addition of benzoquinone (BQ) to the precursors improved conversion efficiency and device stability by improving the crystal structure and morphology of the perovskite. In BQ-incorporated perovskite solar cells, the power conversion efficiency was ~15% and the 80%-lifetime (at which efficiency reduces to 80% of the initial under illumination) was 4,000 hrs. Our recently extrapolated 50%-lifetime is over 20,000 hrs and among the world's top reported values. This approach has been adopted world-wide for solution processed hybrid perovskite photovoltaics. We also demonstrated that our perovskite alloy solar

cells fabricated by mixing several cations and anions were very thermally stable and that our lead-free tin iodide-based perovskite solar cells fabricated with a modified solvent bathing method had very high stability, with almost no degradation under continuous illumination over 1,000 hrs. More recently, our systematic optimization of hybrid perovskite materials and solar cell architectures led to an increase of power conversion efficiency to ~21.5% and extrapolated 50%-lifetime to ~23,000 hrs (manuscript under preparation). *These results exceed the milestone of >20% in power conversion efficiency and >10,000 hrs in 50%-lifetime for Project 1 in the Molecular Photoconversion Devices division's roadmap and are approaching the mid-term milestone.* (iii) In the past year the group has published results of a new approach to improving efficiency of the devices by addition of photochemically active additives which populate grain boundaries in the hybrid perovskites. These reduce the contact potential at the boundaries, and were shown to promote carrier transport and collection. The mechanism for this improvement was demonstrated using scanning probe microscopy and provides a general understanding of a key method to improve device performances. (iv) Working with collaborators in Australia, the United States, and Lithuania, and other countries, our team has established a variety of fundamental understandings of the operation of these devices. We have developed a theory of carrier transport and carrier trapping in the devices, demonstrated the mechanisms for trap formation, and simulated the behaviors with various numerical models including drift-diffusion and density functional theory methods. This fundamental understanding is improving optimization of devices world-wide. These and other results are widely cited by other groups as groundbreaking in the field of

perovskite photovoltaics. *The research has direct connections to and is improving organic light emitting device performance and is opening new approaches to thin film transistor technologies.*

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

### Novel Photocatalysts

Photocatalytic splitting of water to form hydrogen and release oxygen is one of the approaches being explored for inexpensive transportation fuel production and is a key component of Project 2-2 in the Molecular Photoconversion Division. A successful approach requires an improved photocatalyst that will directly absorb sunlight and transfer the energy into breaking a H-O bond in water molecules. Typically, this can be limited by slow reaction kinetics for hydrogen evolution. PI Ishihara and his collaborators at Kyushu University, Imperial College, London, the University of Illinois at Urbana-Champaign, and elsewhere have been working to understand the fundamental properties of electrode materials and to improve these through theory-guided molecular and inorganic solid design. The result is an integrated multiscale modeling approach combined with experiments to demonstrate intelligent design of advanced photocatalysts. The approach has already resulted in dramatic improvements in materials performance. Combining first-principles electronic structure calculations with experimental data and intelligent materials design, the team in collaboration with the Ertekin theory group at the University of Illinois have demonstrated a model for co-catalyst activity in which rhodium (Rh)

atoms are incorporated into titania (TiO<sub>2</sub>) nanosheets. Atomistic first-principles methods were used to reveal the process by which photo-generated charges are transferred to the Rh reaction center. The Rh atom was shown to capture free photoelectrons from the TiO<sub>2</sub> and transfer them to adsorbed H<sub>2</sub>O molecules, resulting in catalytic release of H<sub>2</sub> at increased rates relative to TiO<sub>2</sub> without the Rh dopant. Having demonstrated the basic mechanism, the team then assessed the potential for other transition metal atoms to function in similar ways and to determine which would produce the optimal catalysis of the reaction (Fig. 6.4). Experiments with pure TiO<sub>2</sub> and with doping of both Rh and Pd showed the predictive capability of the model. Design rules were developed for identifying rate-limiting steps in the reaction. This provided the first direct comparison between experiment and computation and the first reliable method for design of advanced co-catalyst dopants for photocatalysis.

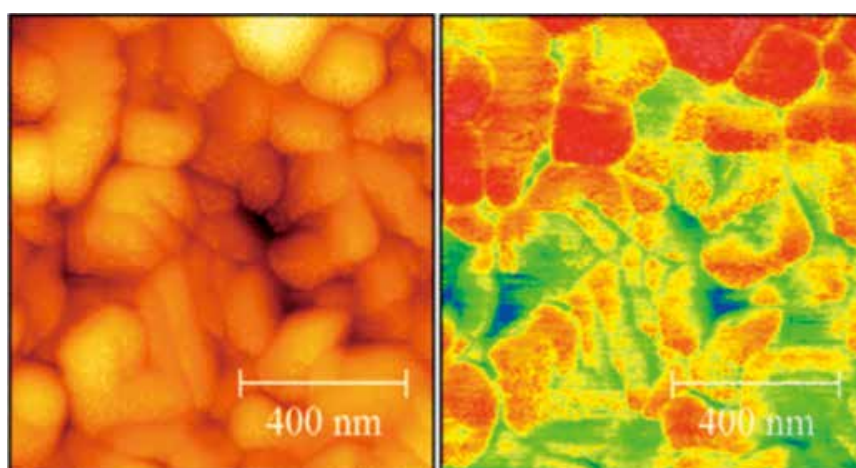
Taking the next step, the model was integrated with a drift-diffusion simulation tool to understand charge transfer at a macroscopic scale. This approach couples the atomic scale first-principles method with the full device scale behavior. Using this method an improved two-layer photocatalyst involving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

The design of advanced photocatalysts has also been extended by the team through their development of new processing methods to create the catalysts that theory predicts should work well. The team showed, for the first time worldwide, that high pressure torsion could stabilize unique new crystal structures of ZnO and TiO<sub>2</sub> and their mixtures with other compounds. The resulting materials are characteristic of high pressure phases of the mixtures. These were shown to have novel engineered optical properties and to function as photocatalysts with enhanced catalytic activity. Improvements were found in GaN-ZnO oxynitride mixtures and tantalite perovskites by a factor of three due to nitrogen and oxygen vacancies. The findings were explained using theoretical calculations and further optimization and intelligent design of new materials was demonstrated using this

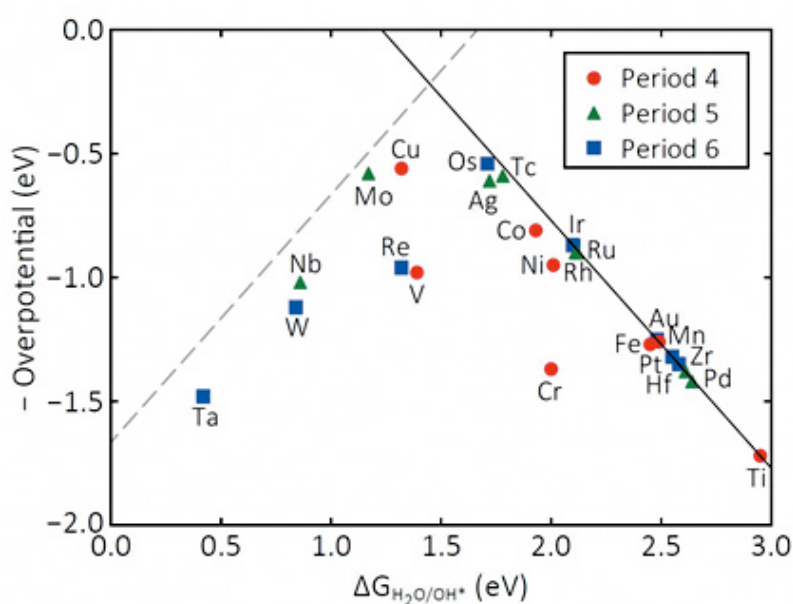
## Selected Research Accomplishments

method. In summary, some of the unique contributions of PI Ishihara's team include: i) Demonstration that single atoms incorporated into TiO<sub>2</sub> nanosheets can catalyze water reduction to produce H<sub>2</sub>, ii) Development and demonstration of the capabilities of a multiscale approach to simulating photocatalysis and allow intelligent design of novel photocatalysts with superior properties. The resulting model is unique on a global scale for understanding photocatalysis,

iii) Visualization of the mechanism for such a process and testing of alternate dopants without the need for experiments a-priori, iv) Development of novel processing methods based on high-pressure torsion resulting in metastable mixtures of compounds with enhanced photocatalytic performances. *These advances address the short-term milestone for project 2 of the Molecular Photoconversion Devices Division.*



**Figure 6.3.** Kelvin-probe force microscopy images of changes to hybrid perovskite materials when doped with benzoquinone. Contact potential differences at grain boundaries decreased under illumination, leading to efficient carrier transport across grain boundaries.



**Figure 6.4.** Calculated activity profiles for a broad spectrum of transition and rare earth metals as cocatalyst dopants.

## Electrochemical Energy Conversion (Lead PI: Prof. Matsumoto)

### Overview

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

### Air electrodes in high temperature electrochemical devices: An atomistic study of composition and mechanisms

This interdisciplinary international effort directed by PI Kilner lies at the intersection of surface science, materials science, electrochemistry and theoretical and molecular chemistry and was enabled by the formation of cross divisional team at I<sup>2</sup>CNER. This team tackled the very difficult problem of understanding the surface properties of multicomponent oxide air electrodes at high temperatures in the complex gaseous environment of ambient air. Air electrodes can typically experience degradation under operation consequently limiting the commercialization of high temperature electrochemical devices for efficient energy conversion. The role of the air electrode is to either incorporate oxygen, by the oxygen reduction reaction (ORR), or evolve oxygen by the oxygen evolution reaction (OER), during operation in either fuel cell or electrolysis mode. The evolution of surface composition, surface reactions, and the degradation mechanism are longstanding puzzles that must be addressed for wide-scale technology adoption. Using a combination of advanced surface analysis techniques and first principles theoretical studies, we have unravelled the significant phenomena that control the performance of the ORR and OER in these multicomponent materials in the complex gaseous environment of ambient air. The most common materials used as air electrodes are the mixed ionic

electronic conducting perovskite oxides with a general formula of  $A_{1-x}A'_xBO_3$ , where the transition metal B cations such as Co or Fe are thought to be essential to the ORR/OER process and the large A and A' atoms, most usually La and Sr respectively, were both thought to be inert. The first part of this investigation showed two previously unknown characteristics, that are universal to a large class of air electrodes and closely linked to their degradation. First, under the conditions of operation the surface quickly reorganizes to a termination consisting entirely of A type cations and O ions, covering the catalytically active B cations. Second, there is a rapid segregation of substituted A' cations to produce a majority A'O (e.g. SrO) rich near-surface region (Fig. 6.5. a, b). Using this knowledge of the surface composition, we computationally modelled the adsorption and incorporation of molecular oxygen onto these segregated electrode surfaces. Our analysis shows that pristine segregated SrO surfaces are inactive for oxygen adsorption, and that systems must rely on active site mediated mechanisms for adsorption to occur. These active sites are the surface oxygen vacancies that provide a window to access the active B site transition metals (Fig. 6.5.c). We have extended this analysis, and again by a combination of experiment and theory we have shown the importance of understanding the role of the other oxygen bearing molecules in the air environment to optimise the ORR reaction. Finally we have shown that in related A' free materials, e.g.  $La_2NiO_4$ , the surfaces are again AO dominated and that, in this case,

and contrary to conventional thought, the surface La cations are an active participant in the ORR reaction. This is due to the electronic configuration of these rare earth elements which shows a marked degree of covalency in their interaction with oxygen. These new insights highlight the critical need for rational design of surfaces to enhance performance; a finding that was previously not recognised points the way to the optimisation of high performance low degradation air electrodes. *Additionally, these results meet the short- and a mid-term milestones for solid oxide cells in Project 1 of the Electrochemistry Energy Conversion division's roadmap.*

### Novel electrocatalyst design based on polymer-wrapping of carbon nanotubes

To overcome the critical limiting feature of low durability of electrocatalysts, PIs Nakashima and Fujigaya have developed the use of polymer-wrapped carbon supports. This unique approach has now been applied to produce a comprehensive set of metal nanoparticles including Pt, Au, Pd, Au-Pd core-shell and Ir or homogeneous coatings of the proton-conductive layers on the surface of carbon supports (Fig. 6.6.a). Notably, the team has demonstrated extremely high durability, with lifetimes of the polymer electrolyte fuel cell (PEFC) for single cell tests exceeding 500,000 cycles at 80°C under humidified conditions (Fig. 6.6.b) and > 400,000 cycles at 120 °C under non-humidified condition, which to the best of our knowledge is the world-top durable fuel cell catalyst. This polymer-wrapping technology opens new routes for developing next generation PEFCs with both exceptional durability enhancement and cost reduction. *These results exceed the stability target for PEFCs in Project 1 of the Electrochemical Energy Conversion division's roadmap, are contributing to the short-term milestone, and are promising toward the final target for 'non-Pt PEFC'.*

