I²CNER

International Institute for Carbon-Neutral Energy Research

2021 Annual Report

I²CNER | wpi World Premier International Research Center Initiative | KYUSHU UNIVERSITY | ILLINOIS

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World Premier International Research Center Initiative (WPI)

World Premier International Research Center Initiative

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 to place itself within the "circle" of excellent human resources

In FY17, concurrent with the end of the 10-year support period for the initially established five WPI centers, Ministry of Education, Culture, Sports, Science and Technology (MEXT) established the new World Premier International (WPI) Academy, which aims to be a leader in internationalizing and reforming Japan's research environment.

Program Summary

The World Premier International Research Center Initiative 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 the best researchers from around the world

Attractive Research and Living Environment of the Highest 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 for researchers
- Facilities and equipment expected in a top 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 long-term, large-scale financial support.

I^{2}CNER was certified as having achieved "World Premier" status by the Program Committee and was inducted into the WPI Academy in April 2020.

For more information:

MEXT Website https://www.mext.go.jp/en/policy/science_technology/researchpromotion/index.htm

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

International Institute for Carbon-Neutral Energy Research (I^{2}CNER) Kyushu University
Toward the realization of a low-carbon society, I^{2}CNER aims to resolve the challenges of the use of hydrogen energy and CO_2 capture and sequestration by fusing together sciences from atomic level to global scale.

Kavli Institute for the Physics and Mathematics of the Universe (Kavli IP MU)
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.

Advanced Institute for Materials Research (AIMR), Tohoku University
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.

Immunology Frontier Research Center (IFReC)
Osaka University
An innovative research center, which pursues the goal of comprehensive understanding of immune reactions through the fusion of immunology, various imaging technologies, and Bioinformatics.

International Center for Materials Nanoarchitectonics (MANA)
National Institute for Materials Science
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.

International Center for Quantum-field Measurement Systems for Studies of the Universe and Particles
The "quantum field" is the origin of everything. QUP will invent and develop new systems for measuring quantum fields.With these new systems, we will bring innovation to the human society, while working on the basic research on the space-time and matter of the universe.

Institute for Integrated Cell-Material Sciences (iCeMS)
Kyoto University
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.

Institute of Transformative Bio-Molecules (ITbM)
Nagoya University
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.

Institute for the Advanced Study of Human Biology (ASHBi) Kyoto University
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.

International Institute for Integrative Sleep Medicine(IIIS)
University of Tsukuba
IIIS 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.

EARTH - LIFE SCIENCE INSTITUTE (ELSI)
Tokyo Institute of Technology
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.

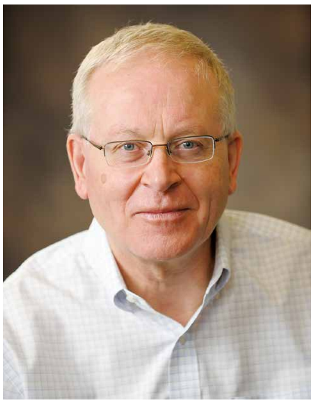
Institute for Chemical Reaction Design and Discovery (ICReDD) Hokkaido University
ICReDD integrates computational, information, and experimental sciences in order to obtain in-depth understanding of chemical reactions, which enables rational design and rapid development of new chemical reactions.

Nano Life Science Institute (NanoLSI)
Kanazawa University
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.

International Research Center for Neurointelligence (IRCN)
The University of Tokyo
IRCN combines life sciences and information sciences to establish the new field of "Neurointelligence". By clarifying the essence of human intelligence, overcoming neuraldisorders, and developing new AI technologies, we will contribute to a better future society.

WPI Academy Centers (other than I^{2}CNER)

Message from the Director



This past year has been an eventful one for I^{2}CNER. When the Institute was inducted in 2020 as a WPI Academy Center, we understood the vision of JSPS and how important it would be for I^{2}CNER to create ripple effects around Kyushu University and Japan. True to the WPI Academy system, we focused on developing deeper connections and engaging with collaborating academic institutions around Japan.

A great achievement this year was I^{2}CNER being awarded Gaisan-Yokyu funding for the new Center for Energy Systems Design. The CESD, which launched November 1, 2022, replicates I^{2}CNER's structure and objectives and – thanks to the great efforts of center director, PI Matsumoto – it is a highly coordinated effort among our PIs and faculty and involves 6 collaborating institutions, Hokkaido University, Tohoku University, Tokyo Institute of Technology, NIMS, RIKEN, and Kumamoto University. Among its areas of focus is data science, for which we are exploiting the data we have generated and plan to generate, not only as an institute but as a research community. We are aggressively pursuing the hire of excellent tenure-track faculty and researchers specifically for the new center.

On November 1, 2021, we launched a new industry-university collaboration in the form of the Mitsui Chemicals, Inc.-Carbon Neutral Research Center (MCI-CNRC). This comprehensive partnership has been working on the development and acquisition of environmental infrastructure technologies that contribute to carbon neutrality as well as pursue the practical use and commercialization of these technologies in relevant fields. The new center, created thanks to the continuous efforts of PI Ishihara, is an exciting opportunity to leverage I^{2}CNER's world-class research alongside Mitsui Chemicals' industry expertise with the goal of incorporating into society the technologies necessary to achieve carbon neutrality.