### Highly-Conductive Proton-Conducting Oxide for Intermediate temperature steam electrolysis

The group of PI Matsumoto made significant advancements on steam electrolysis, currently the most energy-efficient process of water splitting for hydrogen production using renewable energy. We developed BZCY54<sub>89</sub>2, a proton conducting electrolyte exhibiting high performance at intermediate temperatures (400-600 °C). Conductivities at 500 and 400 °C are higher than those of LSGM and GDC which are the most frequently used benchmark for oxide ion conducting solid electrolytes (Fig. 6.7). We determined the

composition to be the best in the series of perovskite-type BaZr<sub>x</sub>Ce<sub>1-x-y</sub>Y<sub>y</sub>O<sub>3-δ</sub> (BZCY) electrolyte materials with protonic conductivity of 10<sup>-2</sup> S/cm or higher at 500°C as well as for thermodynamic stability. The reported BaZr<sub>0.1</sub>Ce<sub>0.7</sub>Y<sub>0.2</sub>O<sub>3-δ</sub> (9 × 10<sup>-3</sup> S/cm at 500°C) as holding the benchmark conductivity is disadvantageous due to its low stability in CO<sub>2</sub> and H<sub>2</sub>O environments. We discovered the cerium/zirconium ratio of 5/4 at the B-site of the perovskite exhibits both a higher conductivity and stability than the benchmark. A steam electrolysis voltage as low as 1.45 V was obtained at current densities of 0.2 and 0.5 A cm<sup>-2</sup> at 550°C and 600°C, respectively, with current efficiency >82% using our developed BaZr<sub>0.44</sub>Ce<sub>0.36</sub>Y<sub>0.2</sub>O<sub>3-δ</sub> electrolyte. From this performance, the calculated amount of electricity required to produce 1 N-m<sup>3</sup> of hydrogen is 4.2 kWh, which is lower than the 5 kWh required for the same amount of hydrogen using ordinary water electrolysis. Regarding the air electrode, we clarified the availability of protons in double perovskite oxide BaGd<sub>0.8</sub>La<sub>0.2</sub>Co<sub>2</sub>O<sub>6-δ</sub> at 300°C from which new air electrode materials tailored for use with protonic electrolytes could be designed. We have established a standard protocol for highly efficient intermediate temperature steam electrolysis, which has been shared with Nippon Shoukubai Co. Ltd through collaborative research initiated in 2013 toward commercialization. *The conductivity of this new material meets the short-term milestone in the Electrochemical Energy Conversion division's roadmap for Project 2.*



## Selected Research Accomplishments

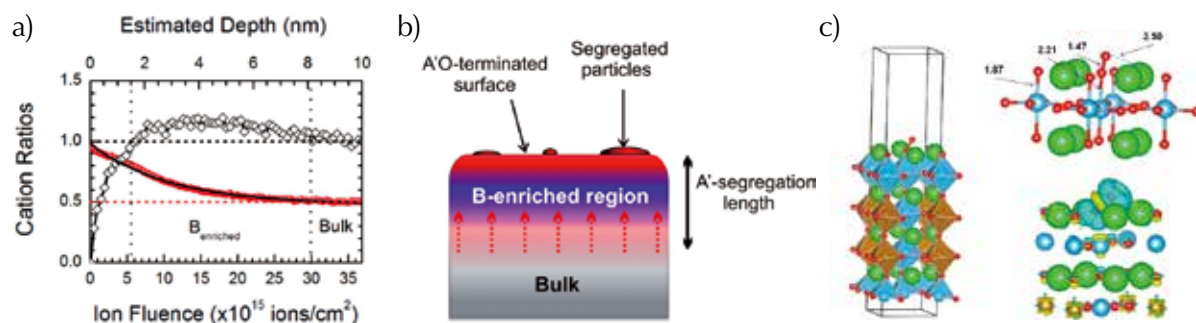


Figure 6.5. a) Measured compositional profile shows segregation of cations to the surface, b) Schematic of measured composition profile. The segregation is closely linked to performance degradation, c) Atomistic modelling has unveiled a vacancy-assisted mechanism for surface oxygen exchange involved in the ORR.

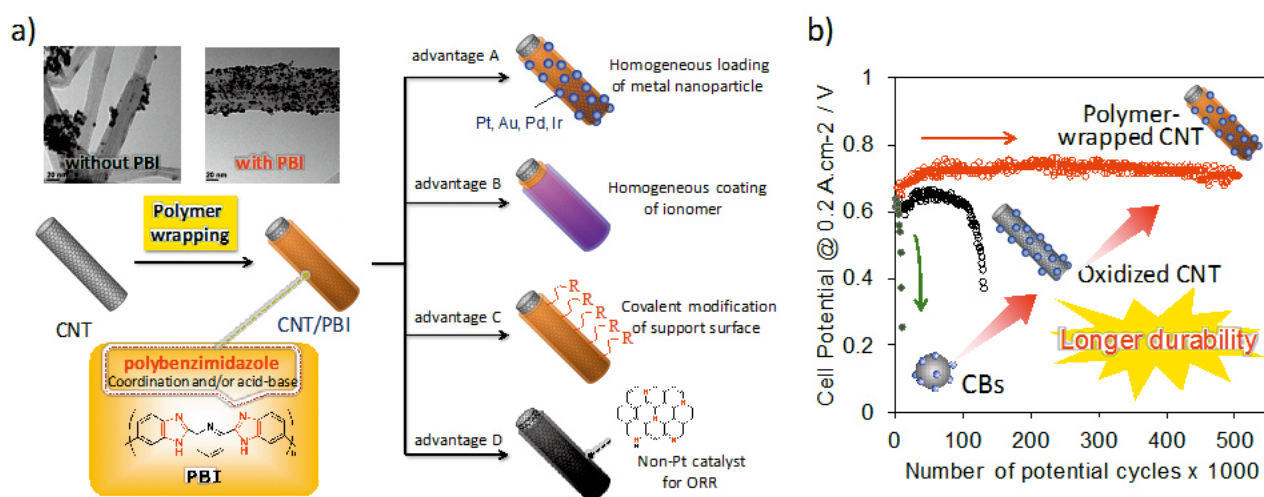


Figure 6.6. New approach to highly durable electrocatalysts based on polymer wrapping. a) Summary of the approach, b) Durability results showing no visible degradation in polymer wrapped systems up to 500,000 cycles.

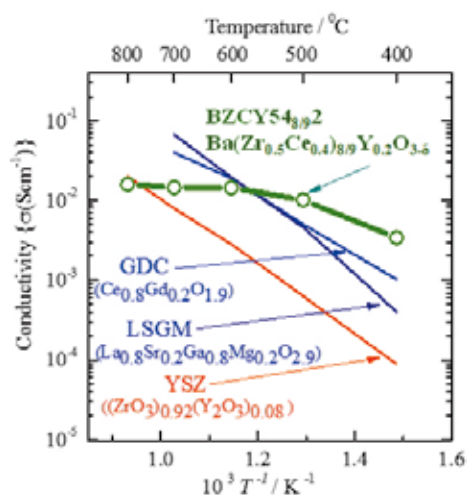


Figure 6.7. Ionic conductivity of (BZCY54.92) compared with existing oxide-ion-conducting electrolyte materials.

## Catalytic Materials Transformations (Lead PI: Prof. Ogo)

### Overview

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<sub>2</sub> emissions in energy, power, or industrial production processes. Projects in the division address the development of: (i) novel biological and biomimetic catalysts for H<sub>2</sub>, CO<sub>2</sub>, and H<sub>2</sub>O activation based on naturally occurring enzymes; (ii) materials development toward the realization of a carbon-neutral power generation cycle.

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

The search for biomimetic hydrogen activation by the Ogo team along with our report of a functional [NiFe]-based catalyst (Fig. 6.8) was crowned the first synthetic analog for H<sub>2</sub> activation in the world. The new catalyst consists of Ni and Fe centers linked by a pair of thiolates, as seen in the natural enzyme. Structural investigations were performed by a range of techniques, including x-ray diffraction and neutron scattering, resulting in detailed crystal structures that can be analyzed to understand the mechanism of catalysis. The hydrido substrate bridges the Fe and Ni, being predominantly associated with the Fe center. The hydridic character of the substrate is manifested by the liberation of H<sub>2</sub> upon reactions with strong acids. By activating hydrogen, this new system is capable of catalytically reducing substrates by both electron transfer and hydride transfer pathways. *This accomplishment along with the development of the model complex of O<sub>2</sub>-tolerant [NiFe]hydrogenase that functions as a non-Pt cathode catalyst for the reductions of O<sub>2</sub> and H<sub>2</sub>O<sub>2</sub> meets the short-term milestone for Project 1 in the Catalytic Materials Transformations Division’s roadmap.*

### One model, two enzymes: activation of hydrogen and carbon monoxide

A second major advance, also coming from the Ogo group, targets bio-mimetic (or bio-inspired) catalysis. The focus remains on transformations of small molecule substrates including H<sub>2</sub>, N<sub>2</sub>, CO<sub>2</sub>, and H<sub>2</sub>O, since these are central to the I<sup>2</sup>CNER mission of producing clean fuels for carbon neutral power generation cycles. Following the division roadmap, research efforts of the Ogo group have made particular progress on single catalysts for transformations of

multiple energy-relevant substrates. The ability to catalyze the oxidation of both H<sub>2</sub> and CO in one pot is highly relevant to our future hydrogen economy since CO is a persistent contaminant of H<sub>2</sub> supplies. The newly reported catalyst is based on a NiIr core, comparable in design to the active site of the iconic [NiFe]-hydrogenases and the CO-dehydrogenases (CODH), two of the most important enzymes in this area. The CO and H<sub>2</sub> bind to the Ir center, as verified by X-ray crystallography. An additional advantage of this design is its compatibility with aqueous media, which allows the operator to control product distribution by manipulating pH. The catalyst has been demonstrated in an actual fuel cell using H<sub>2</sub>, CO, and H<sub>2</sub>/CO as fuels for oxidation at the anode. *This effort satisfies the short-term milestone for project 1 of the Catalytic Materials Transformation Division.*

### CO<sub>2</sub>-free electric power circulation via direct charge and discharge using the glycolic acid/oxalic acid redox couple

This discovery by PI Yamauchi involves a CO<sub>2</sub>-free way to distribute electric power by exploiting an incredibly simple, bio-derived redox couple. The components of the couple are glycolic acid (GC) and oxalic acid (OX), both of which occur widely in nature. Direct electric power storage in GC ensures high stability and transportability under mild conditions in the potential region of -0.5 to -0.7 V vs. the reversible hydrogen electrode (RHE) at 50°C. The most desirable characteristic of this electro-reduction is the suppression of hydrogen evolution even in acidic aqueous media (Faraday efficiency of 70–95%, pH 2.1). Key advantages of this emerging technology are the high energy density of the components and the robustness of titania nanospheres that mediate the electron-transfer. This is the first ever demonstration of direct storage/generation of electric power using

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solution type carriers without CO<sub>2</sub> emission. Aiming at technology development, we first constructed a liquid flow-type electrolyzer as an electric power storage device, namely a polymer electrolyte alcohol electrosynthesis cell (PEAEC) which is applicable for glycolic acid/oxalic acid redox reaction. The aqueous solution of glycolic acid ensures high energy density, up to 528 Ah<sup>-1</sup>, by a consideration of its maximum solubility (~4.93 M at 60 °C), which is almost ten times higher than that of the reported redox flow battery. The energy conversion efficiency of this newly fabricated PEAEC is 59.4% (recently 65%) and it is

the best ever reported on storing electric power into an easily transportable alcoholic solution. Using an alkaline fuel cell (Fig. 6.9), we also achieved CO<sub>2</sub>-free power generation via electro-oxidation of glycolic acid into oxalic acid for the first time. This coupling of power storage and generation based on the alcohol/acid couple holds great promise toward addressing the intermittency problem of renewable electricity. *This achievement is directly relevant to the Catalytic Materials Transformation division's long-term target for Project 2.*

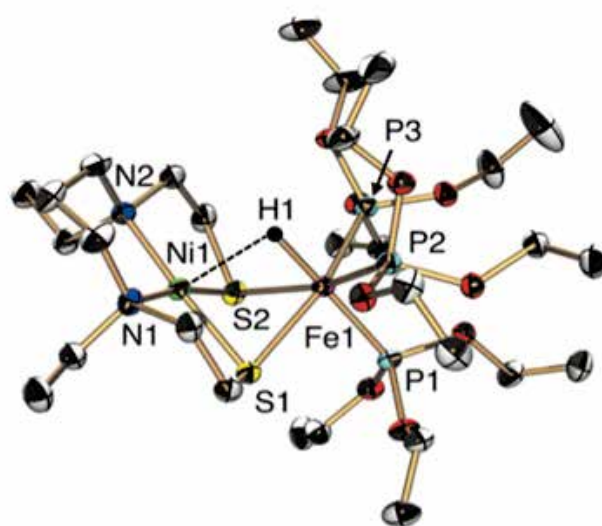


Figure 6.8. Bio-inspired catalyst for hydrogen activation.

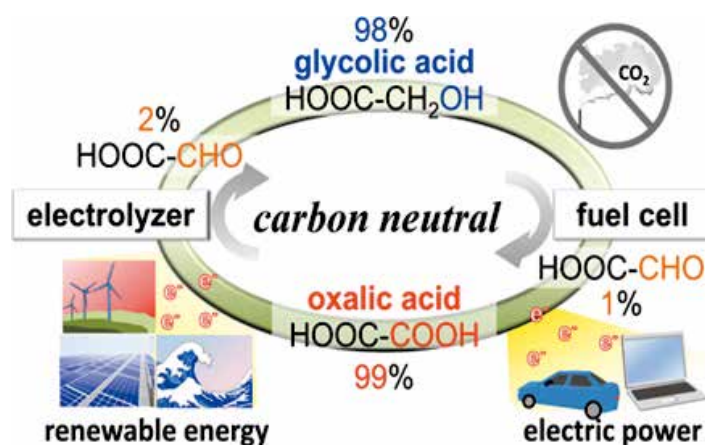


Figure 6.9. Schematic of a carbon-neutral energy circulation by highly selective electrocatalyses using the glycolic acid/oxalic acid redox couple. Numbers indicate product selectivity.