On the topic of hiring, I am pleased to report that post-pandemic, I^{2}CNER reopened to visitors and reinstated our postdoctoral employment opportunities. In fact, I^{2}CNER contributed 20% to the hiring of postdocs and has maintained a healthy number of postdoctoral researchers. In FY2021, we employed 27 postdocs—a dramatic increase from the 20 we employed in FY2020. Contributing to this number is the Kyushu University Negative Emission Technology Center (K-NET), which is well-staffed and pursuing its objectives in research.

We also maintained the success we saw in our first two terms as a WPI Academy Center—fostering a rich culture of research for students. Indeed, I^{2}CNER provides a rich platform for young scientists to impact research in a highly international setting. During FY21, we employed 22 graduate students in our labs, 18 of whom were non-Japanese.

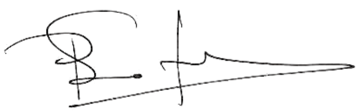
Another important objective for I^{2}CNER is maintaining our connection with our alumni. With this in mind, in July 2021 we established the "I^{2}CNER Alumni Network" – a global network in which all former I^{2}CNER researchers, students, and staff members can register. This is a vital aspect of our strong standing as a truly international institution in the WPI Academy, and we hope this will enable more connections among the I^{2}CNER family worldwide to expand our international network.

For some time now, I^{2}CNER has worked with the Institute of Mathematics for Industry (IMI) and we plan to rekindle and strengthen our interactions, continuing to develop joint and interdisciplinary projects on statistics and related areas. In the works is a symposium on machine learning in materials science, to be held in Tokyo next year. Building such a community among experts in applied mathematics, machine learning, and materials science will be a significant contribution both to engineering at large and to I^{2}CNER's visibility.

Similarly, I^{2}CNER's partnership with the University of Illinois Urbana-Champaign continues its strategic activities. Thanks to continued funding from both universities, this has led to opportunities that have extended even beyond I^{2}CNER. Ongoing efforts are in the areas of data science and mathematics; environmental economics; humanities; library science and data management; sustainable energy; and architecture. UIUC and Kyushu University organized a discussion on diversity, equity and inclusion (DEI) in an effort to bring more inclusivity to both institutions. These new initiatives that were conceived and advanced by the leaders of Kyushu University and the University of Illinois are great examples of brain circulation and the ripple effect of I^{2}CNER within KU.

Our upcoming 2023 I^{2}CNER Annual Symposium, "Optimal Transitions: From Carbon Neutral Energy Research to Energy Markets," is an apt description of our effort to begin building an energy pipeline for the future. Indeed, in our third year as a WPI Academy Center and on the other side of that transition, I^{2}CNER has stabilized itself as a member center, maintaining our postdoctoral numbers at healthy levels and looking to a productive future that will involve transferring our laboratory results to society. We will advance energy solutions that are environmentally friendly and continue renewing our PI composition in a way that fosters a diversity of perspectives and scientific approaches—that is, through fusion.

Professor Petros Sofronis, PhD
Director, I^{2}CNER



About I²CNER

MISSION

At I²CNER, 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 I²CNER's research aims to enable includes solid oxide fuel cells, polymer membrane-based fuel cells, biomimetic and other novel catalyst concepts, and production, storage, and utilization of hydrogen as a fuel. Our research also explores the underlying science of CO_2 capture and storage technology or the conversion of CO_2 to a useful product. Additionally, it is our mission to establish an international academic environment that fosters innovation through collaboration and interdisciplinary research (fusion).

I²CNER's research at the intersection of applied math and engineering has enormous potential to impact all of the Institute's research areas and the overall energy challenge. I²CNER's applied math efforts are based on the its burgeoning relationship with the Institute of Mathematics for Industry (IMI) and various departments at the University of Illinois Urbana-Champaign. The Institute currently has ongoing projects in the areas of mathematics for smart grid, porous materials, computational physics, and social aspects of power systems. Examples include algorithm development for scalable grid optimization problems, study of strategic interactions in electricity markets by accounting for the deepening penetration of variable renewable resources in the grid, and persistent homology to characterize the properties of porous materials for CO_2 storage in rock formations. Projects are also addressing efficiency increase in power generation by modeling expanding flames using theory of parabolic equations.

As the newest center of the WPI Academy (inducted in 2020), we aim to continue to make disruptive advances in the 21st century international energy landscape, as well as strengthen the scientific advancements in Japan in collaboration with the United States and the world.

I²CNER's research is consolidated into three thrusts: Advanced Energy Materials, Advanced Energy Conversion Systems, and Multiscale Science and Engineering for Energy and the Environment.

These thrusts are directly linked to the "Platform for International Collaborations and Partnerships" that has been designed to maintain I²CNER's international identity and the "Platform for Societal Implementation and Industrial Collaboration," whose purpose is to ensure technology transfer through the large and growing network of I²CNER's industrial interactions.

Each thrust is led by a number of Principal Investigators, each with several dozen researchers working toward that thrust's stated research objectives.