## Thermal Science and Engineering (Lead PI: Prof. Takata)

### Overview

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<sub>2</sub> 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<sub>2</sub> emissions.

### Fundamental understanding of phase change heat transfer

Condensation and boiling on smooth and engineered surfaces has received much attention in the past century due to its inherently high heat transfer efficiency. Although widely used in a plethora of industries, the fundamental mechanisms governing the physics of phase change heat transfer are poorly understood. The team of Takata and Miljkovic, working with international collaborators, have challenged this by answering century old questions in the fields of condensation and evaporation (Fig. 6.10) and developing the most comprehensive fundamental understanding of phase change heat transfer anywhere in the world. The knowledge gained from our work is being applied to the development of more compact energy systems, including condensers for Heating, Ventilation, Air Conditioning, Refrigeration (HVAC&R), and power generation industries, anti-icing surfaces, and highly efficient electronics thermal management devices. *This work has achieved the short and mid-term milestones of projects HMT-1 and HMT-2, and it currently targeting the long term milestone of projects HMT-1 and HMT-2.*

### Fundamental understanding of hydrophobic coating degradation

Dropwise condensation of steam on metallic surfaces coated with hydrophobic films has the potential to achieve remarkable heat transfer coefficients resulting in 2% efficiency enhancement on 85% of the baseload power generating infrastructure globally. However, the main challenge of using these coatings for the past 8 decades is their lack of long-term durability. The senior and junior members of the Takata and Miljkovic teams have developed the world's first fundamental

understanding of degradation of hydrophobic coatings during condensation. We elucidated failure mechanisms linked to mechanics of thin-films along with heterogeneous nucleation physics. We used our unique understanding to develop, for the first time, scalable and durable hydrophobic coating approaches, in collaboration with the biggest coatings and paints company in the world (PPG), that can be applied to a variety of industrial energy systems. *This work has achieved the short and mid-term milestones of projects HMT-1, and it currently targeting the long term milestone of projects HMT-1.*

### Achieving dropwise condensation of low surface tension fluids

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

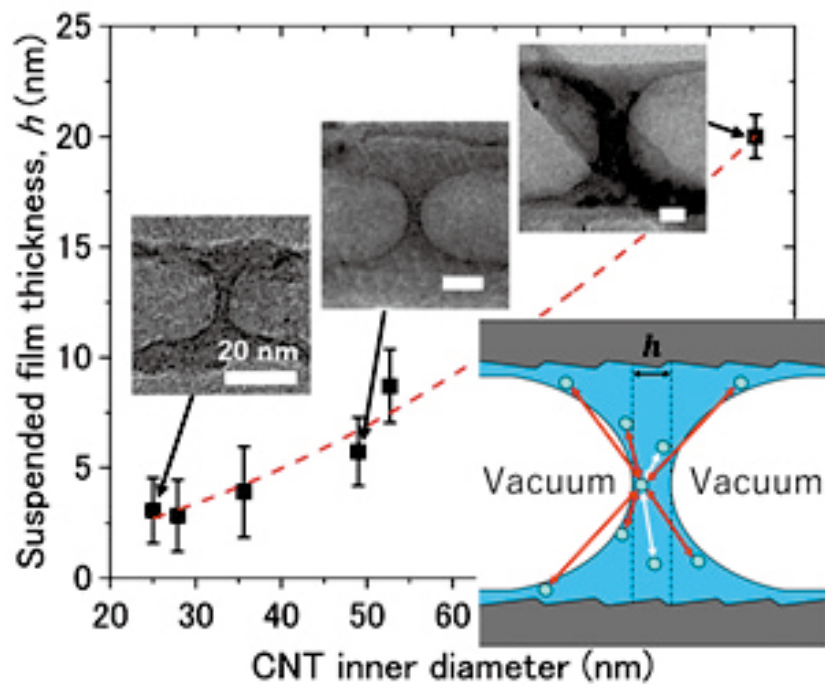


Figure 6.10. TEM images of suspended water film in CNT under high vacuum conditions.

## CO<sub>2</sub> Capture and Utilization (Lead PI: Prof. Fujikawa)

### Overview

The objective of this division is to develop: (i) highly efficient materials for CO<sub>2</sub> separation in power generation and industrial processes; and (ii) electrochemical methods to convert CO<sub>2</sub> into value-added chemicals, such as liquid fuels or their intermediates, in an energy-efficient and cost-effective way. In the area of CO<sub>2</sub> separation, the objective is to develop novel membrane technology to separate CO<sub>2</sub> 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<sub>2</sub> 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<sub>2</sub> conversion, the objective is to develop better catalysts and electrodes. Most current catalysts require a high over-potential to drive electrochemical reduction of CO<sub>2</sub>. 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.

### Membrane materials for CO<sub>2</sub> separation in power generation and industrial processes CO<sub>2</sub>/N<sub>2</sub> separation

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

captured CO<sub>2</sub> from CO<sub>2</sub>/N<sub>2</sub> mixture with a CO<sub>2</sub> concentration of 1000 ppm. This finding expands the relevance of our research goals beyond the capturing of CO<sub>2</sub> at fire-powered plants to the entirely new area of direct CO<sub>2</sub> capture from the air.

### Membrane materials for CO<sub>2</sub>/H<sub>2</sub> separation

Separation of CO<sub>2</sub> over H<sub>2</sub> at integrated gasification combined cycle (IGCC) plants (pre-combustion CO<sub>2</sub> capture) requires membranes with CO<sub>2</sub> permeance and selectivity respectively equal to 100 GPU (1 GPU=7.5×10<sup>-12</sup> m<sup>3</sup>(STP)/(m<sup>2</sup>·s·Pa)) and 30, under CO<sub>2</sub> partial pressure <1.0 MPa and temperature up to 60°C. The I<sup>2</sup>CNER developed alkanolamine-containing polymeric membranes, and especially, the 2-(2-aminoethylamino)ethanol-containing membranes developed by Prof. Taniguchi exhibited CO<sub>2</sub> permeance of 155 GPU with selectivity of 10 at CO<sub>2</sub> pressure of 1.0 MPa and 80 % relative humidity. Investigating the mechanism of preferential CO<sub>2</sub> permeation at the molecular level, we found that the CO<sub>2</sub> permeance is significantly enhanced under humidified conditions. The amine-containing membrane turns into a hydrogel and the CO<sub>2</sub> migrates through the membrane in a bicarbonate ion form. The measured CO<sub>2</sub> permeance exceeds the division's roadmap target of 100GPU, while the selectivity of 10 should be further improved to 30. This performance is better than that of the membranes developed at RITE (permeance of 2.6 GPU and selectivity of 17)

and which are being tested at pilot-scale. It should be noted that CO<sub>2</sub> permeance of 206 GPU with CO<sub>2</sub> selectivity of 103 at 107°C were reported by researchers of Ohio State University at a RITE symposium last January; however these results have not appeared in a refereed journal publication. Currently, our efforts are focused on the development of a hollow fiber membrane module to explore the scaling-up of our membrane project to a demonstration level for technology transfer. I<sup>2</sup>CNER established a facile and scalable technique to prepare hollow-fiber membrane modules by circulating membrane materials inside the hollow-fibers. The resulting membrane modules not only show high CO<sub>2</sub> separation properties but they also exhibit good durability at 50°C and  $\Delta p$  (CO<sub>2</sub>) of 40 kPa for about 300 h.

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

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

## CO<sub>2</sub> Storage (Lead PI: Prof. Tsuji)

### Overview

The objective of this division is to: develop methods of reservoir characterization and modeling, and new effective monitoring of injected/leaked CO<sub>2</sub> to help ensure safe and permanent CO<sub>2</sub> 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<sub>2</sub> injection in aquifer formations, and the requirement for long term monitoring of pressure variations near seismogenic faults.

### Inertial effects in liquid CO<sub>2</sub>-water flow behavior for CO<sub>2</sub> storage

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

### Continuous and accurate monitoring system for injected CO<sub>2</sub>

In Carbon Capture and Storage, the monitoring of injected CO<sub>2</sub> is crucial for (a) predicting the risk of CO<sub>2</sub> leakage from reservoirs, (b) increasing the efficiency of CO<sub>2</sub> injection and reducing the cost, and (c) reducing the risk of injection-induced seismicity. To date time-lapse seismic surveys have been used

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



## Hydrogen Materials Compatibility (Lead PI: Dr. Somerday)

### Overview

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.

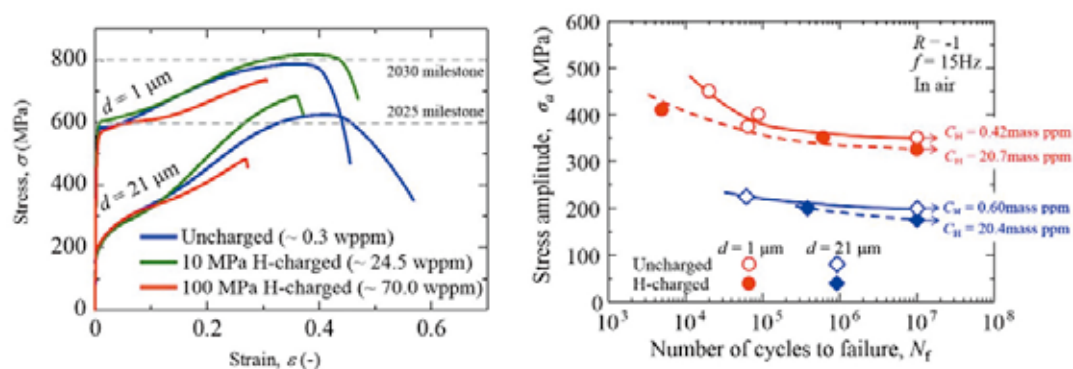
### Next-generation high-strength, low-cost alloy for hydrogen service

Research teams supervised by PI Takaki have pioneered the process of ultra-grain refinement in austenitic stainless steels. By applying this process to the low-cost experimental alloy Fe-16Cr-10Ni, yield strength was increased three-fold (to 600 MPa) relative to the conventional grain sized material (Fig. 6.11. a). As for hydrogen compatibility, two metrics were met: tensile ductility and fatigue life. As shown in Fig. 6.11.a, the strain to failure of ultra-fine grain (UFG) Fe-16Cr-10Ni remains above 30% after exposure to 100 MPa hydrogen. Regarding fatigue life, the fatigue limit (stress amplitude at  $10^7$  cycles) for UFG Fe-16Cr-10Ni is not degraded by hydrogen ( $\sim 20$  wppm), as shown in Fig. 6.11.b. To date, no other austenitic stainless steel can rival this experimental alloy's combined attributes: cost-competitive, high strength, and hydrogen compatible. *This achievement fulfills the mid-term milestone in Project 2 and represents significant progress toward the ultimate target of the Hydrogen Materials Compatibility division.* One technological implication of this achievement is that low-cost, high-strength UFG stainless steels could

replace the benchmark (i.e. SUS316) stainless steel in hydrogen fuel systems. While these results have not been transferred to industry, the commercial-scale production of UFG stainless steels was recently demonstrated by Nippon Steel & Sumitomo Metals Corporation.

### Mitigation of Hydrogen Embrittlement:

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



**Figure 6.11.** Data for Fe-16Cr-10Ni with ultra-fine grain size ( $d = 1 \mu\text{m}$ ) and conventional grain size ( $d = 21 \mu\text{m}$ ). (a) Tensile stress vs. strain data after exposure to hydrogen gas up to 100 MPa, (b) Stress amplitude vs. cycles to failure relationships with hydrogen concentration indicated for each data set.

## Advancing Fusion of Research Fields

I<sup>2</sup>CNER's approach to research bridges multiple spatial, molecular to miles, and temporal scales, nanoseconds to decades, but it also necessities bridging together scientists and engineers from disparate disciplines: chemistry, physics, materials science, mechanics, geoscience, and biomimetics. In other words, I<sup>2</sup>CNER's research activities and goals are by nature interdisciplinary and are carried out across division boundaries and international borders.

### Bioinspiration

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

### Mining Biology for New Hydrogen Processing Catalysts

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

### Materials engineering

PIs Horita and Associate Professor Edalati fusing the disciplines of **materials engineering** with i) **surface science and crystallography** and in collaboration with PI Akiba discovered the defect activation mechanism [4] for hydrogen adsorption of TiFe intermetallics by High Pressure Torsion (HPT), a promising system for renewable stationary energy

storage; ii) **mechanochemistry** and in collaboration with the groups of PIs Ishihara, Yamauchi, and Staykov introduced a new research direction [5] to the development of new visible-light-active photocatalysts by stabilizing high-pressure phases through using the high-pressure torsion (HPT) approach. It was shown that unlike thermodynamically stable phases of TiO<sub>2</sub> and ZnO which are photocatalytically-active only under UV light, the high-pressure TiO<sub>2</sub>-II and rocksalt-ZnO are active under visible light due to their low bandgap in good agreement with the first-principles calculations.

### Applied mathematics for energy

Applied mathematics area was mostly split between *computational gas and combustion dynamics* and *smart grid* research, with two additional groups dealing with models of *porous geomaterials*, and *statistical models of pheno-to-genotype* function (biomathematics).

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

hydrogen production system. Their results showed that the particle distribution was significantly affected by the interaction between the turbulent boundary layer formed on the inner wall of the injector nozzle and the particles, and this behavior could be classified by the particle Stokes number.

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

energy consumption data [14, 15]. They tested DRP designs on thousands of consumer models. The developed consumer model is the first ever proposed in which the incentive payment design method for DRPs is mathematically grounded.

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

**Geomorphology using persistent homology**: PI Tsuji and Prof. Shirai (IMI) used the apparatus of applied topology to characterize pore geometry of rock structures, in particular to estimate their permeability [18]. As pores are notoriously heterogeneous, they deployed persistent homology, created exactly to understand the geometry where the relevant scales are a priori unknown. They were the first in developing novel comparison metrics and predictors based on persistent homology in structural geology studies [19]. By linking such parameters derived from persistence diagrams to hydrologic and elastic properties, this approach has significant potential to facilitate the development of new models to predict physical/elastic/hydraulic properties directly from pore geometry.

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

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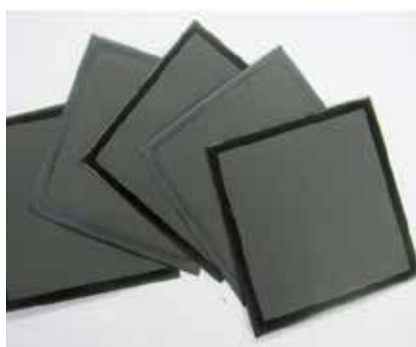
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## Returning Results to Society

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

Representative examples of technology transfer include: i) PI Ishihara’s transfer of dual carbon battery technology for energy recovery from automobiles to Ricoh Co. Ltd., ii) PI Matsumoto’s discovery of optimum chemical compositions of proton-conducting electrolytes and electrodes specifically suitable for steam electrolysis has been transferred to Nippon Shokubai Co., Ltd. for the development of a steam electrolyzer operating at 600°C for mass production of hydrogen from solar energy (Fig. 7.1), iii) PI Takata’s group has provided the Mitsubishi Heavy Industries, Central Glass Corp with fundamental data on thermophysical and transport properties, and heat transfer characteristics of newly developed refrigerants for the design of commercial products

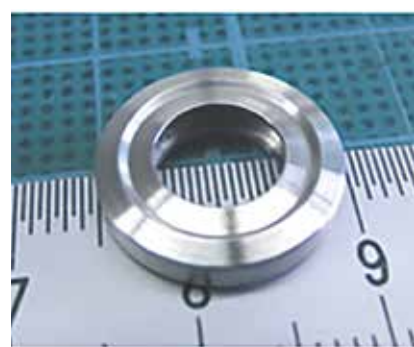
of high temperature heat supply heat pump, iv) Prof. Akiba worked with IWATANI Co. Ltd to develop high performance hydrogen absorbing alloys suitable for stationary hydrogen storage; v) PI Yamauchi’s synthetic method for the preparation of atomically well mixed Fe-Ni nanoalloys has been transferred to Daido Steel, vi) PI Fujikawa’s functional nanomembrane technology for gas separation has been transferred to Nanomembrane Technology Inc. for upscale development, vii) PI Tsuji’s innovative continuous CO<sub>2</sub> monitoring system in collaboration with the Japan Oil, Gas and Metals National Corporation (JOGMEC) has been transferred and deployed in the ongoing CO<sub>2</sub> sequestration project in Saskatchewan, Canada (Fig. 7.2), viii) PI Sugimura’s studies of diamond-like carbon (DLC) coatings in collaboration with Kitz corporation on the wear of candidate coatings in the presence of hydrogen contributed to the development of 100 MPa hydrogen flow valve, which is now in practical use in hydrogen refueling stations, ix) The results of Prof. Itaoka’s investigation on the hydrogen refueling stations and supply infrastructure for Japan have been submitted to the Ministry of Economy, Trade and Industry of Japan in the form of 73-page report in February 2017, and x) PI Fujigaya received funding in FY18 from KU and the Fukuoka Bank for a **startup company** called FUJlcat on novel electrocatalysts.



**Figure 7.1.** Steam electrolysis, PI Matsumoto with Nippon Shokubai Co.



**Figure 7.2.** Continuous CO<sub>2</sub> monitoring system deployed in Canada, PI Tsuji with JOGMEC.



**Figure 7.3.** Novel metal seal for H<sub>2</sub> storage, PI Kubota with TOKI Engineering.

# Network of International Collaborations

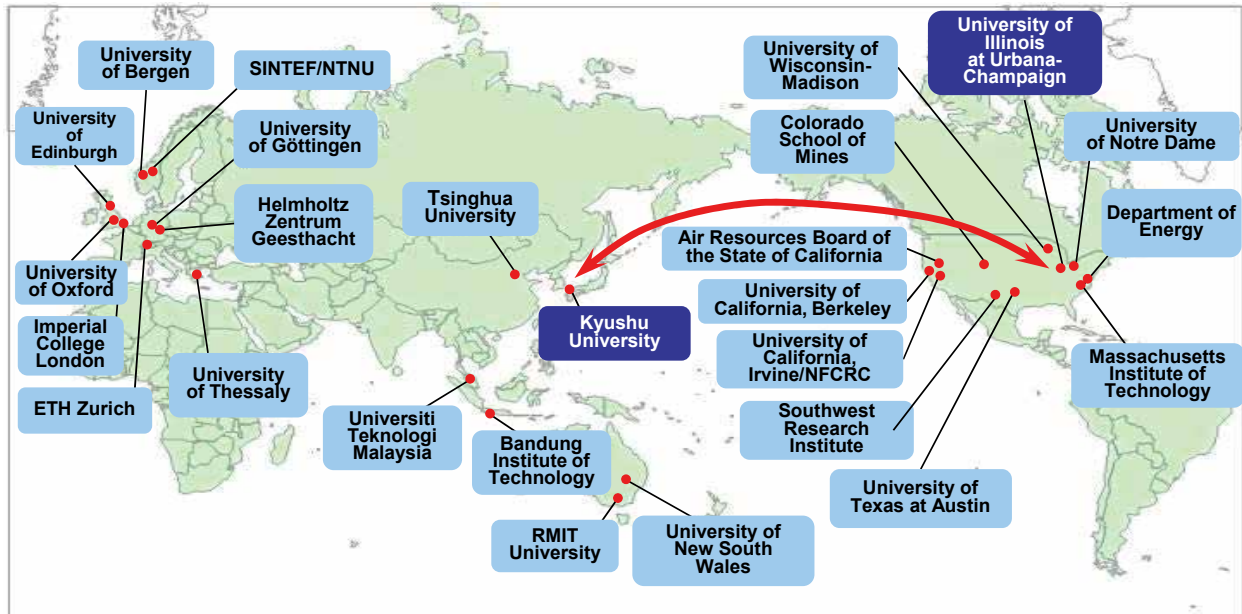
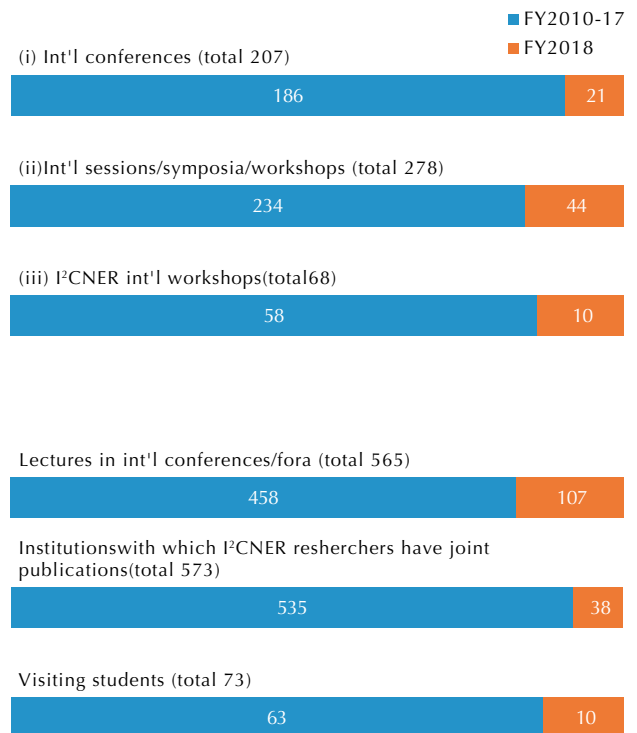


Figure 8. This map includes the home institutions of I²CNER's foreign WPI Faculty as well as those institutions with which I²CNER has academic agreements.

## Globalization by the numbers

In FY2018 there was a vast amount of international activities that enhanced I²CNER's global visibility. The Institute's researchers were responsible for organizing, co-organizing, or serving on the scientific committees for (i) 21 (207 in total since inception) international conferences, (ii) 44 international conference sessions/symposia or workshops (278 in total since inception), and (iii) 10 I²CNER international workshops (68 in total since inception). Our researchers have given 107 keynote, plenary and invited presentations in international conferences and fora (565 in total since inception). Our researchers have joint publications with researchers from 38 new institutions (573 in total since inception). As of March 31, 2019, the Institute has hosted a total of 73 graduate/undergraduate students from various institutions around the world, including Illinois, since its inception. The numbers of visiting students are 1 (FY2010), 9 (FY2011), 6 (FY2012), 7 (FY2013), 7 (FY2014), 6 (FY2015), 10 (FY2016), 17 (FY2017), and 10 (FY2018) of which, 1, 6, 1, 3, 1, 3, 8, 14, and 10 respectively, stayed for more than a month at KU. Of the total 73, 38 students were from Illinois and 23 of these students stayed for more than a month.



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

PIRE, a cooperative program between NSF and JSPS, is one of the most prestigious and competitive awards amongst the international programs of NSF. PIRE provides funding for international joint research carried out between US universities and their counterparts in Japan in order to generate new knowledge and discoveries; promote a diverse, globally engaged U.S./Japan workforce; and build the institutional capacity of U.S./Japan institutions to engage in productive international collaborations. The joint PIRE award to Illinois and I<sup>2</sup>CNER, “Integrated Computational Materials Engineering for Active Materials and Interfaces in Chemical Fuel Production,” is a result of I<sup>2</sup>CNER’s successful fusion of computational science with experiment, and was awarded beginning in FY 2015 for a total of 5 years. The project brings together researchers from Illinois, Kyushu, Northwestern University, Imperial College London, and the University of California at Berkeley (UCB). This project is also an example of the synergistic capabilities of the KU-Illinois partnership. In FY2018, under the 2-month PIRE/x-FU(s)ION (eXchange: FUkuoka, Illinois, califOrnia, Northwestern) exchange program, 6 American students (5 from Illinois and 1 from UCB) carried out research at I<sup>2</sup>CNER from June 4-August 3, 2018.



x-FU(s)ION exchange students participate in a tour of Prof. Selyanchyn’s lab

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

The JSPS Core-to-Core program is designed to create world-class research centers that have lasting partnerships with research institutions around the world in order to advance research in leading-edge fields regarding issues of high international priority. Core-to-Core provides funding for an international joint research project carried out between I<sup>2</sup>CNER, Imperial College, London, Paul Scherrer Institut (PSI, Switzerland), and the Massachusetts Institute of Technology on “Solid Oxide Interfaces for Faster

Ion Transport (SOIFIT)” and was awarded beginning in FY2017 for a total of 5 years. Three of I<sup>2</sup>CNER postdocs visited the counterpart research institutions for more than 1 month: Dr. V. Thoréton in Imperial College, London for 5 weeks; Dr. D. Klotz in MIT for 1.5 months; Dr. K. Ghuman Kaur in PSI for 2 months.

### **Collaborative Foreign Exchange Program**

In July 2013, I<sup>2</sup>CNER established the “Collaborative Foreign Exchange Program” in order to encourage young researchers to visit our overseas collaborating institutions. So far, 21 young researchers had their proposals approved, and 14 of them visited the Illinois Satellite for the extended period between one and nine months. Through this program, in FY2017, Prof. S. Harish stayed at the University of Edinburgh for 5 months and Prof. N. D. Hoa stayed at the Illinois Satellite, each for 5 months. In FY2018, Prof. D. Orejon also spent 4 months at the Illinois Satellite.

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

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



Prof. Cynthia A. Volkert (University of Göttingen) engages in a discussion

## Energy Transitions and the Role of CCS toward a Carbon-Neutral Energy Society (2019 I<sup>2</sup>CNER Annual Symposium)



I<sup>2</sup>CNER Director, Prof. Petros Sofronis, delivers opening remarks

(left to right) Prof. Geert Verbong, Eindhoven University of Technology; Dr. Jill Engel-Cox, U.S. National Renewable Energy Laboratory; Prof. Michael Celia, Princeton University

Since its inception, I<sup>2</sup>CNER has held a symposium on an annual basis, which has evolved over time from an event that celebrates the current research achievements of its thematic research areas (divisions) to an exploratory forum that focuses on a single research topic that is highly relevant in I<sup>2</sup>CNER's research portfolio and the international community. In addition, in order to explore new pathways to best accomplish their thematic research areas, each of I<sup>2</sup>CNER's divisions holds international workshops two days later by inviting several researchers and engineers.