RESEARCH THRUSTS

Advanced Energy Materials

The goal of the Advanced Energy Materials thrust is to develop molecular, nano, and bulk materials based on new science of surfaces, interfaces, and microstructures for applications involving H_2, H_2O, and CO_2. The research is directed to two classes of materials, catalytic and structural. In the area of catalytic materials, our objective is to develop bio-inspired molecular systems for fuel and energy generation that are centered on biological and synthetic catalysts. In addition, we explore the production of fuels and materials of added-value from ubiquitous chemicals through the use of solar energy. In the area of structural materials, the research focuses on the development of the fundamental science that enables optimization of the cost, performance, and safety of materials for H_2 technologies. This includes the association of basic science underlying deactivation of catalytic surfaces to industrial approaches for the mitigation of hydrogen embrittlement. In addition, we aim at advancing our mechanistic insight into the degradation of metals and alloys for technologies that operate at elevated temperatures in the presence of hydrogen. Lastly, it is our objective to develop next-generation tribo-systems with higher efficiency and durability to conserve energy, thus contributing to CO_2 emissions reduction.

Advanced Energy Conversion Systems

The goal of the Advanced Energy Conversion Systems thrust is to develop economically feasible energy systems characterized by high efficiency, fast conversion kinetics, and long lifetimes. The focus is on electrochemical and photochemical conversion that serve for stationary power and fuel generation and mobility, and thermal energy conversion that enables efficient heat transport. For electrochemical conversion, fundamental advances in the understanding of electrocatalysis and ionic and electronic transport properties in solids are needed in order for high conversion rates between electrical and chemical energy to be obtained. The goal of photoelectrochemical conversion is the development of high-performance systems for splitting water, harvesting solar energy, and generating light by exploring inorganic, organic, and hybrid materials from physical, chemical, and biochemical perspectives and by elucidating potential conversion roadblocks and causes of degradation.

Thermal energy conversion is studied by pursuing fundamental understanding of heat and mass transport phenomena in relation to nanoscale thermal transport, phase change heat and mass transfer, and the thermophysical properties of working fluids. Devices thus developed are essential to the integration of renewable energy to the electric grid and the advancement of new energy solution pathways, including hydrogen energy.

Multiscale Science and Engineering for Energy and the Environment

The Multiscale Science and Engineering for Energy and the Environment thrust pulls together the range of challenges facing Japan's and the world's energy transition, namely the transition from largely fossil fueled energy technology to a carbon-neutral or a carbon-free energy supply. In addition, this thrust enables the coordination of carbon reduction technologies, energy efficiency technologies, and guidance for social, political, and investment strategies to coordinate this transition.

This thrust includes the following 4 main clusters;

1. Carbon capture technologies based on membrane separation for zero and negative emission

We are developing technologies for CO_2 capture based on membrane separation, which is considered to have the lowest capture energy. In order to control global warming, CO_2 is not only captured from largescale emission sources, but also CO_2 from (1) air and (2) exhaust gas with diluted CO_2 by membrane separation for negative emission, and CO_2 removal at biogas upgrading. We are also considering modularization along with the development of these technologies.

2. Carbon storage and management using the earth

As a CO_2 reduction approach using the Earth, CO_2 geological storage that directly injects CO_2 into the subsurface reservoir has been recognized. By considering (1) amount of CO_2 reduction, (2) time to achieve CO_2 reduction and (3) cost for CO_2 reduction, CO_2 reduction and managements using the Earth could be a realistic approach.

3. Energy efficient technologies

To contribute toward the world's energy transition, we are working on the development of energy-efficient technologies, which includes heat mass transfer enhancement in adsorption systems, development of low-temperature thermally powered adsorption heat pump/refrigeration systems, and biofuel and edible protein production and negative CO_2 emissions.

4. Socio-techno-economic and policy analysis

In order to progress an energy transition that incorporates and develops technologies which can effectively deal with climate change, there is a need for analysis of technical, economic, and social aspects. I[2]CNER is furthering this analysis across the spectrum of available technologies, with a focus on the technologies being developed within I[2]CNER. In addition to the evaluation of the technical aspects such as technological applicability and efficiency, we also consider their economic and social merit. The analytical approaches we undertake include modeling, systems analysis, statistical analysis, applied mathematical analysis, social surveys, and stakeholder engagement.

RESEARCH PLATFORMS

Platform for International Collaborations and Partnerships

This platform is intended to maintain and foster I[2]CNER's international identity. The members of this platform, who are world experts with a solid record of international research experiences, collaborate with I[2]CNER's researchers from all three thrusts. Because this platform and the three thrusts are interwoven and the thrusts' themes overlap, this is an effective way to promote interdisciplinary collaborations across the Institute and around the world.

Platform for Societal Implementation and Industrial Collaboration

The three major research thrusts contribute directly to the transition of future I[2]CNER scientific advances to applicable technology transfer through a large and growing network of I^2CNER industrial interactions. This platform ensures a high level of tech transfer, provides policy guidance for science and technology investments, and addresses potential social acceptance and social impact issues. With its strengths in both advanced energy science and energy analysis, I^2CNER provides critical direction and support to Japan's energy transition over the next 30 years to meet the 2050 carbon reduction goals with minimal social and economic disruptions.

AFFILIATED RESEARCH INSTITUTES

Research Center for Next Generation Refrigerant Properties (NEXT-RP)

Through coordination of efforts of the international community, this unique center focuses on the development of next-generation refrigerants. More specifically, the objectives of the center include the accurate evaluation of thermophysical properties and fundamental performance of heat exchange and air conditioning and refrigeration (ACR) cycles for zero-ODP (ozone depletion potential) and low-GWP (global warming potential) refrigerants. Through development of base knowledge and thermophysical properties technology the NEXT-RP aims to contribute to Japanese ACR industries in enhancing their competitiveness in the global market.

Mitsui Chemicals, Inc.-Carbon Neutral Research Center (MCI-CNRC)

This new industry-university center was launched November 1, 2021 within I^2CNER. The comprehensive collaboration aims to develop and acquire cutting-edge environmental infrastructure technologies that contribute to carbon neutrality as well as pursue the practical use and commercialization of these technologies in relevant fields. The center will utilize the world-leading expertise I^2CNER has developed—including green hydrogen as well as carbon capture, utilization and storage (CCUS)—and combine this with the development- and industrialization-related expertise from Mitsui Chemicals. This will lay the groundwork for focused and efficient research into the elemental technologies needed to achieve carbon neutrality, with the goal of quickly integrating the technologies into society.

Moonshot K-NET

In 2020, Japan's New Energy and Industrial Technology Development Organization ("NEDO") selected 13 research and development (R&D) projects aimed at achieving the Moonshot Goal of "realization of sustainable resource circulation to recover the global environment by 2050."

Professor Shigenori Fujikawa's project, "Development of Global CO_2 Recycling Technology Towards 'Beyond-Zero' Emission," was adopted as one of the 13 projects under the Moonshot goal of targeting recovery of the global environment. In this project, a membrane-based CO_2 capture unit with ultra-high CO_2 selectivity and permeability is being developed based on innovative nanomembrane technology. At the same time, the team is developing a unit to convert the collected CO_2 into carbon fuel with high efficiency. These two units will be connected to build a "Direct Air Capture and Utilization (DAC-U) system" that integrates CO_2 capture from the atmosphere to carbon fuel conversion. This system has high scalability because the units can be connected arbitrarily, and its performance can be adjusted according to conditions from small to large scale. Through this work, the researchers hope to create an innovative DAC-U system that contributes to solving climate change problems and helps build a new future society.

I²CNER Carbon Neutral Vision

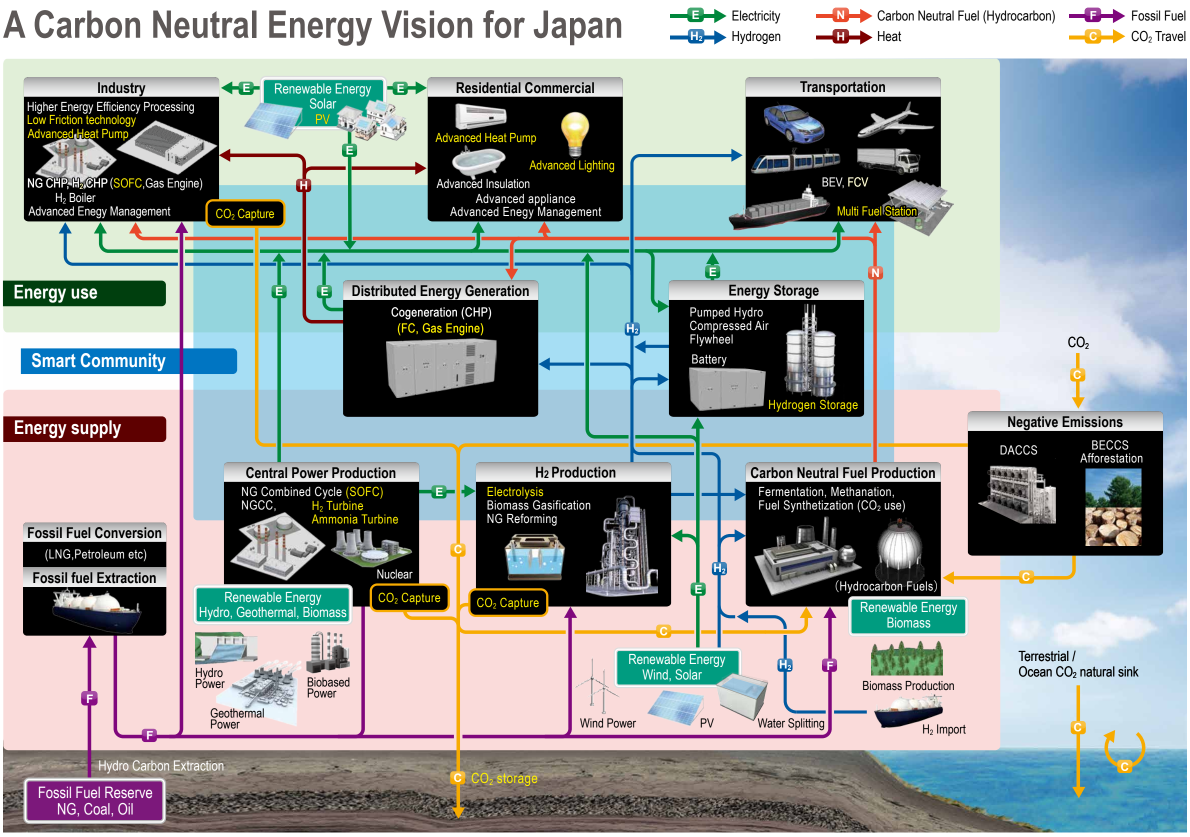


Figure 4.1. Parameter Space of Technology Options.