The 2019 I<sup>2</sup>CNER Annual Symposium, which was titled "Energy Transitions and the Role of CCS toward a

Carbon-Neutral Energy Society", was held on January 31, 2019 and was attended by 150 participants (26 from overseas). This symposium brought together top level researchers both from Japan and abroad to discuss the issues surrounding the transition to a low-carbon energy future, considering both the deployment of renewable energy and the role of CCS. Through discussion and exchange of ideas in the symposium, participants explored ideal technological combinations, policy approaches, as well as emerging opportunities, and assessed where I<sup>2</sup>CNER's research activities should be focused on a moving-forward basis. The symposium included 6 invited lectures including a lecture titled "Clean Energy Technologies



for Economic Transitions” by Dr. Jill Engel-Cox, Director of Joint Institute for Strategic Energy Analysis at National Renewable Energy Laboratory, and a lecture titled “CCS and its Role in the Low-Carbon

Energy Transition” by Prof. Michael Celia, a Nobel Laureate from Princeton University’s Department of Civil and Environmental Engineering.

**January 31, 2019**

**Opening Remarks**

**Dr. Chiharu Kubo**, President, Kyushu University

**Dr. Akira Ukawa**, WPI Program Director, Japan Society for the Promotion of Science

**Mr. Ross Matzkin-Bridger**, Energy Attaché, U.S. Embassy Tokyo, and Director, U.S. Department of Energy’s Japan Office

**Prof. Petros Sofronis**, Director, I<sup>2</sup>CNER, Kyushu University

Speaker	Title
<b>Prof. Geert Verbong</b> (Eindhoven University of Technology)	<i>Invited Lecture</i> Understanding Transitions: the Case of the Energy Transition
<b>Dr. Jill Engel-Cox</b> (U.S. National Renewable Energy Laboratory)	<i>Invited Lecture</i> Clean Energy Technologies for Economic Transitions
<b>Prof. Kenshi Itaoka</b> (I <sup>2</sup> CNER, Kyushu University)	I <sup>2</sup> CNER Energy Transition Efforts for a Carbon-Neutral Energy Society
<b>Prof. Michael Celia</b> (Princeton University)	<i>Invited Lecture</i> CCS and its Role in the Low-Carbon Energy Transition
<b>Prof. Takeshi Tsuji</b> (I <sup>2</sup> CNER, Kyushu University)	Monitoring for Effective and Safe CO <sub>2</sub> Storage
<b>Mr. Hitoshi Nissaka</b> (Ministry of the Environment)	<i>Invited Lecture</i> Overview of Climate Change Measures and Proactive Initiatives for Realizing CCS in Japan
<b>Dr. Makoto Akai</b> (National Institute of Advanced Industrial Science and Technology)	<i>Invited Lecture</i> CCS as a Vital Option towards a Sustainable Future
<b>Dr. David Reiner</b> (University of Cambridge)	<i>Invited Lecture</i> Energy Transitions, Moral Hazard and Magical Thinking

**Wrap up and Implications**

**Prof. Andrew Chapman** (I<sup>2</sup>CNER, Kyushu University)

**Prof. Michael Celia** (Princeton University)

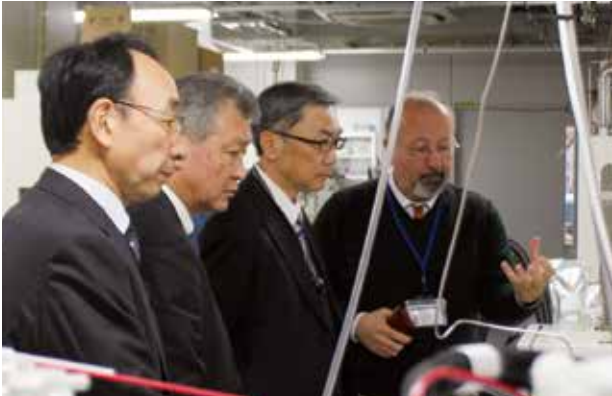


An audience member poses a question



Participants discuss during the poster session

## Distinguished Visitors



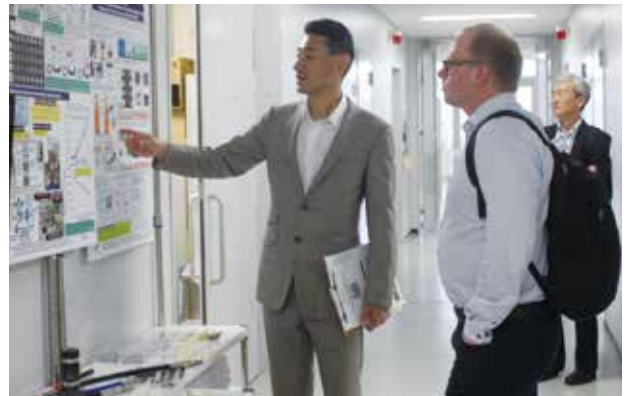
**January 12, 2018** Mr. Fuminori Kishino (second from right), General Manager, Power and Industrial Systems R&D Center, Toshiba



**April 9, 2018** Mr. Nicholas Hill (third from left), U.S. Embassy's Minister Counselor for Economic Affairs



**April 24, 2018** Dr. Yves BRECHET (second from left), High Commissioner, French Alternative Energies and Atomic Energy Commission (CEA), France



**October 23, 2018** Dr. Espen Steinseth Hamborg (middle), Principal Researcher Process Technology Downstream, Equinor



**March 1, 2019** Prof. Sea-Fue Wang (right), President, National Taipei University of Technology, Taiwan



I<sup>2</sup>CNER has always hosted a large number of visitors and students but in 2017 and 2018 I<sup>2</sup>CNER increased its student outreach efforts and hosted several more school field trips.

## Seminars

### The I<sup>2</sup>CNER Seminar Series (ISS)

One of the most important goals of the I<sup>2</sup>CNER Seminar Series is to engage key members of the international community from academia, national laboratories, industry, and government agencies (policy makers). In FY2018, the Institute hosted a total of 10 speakers (7 non-Japanese) in 10 I<sup>2</sup>CNER Seminars. Cumulatively, 161 speakers have presented at 157 I<sup>2</sup>CNER Seminars.

#### Selected ISS speakers

**August 2, 2018**

**Prof. Nicholas Kotov**

Professor, University of Michigan, USA

*Title: Self-Organization of Biomimetic Nanoparticles*

**October 10, 2018**

**Prof. Pailin Ngaotrakanwivat**

Assistant Professor, Burapha University, Thailand

*Title: WO<sub>3</sub>-CuS Photochromic smart window*

**November 7, 2018**

**Prof. John Andrews**

Professor, School of Engineering RMIT University, Australia

*Title: The role of hydrogen energy technologies in combating climate change: Is a 'proton battery' the answer?*

**December 5, 2018**

**Prof. Luca Brandt**

Professor, Fluid Mechanics KTH Stockholm, Sweden

*Title: Numerical simulations of turbulent flows of particle suspensions*

**December 7, 2018**

**Prof. Janusz S. Szmyd**

Head - Dept. of Fundamental Research in Energy Engineering AGH University of Science and Technology, Poland

*Title: Numerical Modelling of Transport Phenomena in SOFC Systems*

**March 15, 2019**

**Prof. Nobuhiro Kosugi**

Director, Institute of Materials Structure Science KEK, Japan

*Title: Progress in molecular X-ray absorption spectroscopy*

### Institute Interest Seminar Series (IISS)

Since the inception of the Institute, young researchers have been giving presentations at the Institute Interest Seminar Series (IISS), the goal of which is to initiate interdisciplinary collaborations and train young researchers to present before general scientific audiences outside their areas of expertise. In FY 2018, a total of 44 speakers presented at 23 Institute Interest Seminars. Cumulatively, 256 speakers have presented at 158 Institute Interest Seminars.

#### Selected IISS speakers

**April 20, 2018**

**Yutaku Kita (Ph.D. Student)**

Thermal Science and Engineering Division

*Title: Drop Mobility on Microtextured Surfaces with Wettability Contrasts*

**May 31, 2018**

**Dr. Hadi Farabi Asl**

Energy Analysis Division

*Title: Research background and current research topics in EAD, I<sup>2</sup>CNER*

**June 14, 2018**

**Dr. Miho Isegawa**

Catalytic Materials Transformations Division

*Title: DFT investigation on H<sub>2</sub> and O<sub>2</sub> activation by bio-inspired NiFe complexes*

**July 5, 2018**

**Dr. Vlad Bogdan Niste**

Hydrogen Materials Compatibility Division

*Title: Adapting lubricant additive reactivity to control the hydrogen embrittlement of bearing steels*

**October 25, 2018**

**Dr. Dino Klotz**

Electrochemical Energy Conversion Division

*Title: Generalized Electrochemical Impedance Spectroscopy (GEIS) in Solid State Ionics*

**December 13, 2018**

**Dr. Qing Wang**

Molecular Photoconversion Devices Division

*Title: Photo/electro-catalytic activity of ceramics produced by high pressure torsion*

**March 4, 2019**

**Dr. Tatsunori Ikeda**

CO<sub>2</sub> Storage Division

*Title: Monitoring of seismic velocity in CO<sub>2</sub> storage sites using a continuous and controlled seismic source*

## Selected Awards

DATE	AWARD / PRIZE	AWARDING ORGANIZATION	AWARD RECIPIENT
Apr. 2018	<b>Prize for Science and Technology, The Commendation for Science and Technology</b>	Minister of Education, Culture, Sports, Science and Technology	Chihaya Adachi
May 2018	<b>The Hult Prize</b>	Hult Prize	M. L. Palash, Mahbubul Muttakin, Md. Amirul Islam, Tahmid Hasan Rupam
Jun. 2018	<b>ASME ICNMM Outstanding Leadership Award</b>	American Society of Mechanical Engineers	Yasuyuki Takata
Jun. 2018	<b>DOE Early Career Award</b>	The Department of Energy	Nicola H. Perry
Sep. 2018	<b>Incentive Award</b>	The Japan Society for Analytical Chemistry	Yukina Takahashi
Nov. 2018	<b>The Early Career Scientist Award</b>	The International Union of Geodesy and Geophysics (IUGG)	Takeshi Tsuji



(from left) Mahbubul Muttakin, Md. Amirul Islam, Tahmid Hasan Rupam and M. L. Palash receiving The Hult Prize



Prof. Takata receiving ASME ICNMM Outstanding Leadership Award



Prof. Takahashi receiving Incentive Award

# Outreach Activities

## Publications

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

As a part of our efforts to promote the research activities of I<sup>2</sup>CNER to the next generation of scientists (e.g. high school students), we publish a newsletter entitled “Hello! I<sup>2</sup>CNER.” The newsletter, which highlights the research activities of one of the Institute’s research divisions in each issue, is published about three times per year. It is our goal for this publication to help increase general interest in carbon-neutral energy research amongst the next generation of scientists. In order to provide a more formal perspective on the potential impact I<sup>2</sup>CNER’s research could have on the world, each issue of Hello! I<sup>2</sup>CNER is published simultaneously with another publication, Energy Outlook. The main objective of Energy Outlook is to present to the public the perspectives of industry and government on energy issues. To this end, the main article in nearly every Energy Outlook is an interview of an industry or government official by an I<sup>2</sup>CNER researcher, which provides the public with a candid view of how an industry or a branch of the government deals with a given energy issue. This regular interaction with industry and government officials not only allows I<sup>2</sup>CNER to facilitate public awareness of new technologies, which is a vital part of outreach for the Institute, but also provides I<sup>2</sup>CNER researchers with opportunities to gauge the relevance of their ongoing basic research projects against industry and government perspectives.



## Important energy issues (Special Interviews from Energy Outlook)

### ***Building Japan’s Energy System: The Strategic Thinking We Need and Initiatives for Implementing It***

When we look at reducing CO<sub>2</sub> emissions from the standpoint of separating and capturing CO<sub>2</sub> from large-scale sources, we can divide the associated technologies into three broad categories: liquid absorbents, adsorbents, and separation membranes. The performance of liquid absorbents has pretty much reached a limit, so there’s not much room for improvement there. Similarly, adsorbents that use porous materials like zeolite<sup>\*1</sup> are also close to their limit. RITE is conducting research into a solid absorbent bearing amines<sup>\*2</sup>, but that also has its limits. CO<sub>2</sub> capture from natural gas, which is already at high pressure, and from pre-combustion exhaust gases in IGCC<sup>\*3</sup> (integrated coal gasification combined cycle) does not require pressurization, so separation membranes are ideal for those tasks. If the goal is to promote separation membranes, a good approach would be to package construction of coal-fired thermal power plants with CO<sub>2</sub> capture systems. There’s a large market for natural gas, and the technology could become a means of reducing CO<sub>2</sub> emissions that offers cost advantages.

In its pursuit of basic research into separation membrane materials, I<sup>2</sup>CNER is focusing on efficient

CO<sub>2</sub> capture using separation membrane methods, specifically CCU<sup>\*4</sup> and CCS<sup>\*5</sup> (carbon capture and utilization/storage). Our goal is for basic technologies to be commercialized in the future, and in the field of fuel cells, there are researchers who are already working on demonstration testing. In addition to CCS research, I<sup>2</sup>CNER is also conducting research into CCU, in which CO<sub>2</sub> undergoes electroreduction to convert it into CO. If we can get to that stage then there are already technologies available for chemically converting it into a valuable resource. We already have enhanced recovery of oil and gas using captured CO<sub>2</sub> (EOR and EGR)<sup>\*6</sup>.

Japan has found itself in an extremely special energy situation since the Great East Japan Earthquake of 2011. We need to create an energy system for Japan with an optimal mix of energy sources based on evidence in the form of exhaustive calculations. We need to create institutions that can formulate a proper strategy, and then disseminate and implement that strategy.

### Notes

<sup>\*1</sup> Zeolite: A general name for crystalline aluminosilicates. In addition to molecular sieve effects that result from pores deriving from the material’s skeletal structure, zeolites’ characteristics include adsorptive capability.

<sup>2</sup> Amine: A general name for compounds in which hydrogen atoms in ammonia are replaced by a hydrocarbon group or an aromatic atom group. Amines exhibit affinity with CO<sub>2</sub>.

<sup>3</sup> IGCC (integrated coal gasification combined cycle): A power generation system that improves the efficiency of conventional coal-fired thermal power by gasifying coal as an input for combined-cycle generation.

<sup>4</sup> CCU (carbon capture and utilization): The process of reusing captured and sequestered CO<sub>2</sub>.

<sup>5</sup> CCS (carbon capture and storage): The process of separating and capturing CO<sub>2</sub> and then storing it underground.

<sup>6</sup> EOR/EGR (enhanced oil/gas recovery): A technique for pressurizing CO<sub>2</sub> that has been separated and captured in order to improve oil and natural gas recovery efficiency.

**Exploring Renewable Energy: A Discussion on Incorporating Sustainable Resources into Our Everyday Lives**

Currently, renewable energy has grown to be more commercial, particularly certain types including solar, wind, and hydropower. We need to focus on the industrial sector, and the agricultural sector as these are some of the areas where renewable energy hasn't been fully addressed yet. Many cities and states are starting to think about going 100% renewable or 100% low carbon. That is very easy to say, but it is very hard to really achieve. There are two different approaches to energy supply that do not rely on conventional fossil fuels. To achieve the goal of renewable energy, it is necessary to combine the fully centralized approach and the decentralized approach. It depends on the location itself and what baseline you begin with in the area. We need to consider what kind of existing grid systems are already there, how centralized the system is now, and what existing power systems are already built.

Separating consumer activity in Japan's energy market by intention, divided into three major groups. We found that only a small percentage were early adopters. Then, there is a very big group in the middle and an equally large group at the bottom that just wait for the government to say they have to begin using a particular system.

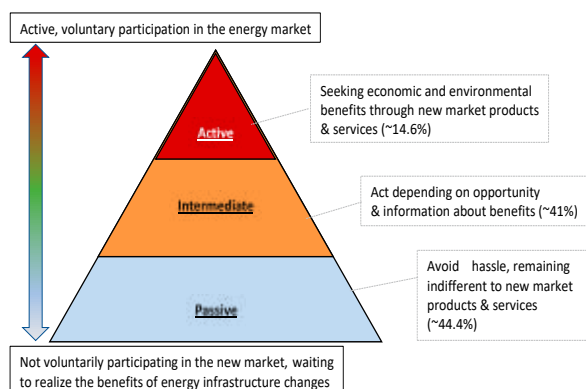


Figure 9. Consumer activeness tiers in the Japanese energy market.

One of the big challenges is for the technology people to work with the social scientists, economists, and others to think about how to bring these solutions forward in a way that people are going to be excited about and accepting of them and not resistant.

**Inspiring Future Generations: The Importance of Carbon Capture Storage and Understanding Human Environmental Impacts**

It's an important point – the fact that you approach this with a seismology background. I think it gives a different perspective and you are thinking about one of the major issues with CCS which is: 'How should we think about the risk of creating earthquakes by injecting huge amounts of fluid underground?'. You need expertise in earthquakes and seismology in order to think about that problem in the right way. The major technology that is currently expected to be able to do that is the combination of bioenergy with CCS, that is an order of 10 gigatons a year ramping up. All of these scenarios for how we can realistically solve the carbon problem involve massive amounts of CCS. The challenge that we have is to go from where we are today, to what these future projections are assuming will happen.

Negative emissions<sup>7</sup> is a very important concept for carbon reduction. At the moment, there is no viable human-made technology that works at scale for the extraction of huge amounts of CO<sub>2</sub> from the atmosphere. That's why the technology that is referred to as 'BECCS'<sup>8</sup> (bio-energy with carbon captured storage) is what's pointed to in these reports. That's the technology that we know has some reasonable chance to work right now. It is important to reduce large amounts of CO<sub>2</sub>, and CCS could achieve the large-scale CO<sub>2</sub> emission reduction. However, the general perception is that CCS has not gained traction worldwide toward decarbonizing the environment. In the U.S., there are interesting possibilities at the moment. About a year ago in 2018, a new tax bill was passed. In that tax bill are tax credits for CCS. The tax credits are at a significant level, up to \$50 per ton if you capture the CO<sub>2</sub> and use it for direct storage, and up to \$35 a ton if you use it for enhanced oil recovery. The role of academic institutions, such as I<sup>2</sup>CNER, is that they increase the motivation of young researchers to work on research in the CCS in the area. We continue our research activities for carbon emission reduction, and also try to educate young scientists to save our planet earth.

**Notes**

<sup>7</sup> Negative emissions: A reduction in the amount of CO<sub>2</sub> that is in the atmosphere.

<sup>8</sup> BECCS (bio-energy with carbon captured storage): A technology that has the potential to mitigate greenhouse gases.

## Outreach Events

### **2018 E-MRS Spring Meeting (June 18-22, 2018)**

WPI was represented by four WPI centers, including I<sup>2</sup>CNER, at the European Materials Research Society (E-MRS) 2018 Spring Meeting in Strasbourg, France from June 18 to 22. Founded in 1983, today the E-MRS has more than 4,000 members. I<sup>2</sup>CNER, along with AIMR, iCeMS and MANA, ran the WPI booth throughout the event, and hosted a reception entitled "Come together + Japanese Drink Tasting" on June 19, where researchers from the four WPI centers mingled with other E-MRS attendees. On the June 20, the WPI program was jointly featured in a workshop titled "STAM-WPI Joint Symposium." Prof. Watanabe from I<sup>2</sup>CNER gave his presentation to showcase his latest research findings.

### **Innovation Japan 2018-University show (August 30-31, 2018)**

From August 30 to 31, 2018, the "Innovation Japan 2018 – University Show," which was organized by the Japan Science and Technology Agency (JST), was held at Tokyo Big Sight in Tokyo, and Prof. Ikuo Taniguchi (CO<sub>2</sub> Capture and Utilization Division) ran a booth. "Innovation Japan" is one of the largest industry-academia matching events in Japan which has more than 20,000 visitors each year. The main purpose of the event is promoting technology transfer and passing on research outcomes from universities and official organizations to the society. Supporting industry-academia matching toward the practical use is also one of the missions. Prof. Taniguchi explained his research on "Low-temperature processable degradable plastics" to the visitors. He conducted a plastic pressure molding test and demonstrated that it can be shaped at room temperature. Many participants from both industries and research institutions visited his booth seeking a possibility of future collaborative research.

### **59th Science Café at Fukuoka (September 21, 2018)**

Prof. Ki-Seok Yoon (Catalytic Materials Transformations Division) gave a lecture at the "59th Science Café @ Fukuoka," which was held in a business event space in the heart of the city at 7 p.m. on September 21, 2018. The 59th Science Café @ Fukuoka drew an audience of approximately 40 people. In his presentation titled, "Unveiling the H<sub>2</sub>-oxidation and CO<sub>2</sub>-fixation of Hydrogen-oxidizing bacteria" Prof. Yoon introduced his research on new O<sub>2</sub>-tolerant H<sub>2</sub>-oxidizing and CO<sub>2</sub>-fixing enzymes, which can contribute to the development of novel biomimetic catalysts for H<sub>2</sub>-activation and CO<sub>2</sub>-fixation. The lecture was followed by a roundtable talk, in which participants discussed their views on immediate energy issues and showed keen interest in the development of the latest eco-conscious technologies.

### **15th Anniversary Event of JSPS at San Francisco (January 24-25, 2019)**

Director Petros Sofronis and Prof. Toshinori Matsushima (Molecular Photoconversion Devices Division) from I<sup>2</sup>CNER gave presentations at the 15th anniversary event of the Japan Society for the Promotion of Science's (JSPS) San Francisco office. The event, "World Premier Research in Japan", was held at the University of California, Berkeley and Stanford University on January 24 and 25, respectively.

Since its establishment in 2003, JSPS San Francisco has been promoting academic and research exchange between the U.S. and Japan, and has been working to invite leading researchers from the U.S. to Japan. At this event, 4 WPI centers, Kavli IPMU, AIMR, I<sup>2</sup>CNER, and ITbM, were invited as examples of highly internationalized research institutions with the best-in-class research achievements in Japan. The two-day event attracted 110 people including faculty, researchers, students, and personnel from industries.



Prof. Yoon gives his lecture at the 59th Science Café at Fukuoka



Prof. Matsushima gives his presentation at the 15th Anniversary Event of JSPS at San Francisco

## Press Releases and Media Coverage

### Selected Press Releases

DATE	DESCRIPTION
May. 25, 2018	<b>Prof. Yukihiro Higashi</b> (Research Center for Next Generation Refrigerant Properties) Developed new equation of state for low- Global Warming Potential refrigerant and registered in world standard database “NIST REFPROP”
Jul. 3, 2018	<b>Profs. Chihaya Adachi and Hajime Nakanotani</b> (Molecular Photoconversion Devices Division) Exciton limits are meant to be broken: OLED surpasses 100% exciton production efficiency
Jul. 19, 2018	<b>Prof. Andrew Chapman</b> (Energy Analysis Division) Describing research about Kuznets Curve application and findings for CO <sub>2</sub> emissions and urban development
Jul. 19, 2018	<b>Prof. Andrew Chapman</b> (Energy Analysis Division) Kyushu and Matsuyama University successful in deriving a new method for estimating urban emissions

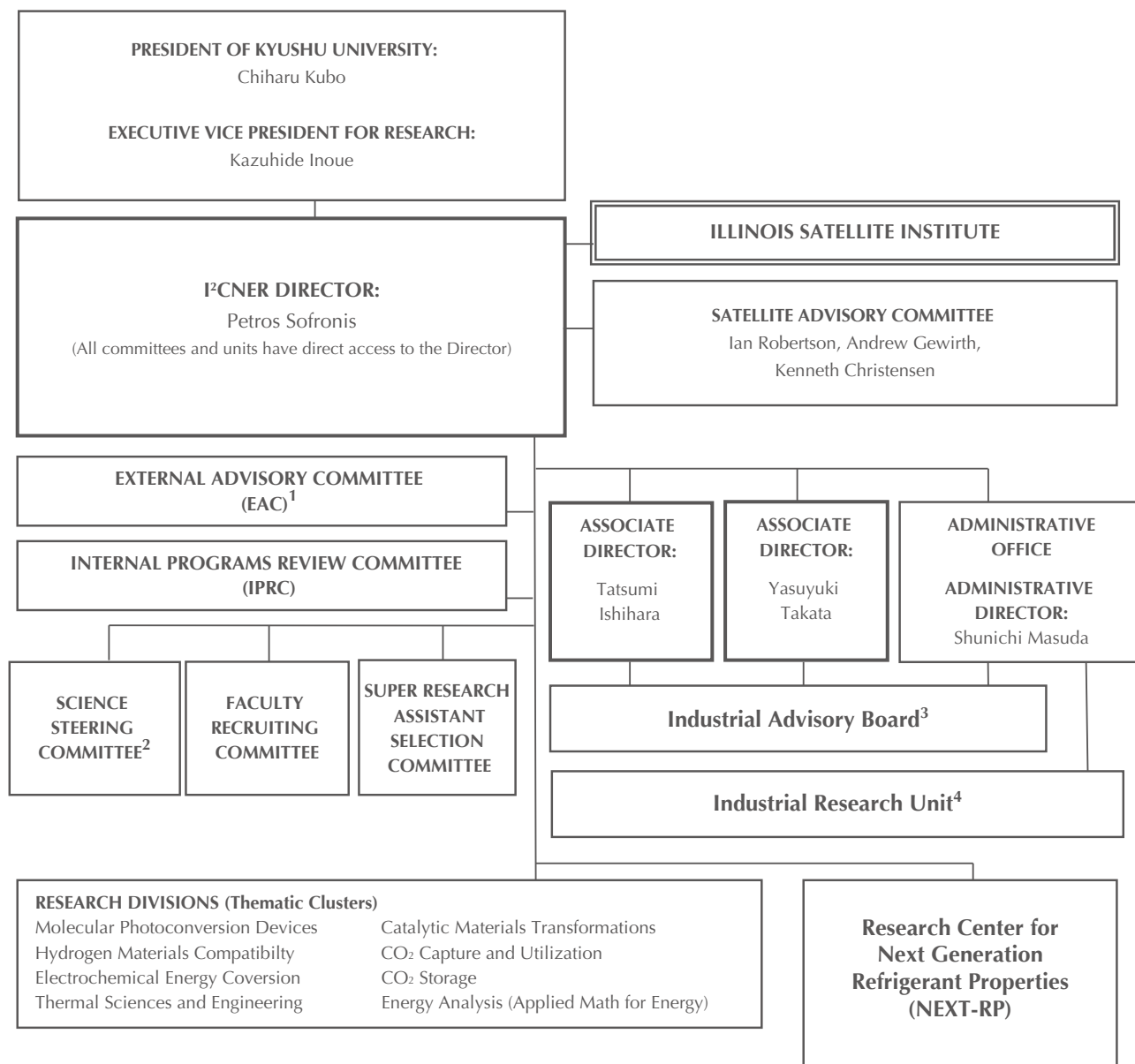
### Selected Media Coverage

DATE	MEDIA OUTLET	DESCRIPTION
Jul. 2018	Nikkei Sangyo Shimbun (Jul. 6)	<b>Profs. Chihaya Adachi and Hajime Nakanotani</b> Newspaper article covering the press release “Exploiting singlet fission in organic light-emitting diodes”
Jul. 2018	Nihon Keizai Shimbun (Jul. 19)	<b>Prof. Andrew Chapman</b> Newspaper article covering the press release “An analysis of urban environmental Kuznets curve of CO <sub>2</sub> emissions: Empirical analysis of 276 global metropolitan areas”
Jan. 2019	Kyushu Asahi Broadcasting (Jan. 8) NHK Fukuoka (Jan. 8 and 9) RKB Mainichi Broadcasting (Jan. 8)	<b>Prof. Atsushi Takahara</b> TV news covering a new electric vehicle made of a newly-developed, light and tough polymer



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

## Organizational Structure



1) The **External Advisory Committee (EAC)** makes recommendations on the current status of the Institute and its future directions, and provides the Director with a written report detailing their findings and recommendations. The full list of members as of April 1, 2019 is as follows:

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

2) The **Science Steering Committee (SSC)** is chaired by the Director, and its members are the two Associate Directors and the lead PIs of the thematic research divisions. The SSC is the body that reviews and advises on all matters of the Institute, e.g. planning and operation of research activities, budget implementation, international collaborations, and outreach.