Background

Our vision of a carbon-neutral energy society includes the need to identify future technology options by sharing a common image of a future for Japan with people in and outside of I²CNER. In October 2020, the Prime Minister of Japan made a speech to the Diet in which he declared, "I hereby declare that Japan aims to reduce its greenhouse gas emissions to net zero by 2050 as a whole, that is, to achieve a carbon-neutral, decarbonized society by 2050." The shift of the GHG target for 2050 from an 80% emission reduction to carbon neutrality requires not only expediting our efforts to reduce GHG emissions but also requires a drastic change for our energy system from a fossil fuel energy regime to a zero-carbon energy regime. In addition, a net zero society implies that net zero emissions can be achieved by implementing GHG "removals" that can offset any GHG "emissions" left over at the end of emission reduction efforts.

The I²CNER vision for a low-carbon society for Japan is revised based on setting a carbon neutrality target of a 90-100% reduction of GHG emissions by 2050. This target is particularly relevant to energy security concerns caused by Japan's current heavy reliance on imported fossil fuels, which are costly resources. To achieve the target by developing new technology, we also consider economic efficiency and safety issues. On the whole, we consider 3E+S (Environment, Energy Security, Economy, and Safety) as the fundamental pillar of our vision.

In drawing our vision, we consider two major principles: 1) efficiency increase ("EI") in energy conversion and energy use and 2) lowering of carbon intensity ("LCI") of fuel and electricity to adopt and develop future technologies. EI should be pursued in energy transformation systems, end use systems including home appliances, and industrial processes. EI can be applied to existing systems but is also achieved by replacing existing systems with new technology. LCI in electricity and fuel supply-use pathways is achieved using renewables, nuclear, or CO_2 capture, utilization and sequestration (CCUS).

LCI typically requires the deployment of new facilities, new infrastructure, or both. In addition, 3) the negative emission ("NE") technologies to realize "removal" need to be employed to cancel out the residual GHG emissions in our new vision. "NE" is achieved by capturing CO_2 directly from the atmosphere and storing it underground (via DACCS), capturing CO_2 from the flue gas of combusting biomass and storing it underground (i.e., BECCS), or enhancing CO_2 absorption and fixation by afforestation or land use management.

I²CNER Scenarios for a Carbon-Neutral Energy Society

The scenarios which could lead to carbon neutrality considering the 3E+S attributes would not have a wide variance range because the target year of 2050 is rapidly approaching and difficulty attached to the quick deployment of some important technologies is recognized, based on our past experience to narrow high-potential options.

EI technology developments are at the base of emission reduction scenarios. Therefore, they are included across all scenarios. To achieve a huge emission reduction, LCI technologies could have the greatest impact. However, even a large deployment of LCI technologies cannot enable carbon neutrality due to some types of GHG emissions such as emissions from farmland and other GHG gases (CH_4 and N_2). Therefore, introduction of negative emission (NE) technologies is necessary to offset these unavoidable GHG emissions.

One of the most likely scenarios for the future energy systems is named Scenario A (the main scenario). This scenario does not include the extreme deployment of some technologies, except for solar PV, and reflects past deployment progress and current and future development progress for technologies. Among LCI technologies, nuclear still has a large potential to reduce CO_2 emission since a large unused capacity exists. However, restarting unused nuclear capacity has been relatively slow due to public concerns about safety. Therefore, nuclear is not prioritized in the main scenario, reflecting the current situation for permitting the restarting of existing nuclear capacity. However, a scenario maximizing the use of the existing nuclear capacity assuming an extension of operational periods is also detailed (Scenario B - Nuclear Scenario).

The common features across the scenarios are 1) deployment of EI, 2) maximizing use of solar energy as an LCI technology, 3) deployment of NE technologies, 4) expansion of electrification in energy use sectors (transportation, industry and commercial and residential), 5) a large introduction of hydrogen energy and 6) effective application of CCS.

As for 4), expansion of electrification can take advantage of the decarbonatization of the power generation sector. As for 5), hydrogen demand would be boosted due not only to fuel for FCVs but also for hydrogen power generation, hydrogen steel reduction, and carbon neutral gas synthesized by CO_2 and H_2. In terms of 6), CCS deployment has been delayed due to a delay in storage site preparation and lack of incentives for additional investment to equip CO_2 sources with CCS facilities. Since the lead time to implement CO_2 storage facilities tends to be long and the availability of drilling rigs tends to be limited, it is expected that CO_2 storage capacity in Japanese geological formations will be limited 200 million tons of CO_2/year. This limitation hinders the employment of CO_2 storage related activities such as CCS for power generation, CCS for industry, and CCS for NE (DACCS and BECCS). In our scenarios, CO_2 storage capacity necessary for CCS is mainly prioritized for industrial CCS where no significant emission mitigation measures are available and NE CCS (DACCS and BECCS) instead of using CCS for power generation where various LCI technologies such as solar PV and wind power are available.

In terms of Scenario A (the main scenario), we are analyzing the inherent compromises which emerge between system cost, energy security, and overall feasibility of the deployment of LCI technologies, along with system EI over time. This scenario uses 70% of the economically feasible PV for power generation and 20% for hydrogen production. For wind power generation, 10% of the economically feasible potential is employed, reflecting the fact that wind power has not been deployed as quickly as PV under the Feed-in Tariff (FIT). A relatively small amount of CCS is introduced to the power generation sector for natural gas combined cycle (NGCC). Coal power is assumed to phase out by 2040.

Scenario B (nuclear scenario) utilizes nuclear power at a much higher level than for Scenario A (which only engages nuclear for 4% of the electricity supply in 2050), assuming all existing nuclear power plants

– except for those which will be abolished – will be restarted by 2030 with an extension in operational years from 40 to 60 years. This assumption results in nuclear power accounting for 21% of the electricity supply in 2050. This level of nuclear power makes CCS unnecessary in the power sector such that CCS capacity is used for more NE, which enables the offset of residual GHG emissions at a higher level than is realized in Scenario A. In short, the CO_2 storage capacity saved due to nuclear is more effectively used for NE.

Scenario A (Main Scenario): Development of important EI technologies and maximum deployment of solar power together with low carbon hydrogen energy system and NE. Approximately 92% reduction in GHG emissions by 2050, relative to 2010.

Contribution to EI

Heat pump (*GHG impacts of "Energy Efficiency"* *) and FC co-generation (*GHG impacts of "Power Generation"* *) for residential and commercial from 2020. Low-temperature heat utilization for industry from 2020, Fuel cell (*GHG impacts of "Power Generation"* *) for transportation from 2020.

Contribution to LCI through renewables

Low-cost and high-efficiency PV (*GHG impacts of "Renewables"* *) from 2030. Hydrogen storage and new battery technology (*GHG impacts of "Energy Carriers and Storage"* *) to adjust intermittent PV and wind power from 2030. High-efficiency electrolysis (PEM and high-temperature steam) (*GHG impacts of "Energy Carriers and Storage"* *) using renewable electricity to provide low-carbon hydrogen from 2030. SOFC using hydrogen and hydrogen turbine (*GHG impacts of "Power Generation"* *) for electricity generation industry from 2030 to 2050. I²CNER's hydrogen-compatible material research (*GHG impacts of "Hydrogen Compatible Steel"* *) and hydrogen physical property research (*GHG impacts of "Hydrogen Compatible Steel"* *) underpin the hydrogen energy systems.

Contribution to LCI and NE through CCS

Low-cost membrane CO_2 capture technology (*GHG impacts of "CO_2 Capture and Storage"* *) for NGCC, industrial CCS and DACCS and BECCS from 2030. Development of simulation technology for CO_2 monitoring and storage site characterization (*GHG impacts of "CO_2 Capture and Storage"* *) from 2030 through seismic approaches.

*The technology category in which I²CNER's research will produce CO_2 emission reduction impacts

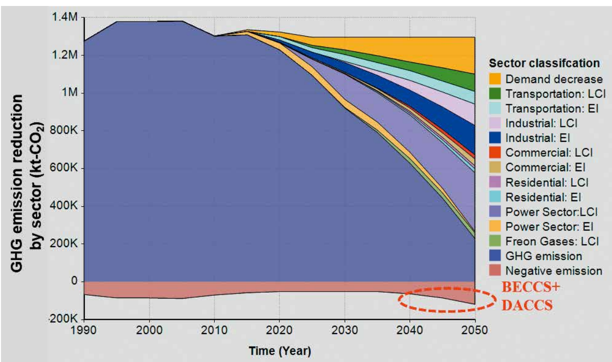


Figure 4.2. CO_2 reduction relative to 2010 by sector in Scenario A.

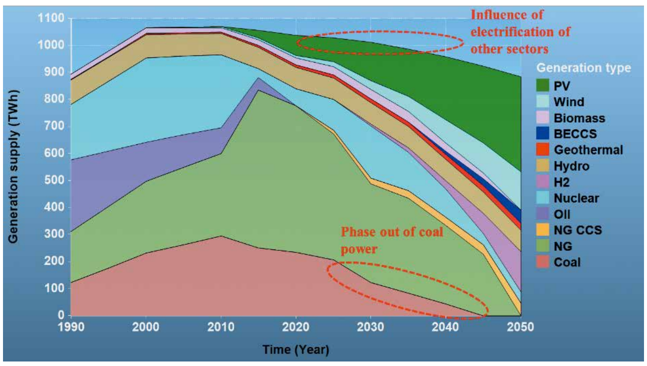


Figure 4.3. Electricity mix by generation type in Scenario A.