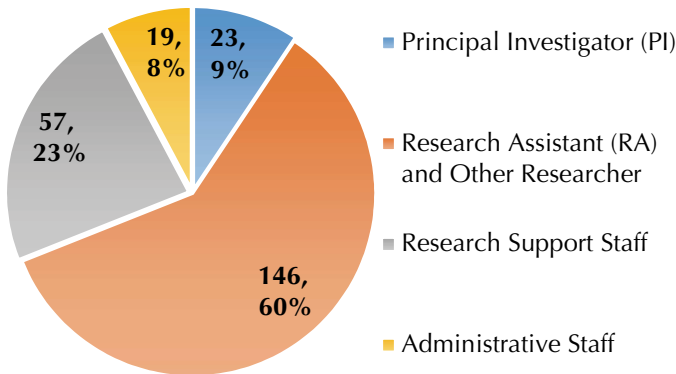
3) In FY2017, I<sup>2</sup>CNER established the **Industrial Advisory Board (IAB)**, whose members are prominent executives from industry, government agencies, and national laboratories that advise I<sup>2</sup>CNER on opportunities for interactions with industry and technology transfer. The first IAB meeting was held on February 1, 2018 and was attended by 9 out of 10 IAB members. The meeting provided invaluable inputs to I<sup>2</sup>CNER researchers in regards to research areas that industries would have interest for promoting the development of new technologies. The full list of members as of April 1, 2019 is as follows (in no particular order):

- Dr. Hiroyuki Yamamoto, General Manager, Technical Research Center in Mazda Motor Corporation
- Dr. Akira Yamada, Senior Corporate Adviser, Mitsubishi Heavy Industries, Ltd.
- Dr. Akira Yabe, Lead of Energy System and Hydrogen Unit, Technology Strategy Center in New Energy and Industrial Technology Development Organization (NEDO)
- Dr. Mark Selby, Chief Technology Officer, Ceres Power, USA
- Mr. Tatsumi Maeda, Advisor, KYOCERA Corporation
- Mr. Kazutoshi Ida, Managing Director, K.K. AIR LIQUIDE LABORATORIES
- Dr. Kuniaki Honda, Adviser, Hydrogen Energy Systems Society of Japan
- Dr. Katsuhiko Hirose, Project General Manager, Hydrogen & Fuel Cell Promotion Group in R&D Management Division of TOYOTA Motor Corporation
- Dr. Akio Fujibayashi, Technical Fellow, Steel Research Laboratory in JFE Steel Corporation
- Mr. Sumitoshi Asakuma, Director & Managing Executive Officer, Sumitomo Bakelite Co., Ltd.

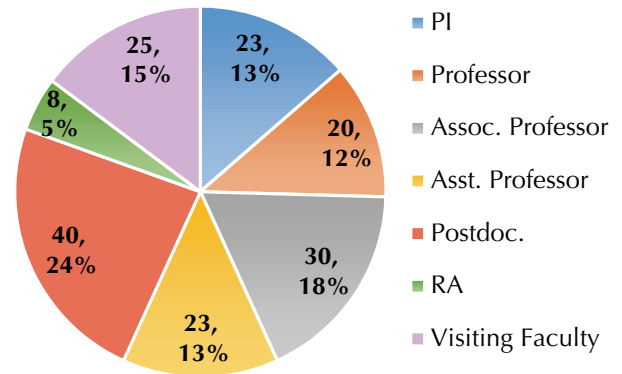
4) The **Industrial Research Unit** was established in FY2017 with its purpose being to advance technology transfer with corporations and pursue stronger relationships with industry and government programs. This “Unit” comprises of several industry-sponsored research projects, wherein a team of I<sup>2</sup>CNER researchers and embedded-industry-affiliates work on a particular research area of mutual interest. Through this new unit, I<sup>2</sup>CNER will expand its outreach to promote the deployment of its technology to industries that will fund I<sup>2</sup>CNER projects in the future. The first such project is “Mobile Energy Storage for Low-Carbon Society” sponsored by Mazda Motor Corporation for 71 million JPY with a duration of three years beginning in FY17. Additionally, the IHI Corporation has sponsored 5 million JPY on the “Study of High-temperature Co-electrolysis of CO<sub>2</sub> and H<sub>2</sub>O.”

## Personnel (as of April 1, 2019)

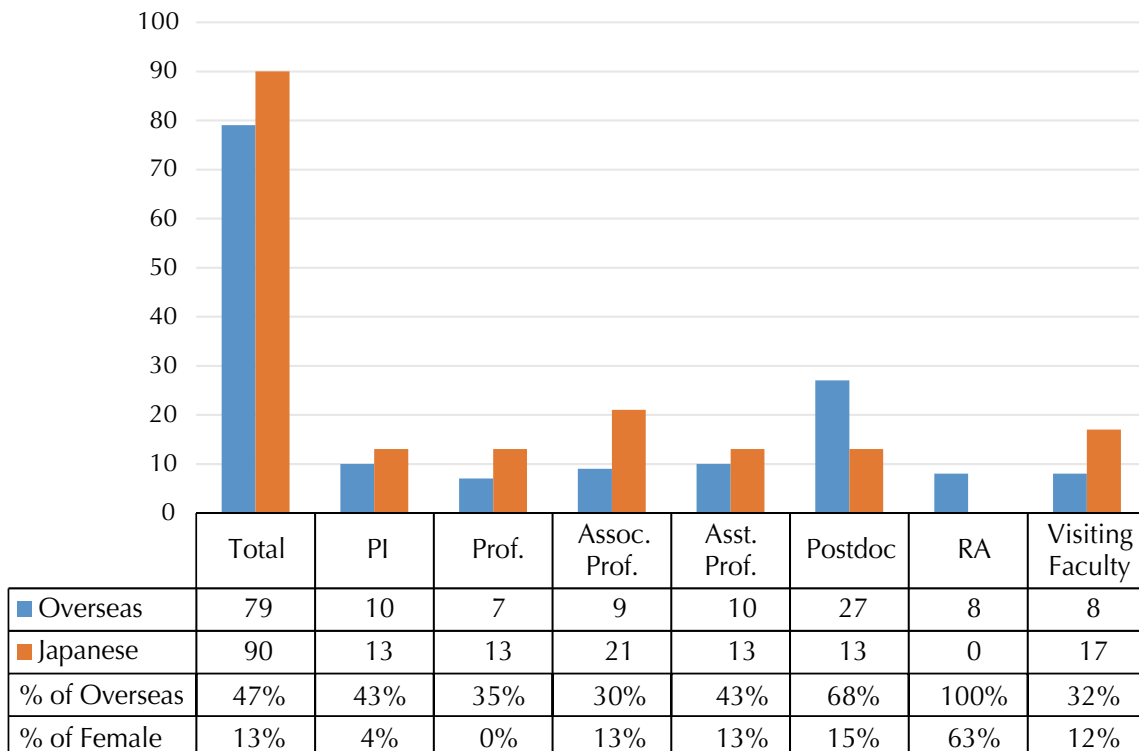
### Breakdown of Personnel (Total: 245)



### Researchers by Title (Total: 169)

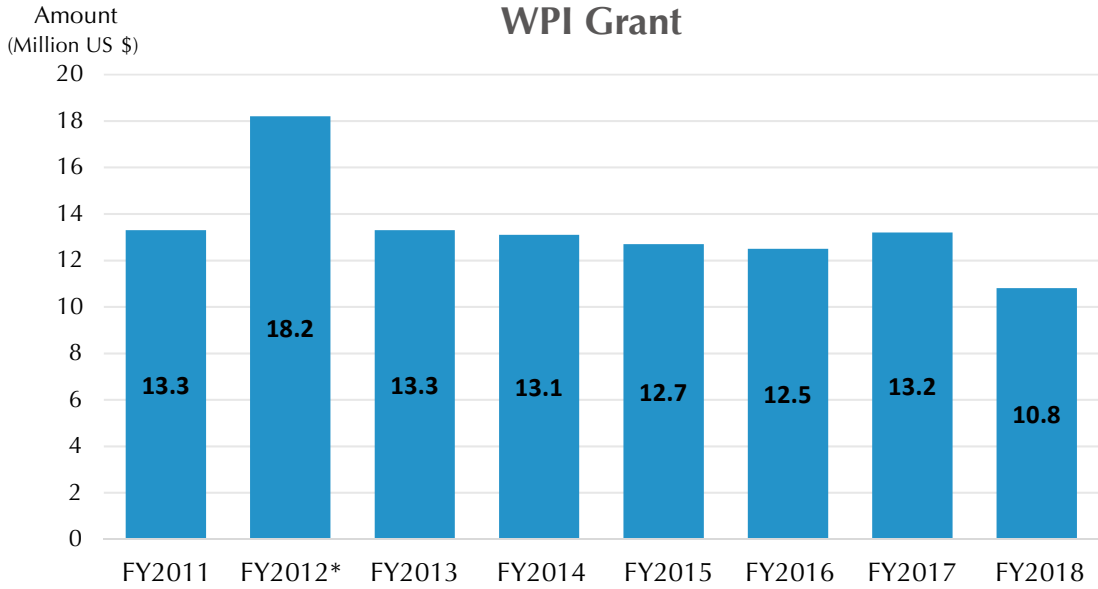


### Statistics of Researchers by Title

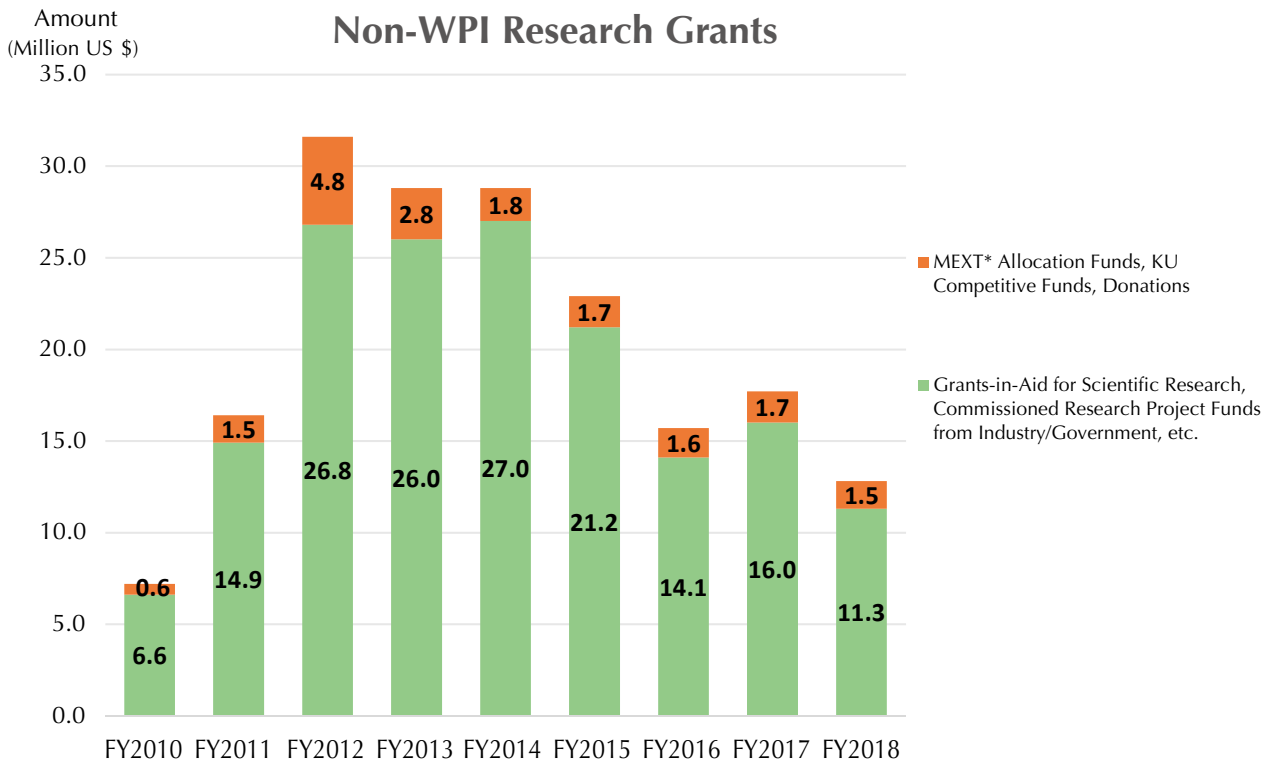


# Finances

1USD = 100JPY



\*WPI Grant of FY2012 includes the supplementary budget worth 5 million USD



\*MEXT is an acronym for Ministry of Education, Culture, Sports, Science and Technology

## Researcher List (as of April 1, 2019)

### Administration

#### Director

Prof. Petros Sofronis

#### Associate Directors

Prof. Tatsumi Ishihara

Prof. Yasuyuki Takata

### Principal Investigators

#### Molecular Photoconversion Devices

Prof. Tatsumi Ishihara (Division Lead PI)

Prof. Chihaya Adachi

Prof. Thomas Lippert, *Paul Scherrer Institut, Switzerland*

Prof. Ken Sakai

Assoc. Prof. Aleksandar Staykov

#### Hydrogen Materials Compatibility

Dr. Brian Somerday (Division Lead PI), *Southwest Research Institute, USA*

Prof. Reiner Kirchheim, *University of Göttingen, Germany*

Prof. Masanobu Kubota

Prof. Petros Sofronis

Prof. Joichi Sugimura

#### Electrochemical Energy Conversion

Prof. Hiroshige Matsumoto (Division Lead PI)

Prof. Andrew A. Gewirth, *University of Illinois at Urbana-Champaign, USA*

Prof. Tsuyohiko Fujigaya

Prof. John A. Kilner, *Imperial College London, UK*

Prof. Kazunari Sasaki

Prof. Harry L. Tuller, *Massachusetts Institute of Technology, USA*

#### Thermal Science and Engineering

Prof. Yasuyuki Takata (Division Lead PI)

Prof. Bidyut Baran Saha

Prof. Hiroaki Watanabe

Prof. Xing Zhang, *Tsinghua University, China*

#### Catalytic Materials Transformations

Prof. Seiji Ogo (Division Lead PI)

Prof. Miho Yamauchi

#### CO<sub>2</sub> Capture and Utilization

Assoc. Prof. Shigenori Fujikawa (Division Lead PI)

#### CO<sub>2</sub> Storage

Prof. Takeshi Tsuji (Division Lead PI)

Prof. Kenneth Christensen, *University of Notre Dame, USA*

### Full-time Faculty & Postdoctoral Associates

#### Molecular Photoconversion Devices

Assoc. Prof. Toshinori Matsushima

Assoc. Prof. Songmei Sun

Assoc. Prof. Motonori Watanabe

Asst. Prof. Edalati Kaveh

Asst. Prof. Minkyu Son

Dr. Nuttavut Kosem

Dr. Sijun Luo

Dr. Wei Ma

Dr. Arnau Call Quintana

Dr. Qing Wang

Dr. Tang Yongpeng

#### Hydrogen Materials Compatibility

Dr. Vlad Bogdan Niste

Dr. Pravakaran Saravanan

#### Electrochemical Energy Conversion

Prof. Naotoshi Nakashima

Dr. Junfang Cheng

Dr. Takaya Fujisaki

Dr. Kulbir Kaur Ghuman

Dr. Dino Klotz

Dr. Leonard Kwati

Dr. Youngsung Lee

Dr. Jin Nishida

Dr. Ganasan Pandian

Dr. Veeramani Vedyappan

#### Thermal Science and Engineering

Asst. Prof. Sivasankaran Harish

Asst. Prof. Biao Shen

Dr. Sumitomo Hidaka

#### Catalytic Materials Transformations

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Assoc. Prof. Yukina Takahashi

Assoc. Prof. Ki-Seok Yoon

Asst. Prof. Miho Isegawa

Dr. Tatsuya Ando

Dr. Takashi Fukushima

Dr. Sho Kitano

#### CO<sub>2</sub> Capture and Utilization

Assoc. Prof. Ikuo Taniguchi

Asst. Prof. Roman Selyanchyn

#### CO<sub>2</sub> Storage

Asst. Prof. Tatsunori Ikeda

Asst. Prof. Keigo Kitamura

Dr. Andri Hendriyana

#### Energy Analysis

Prof. Kenshi Itaoka

Assoc. Prof. Andrew Chapman

Asst. Prof. Nguyen Dinh Hoa

Dr. Hadi Farabi Asi

#### Research Center for Next Generation Refrigerant Properties

Prof. Yukihiro Higashi

#### Mazda Mobile Energy Storage for Low-Carbon Society (Industrial Research Unit)

Assoc. Prof. Hackho Kim

### Satellite Faculty & Postdoctoral Associates

#### Molecular Photoconversion Devices

Prof. Angus Rockett

Assoc. Prof. Elif Ertekin

### Electrochemical Energy Conversion

Prof. Andrew Gewirth  
Asst. Prof. Nicola Helen Perry

### Thermal Science and Engineering

Asst. Prof. Nenad Miljkovic

### CO<sub>2</sub> Capture and Utilization

Prof. Paul J. A. Kenis

### CO<sub>2</sub> Storage

Prof. Kenneth Christensen  
Dr. Yaofa Li

### Energy Analysis

Prof. James Stubbins  
Asst. Prof. Katy Huff

### Part-time Faculty & Postdoctoral Associates

#### Molecular Photoconversion Devices

Prof. Taner Akbay  
Prof. Etsuo Akiba  
Prof. Keiji Tanaka  
Prof. Kazunari Yoshizawa  
Assoc. Prof. Ken Kojio  
Assoc. Prof. Hai-Wen Li  
Assoc. Prof. Hisao Matsuno  
Assoc. Prof. Hajime Nakanotani  
Assoc. Prof. Hironobu Ozawa  
Assoc. Prof. Atsuumi Shundo  
Assoc. Prof. Atsushi Takagaki  
Asst. Prof. Yoshifumi Amamoto  
Asst. Prof. Kenichi Goushi  
Asst. Prof. Kosei Yamauchi  
Dr. Kazutaka Kamitani  
Dr. Byeong Su Kang  
Dr. Hajime Kusaba  
Dr. Huan Li  
Dr. Hui Ling Tan  
Dr. Tze Hao Tan  
Dr. Zhe Tan  
Dr. Kuan-Ting Wu  
Dr. Toshihiko Yokota

#### Hydrogen Materials Compatibility

Prof. Hisao Matsunaga  
Prof. Yoshinori Sawae  
Prof. Toshihiro Tsuchiyama  
Assoc. Prof. Kazuyuki Yagi  
Assoc. Prof. Tetsuo Yamaguchi  
Asst. Prof. Kaname Matsue  
Asst. Prof. Takehiro Morita  
Asst. Prof. Hiroyoshi Tanaka  
Dr. Takuro Masumura

#### Electrochemical Energy Conversion

Prof. Kohei Ito  
Assoc. Prof. Stephen Lyth  
Assoc. Prof. Junko Matsuda  
Assoc. Prof. Masamichi Nishihara  
Assoc. Prof. Tomohiro Shiraki  
Dr. George Harrington  
Dr. Yuki Terayama

### Thermal Science and Engineering

Prof. Masamichi Kohno  
Prof. Takahiko Miyazaki  
Prof. Shoji Mori  
Prof. Koji Takahashi  
Assoc. Prof. Jin Miyawaki  
Assoc. Prof. Naoya Sakoda  
Assoc. Prof. Kyaw Thu  
Asst. Prof. Yutaku Kita  
Asst. Prof. Qin-Yi Li

### Catalytic Materials Transformations

Assoc. Prof. Takahiro Matsumoto  
Assoc. Prof. Tatsuya Uchida  
Asst. Prof. Mitsuhiro Kikkawa  
Asst. Prof. Takeshi Yatabe  
Dr. Takuo Minato

### Visiting Professors & Scholars

#### Hydrogen Materials Compatibility

Prof. Nikolaos Aravas, *University of Thessaly, Greece*  
Prof. Robert O. Ritchie, *University of California, Berkeley, USA*  
Dr. Akihide Nagao, *JFE Steel Corporation, Japan*

#### Electrochemical Energy Conversion

Asst. Prof. Helena Tellez-Lozano

#### Thermal Science and Engineering

Prof. Sushanta Mitra, *University of Waterloo, Canada*  
Prof. Akira Yamada, *Mitsubishi Heavy Industries, Ltd, Japan*  
Assoc. Prof. Daniel Orejon, *University of Edinburgh, UK*  
Dr. Mahfuza Sharifa Sultana

#### Catalytic Materials Transformations

Dr. Kinya Kumazawa, *Japan Institute for Promoting Invention and Innovation*

#### CO<sub>2</sub> Capture and Utilization

Prof. Benny Freeman, *University of Texas, Austin, USA*  
Dr. Toyoki Kunitake, *Kitakyushu Foundation for the Advancement of Industry Science and Technology, Japan*

#### CO<sub>2</sub> Storage

Assoc. Prof. Diogo Bolster, *University of Notre Dame, USA*  
Asst. Prof. Jiang Fei, *Yamaguchi University, Japan*  
Asst. Prof. Jihui Jia, *China University of Petroleum*  
Dr. Osamu Nishizawa

#### Energy Analysis

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Prof. Kuniaki Honda  
Prof. Atsushi Kurosawa, *Institute of Applied Energy, Japan*  
Prof. Ken Okazaki, *Tokyo Institute of Technology, Japan*  
Assoc. Prof. Jack Brouwer, *University of California, Irvine, USA*  
Dr. Makoto Akai, *National Institute of Advanced Industrial Science and Technology, Japan*  
Dr. Katsuhiko Hirose, *Toyota Motor Corporation, Japan*  
Dr. Seiichiro Kimura, *Renewable Energy Institute, Japan*

#### Research Center for Next Generation Refrigerant Properties

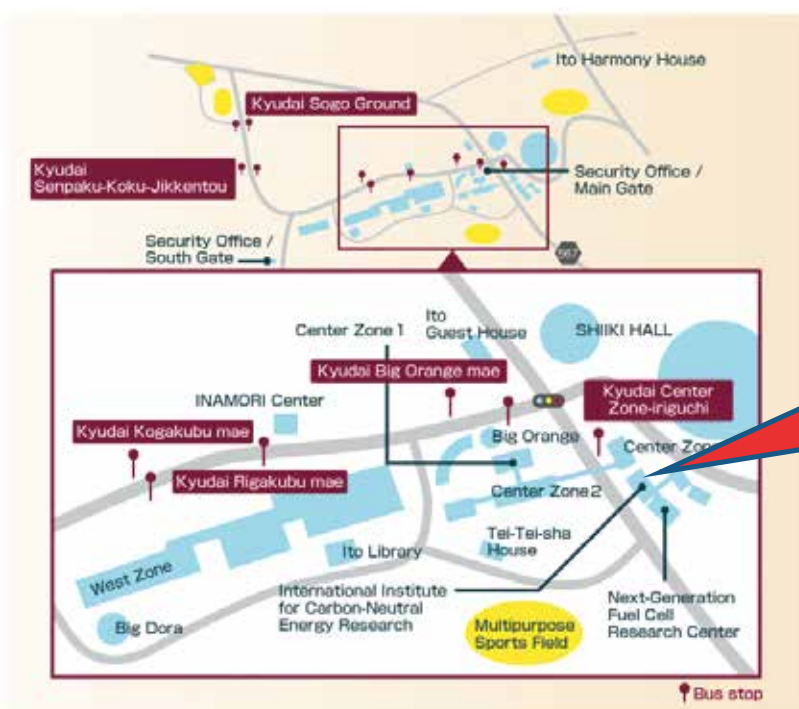
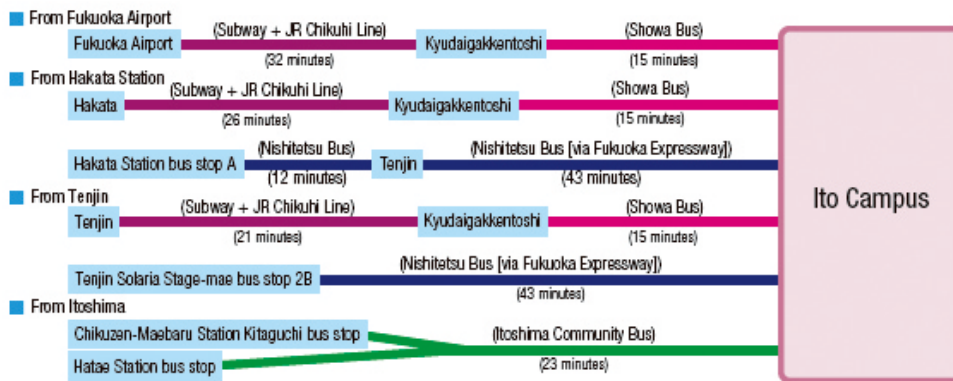
Prof. Ryo Akasaka, *Kyushu Sangyo University, Japan*  
Prof. Akio Miyara, *Saga University, Japan*  
Assoc. Prof. Chieko Kondo, *Nagasaki University, Japan*

#### Mazda Mobile Energy Storage for Low-Carbon Society (Industrial Research Unit)

Assoc. Prof. Suguru Ikeda, *Mazda Motor Corp., Japan*

# Access Map

## Map of Fukuoka City



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The overhead view of the new I<sup>2</sup>CNER building portrays the \*Keeling Curve, which rises over time, to indicate that I<sup>2</sup>CNER's research will eventually contribute to the downward turn of this curve.

\*In 1958, Charles David Keeling began making daily measurements of the concentration of atmospheric carbon dioxide (CO<sub>2</sub>) at the Mauna Loa Observatory on the Big Island of Hawaii. Keeling's measurements are the first significant evidence of rapidly increasing carbon dioxide in the atmosphere.