Scenario B (Nuclear): Development of important EI technologies and maximizing use of existing nuclear plants together with low-carbon hydrogen energy system and NE. Approximately 94% reduction in GHG emissions by 2050, relative to 2010. If the public concerns on nuclear safety can be addressed, this scenario becomes more feasible, resulting in (i) providing more zero carbon electricity (nuclear) and reducing necessary renewable deployment; (ii) avoid employing CCS in the power generation sector; (iii) providing more CO_2 storage capacity for NE.

Contribution to EI

Heat pump (*GHG impacts of "Energy Efficiency"* *) and FC co-generation (*GHG impacts of "Power Generation"* *) for residential and commercial from 2020. Low-temperature heat utilization for industry from 2020, Fuel cell (*GHG impacts of "Power Generation"* *) for transportation from 2020.

Contribution to LCI through renewables

Low-cost and high-efficiency PV (*GHG impacts of "Renewables"* *) from 2030. Hydrogen storage and new battery technology (*GHG impacts of "Energy Carriers and Storage"* *) to adjust intermittent PV and wind power from 2030. High-efficiency electrolysis (PEM and high-temperature steam) (*GHG impacts of "Energy Carriers and Storage"* *) using renewable electricity to provide low-carbon hydrogen from 2030. SOFC using hydrogen and hydrogen turbine (*GHG impacts of "Power Generation"* *) for electricity generation industry from 2030 to 2050. I²CNER's hydrogen-compatible material research (*GHG impacts of "Hydrogen Compatible Steel"* *) and hydrogen physical property research (*GHG impacts of "Hydrogen Compatible Steel"* *) underpin the hydrogen energy systems.

Contribution to LCI and NE through CCS

Low-cost membrane CO_2 capture technology (*GHG impacts of "CO_2 Capture and Storage"* *) for industrial CCS and DACCS and BECCS from 2030. Development of simulation technology for CO_2 monitoring and storage site characterization (*GHG impacts of "CO_2 Capture and Storage"* *) from 2030 through seismic approaches.

*The technology category in which I²CNER's research will produce CO_2 emission reduction impacts

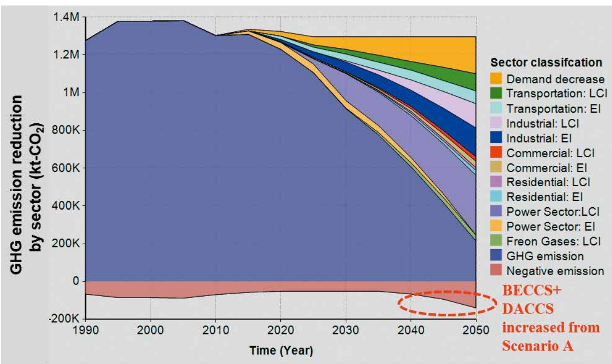


Figure 4.4. CO_2 reduction relative to 2010 by sector in Scenario B.

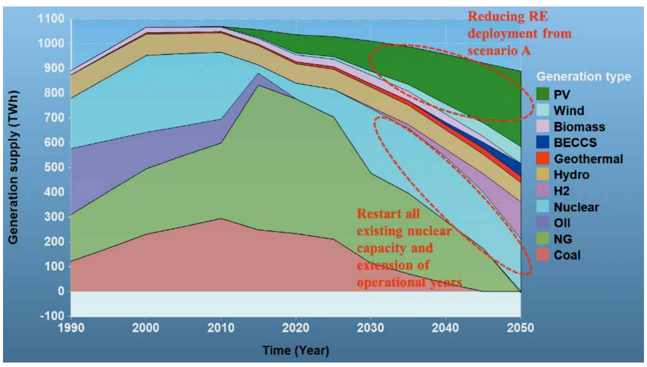


Figure 4.5. Electricity mix by generation type in Scenario B.

The figure for CO_2 reduction in Scenario B is very similar to that of Scenario A. The difference in energy system makeup is defined in the electricity mix figures (Figures 4.3 and 4.5). Both energy systems show strong CO_2 reductions in the Power Sector LCI wedge in the CO_2 reduction figures (Figure 4.2 and Figure 4.4) as nuclear and CCS are classified in the same Power Sector LCI wedge.

I²CNER's Contribution to the 2050 CO_2 Reduction Target

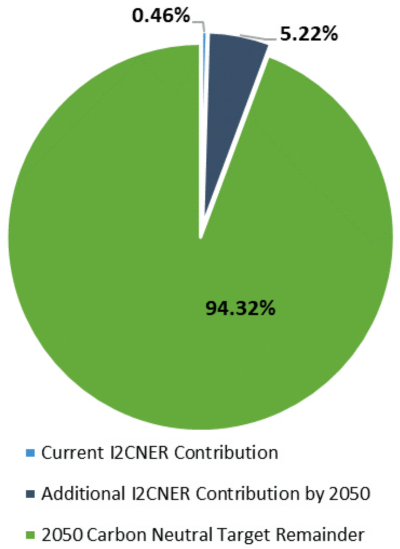
Based on our analysis of current and future achievements, approximately 0.46% of the total required CO_2 reductions via current achievements, and approximately 5.22% of the total required reductions through our future achievements, can be realized by I²CNER technologies and innovations if they are applied to appropriate energy systems (limiting the contribution of any one technology to 50% of the resultant market).

In addition to I²CNER's direct contributions, all I²CNER activities also contribute to the overall relevant industry efforts (a further 32.1% of the 2050 target, shown in dark grey in Fig. 5b) through the provision of underpinning technologies and analyses. The reason for the increase of I²CNER's future contributions (from 4.71% reported in the 2019 Annual Report to 5.22%) is that the new I²CNER Scenarios for a Carbon Neutral Energy Society need much larger introductions of renewable energy in 2050, wherein much of I²CNER's research is conducted directly or indirectly, than the previous scenarios. This implies the research direction of I²CNER is suitable for an energy transition to a carbon-neutral energy society.

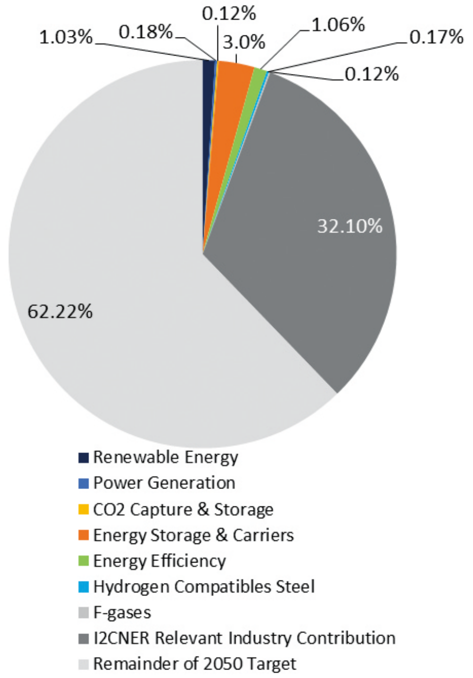
As shown in Fig. 5c, the leading contributors to I²CNER's 2050 CO_2 reduction efforts include energy storage and carriers, encompassing electrolysis and the reversible fuel cell; renewable energy through organic-inorganic hybrid perovskite solar cells; and energy efficiency, utilizing energy-saving heat loop-tube technologies and friction-reducing coatings.

The changes of I²CNER's contribution from the previous assessment reported in the 2019 Annual Report are primarily due to the scenario influences, shown as follows. The contribution of energy storage and carriers increases (from 2.28% to 3.0 %) due to necessity of a larger introduction of low carbon hydrogen. The contribution of CO_2 capture and storage decreases significantly (from 0.77% to 0.12 %) due to a long lead time of implementation and limited availability of storage sites. The contribution of energy efficiency (1.06%) is almost the same. The contribution of renewable energy increases (from 0.79% to 1.03 %) due to a larger introduction of PV. The contribution of renewable energy increases (from 0.79% to 1.03 %) due to a larger introduction of PV. The contribution of hydrogen compatibles steel increases (from 0.12% to 0.17%) again due to a larger introduction of low carbon hydrogen. The contribution of power generation (0.18%) is similar because a decrease of natural gas power generation (SOFC) and an increase of hydrogen power generation (hydrogen turbine) cancel out. The contribution of F-gases (0.12%), which are development of new refrigerants for heat pump with lower GWP, is newly counted. Finally, the contribution to the overall relevant industry efforts decreases (from 35.7% to 32.1%) due to a larger introduction of renewable energy where the share of I²CNER's direct contribution is larger than that of other research areas. EAD continues to analyze each technology thrust within I²CNER in line with our energy system scenarios to ensure that our contribution toward CO_2 reduction and to underpinning industry efforts is maximized.

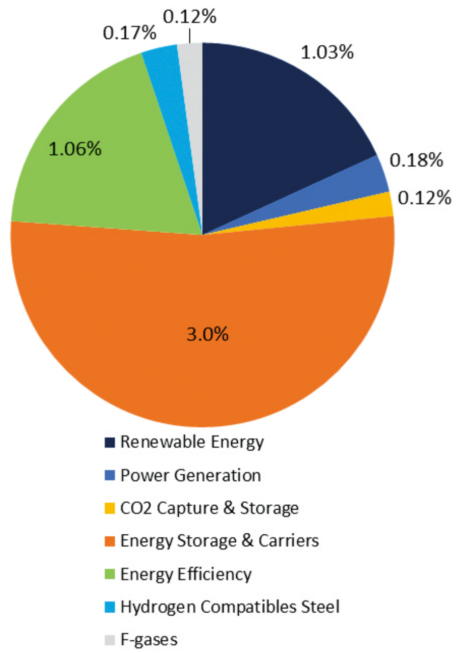
I^2CNER's Contribution to the 2050 CO_2 Reduction Target



(a) Current and Future Contributions



(b) Overall Contributions to 2050 CO_2 Reduction Target



(c) Overall I^2CNER Contributions to 2050 CO_2 Reduction Target

Figure 6. I^2CNER's current and future contributions to CO_2 reduction in Japan.

Advanced Energy Materials

1. C–H arylation of benzene with aryl halides using H_2 and a water-soluble Rh-based electron storage catalyst (PI Ogo and Prof. Yoon)

This work [1] reports the first example of C-H arylation of benzene under mild conditions, using H_2 as an electron source (turnover numbers (TONs)=0.7-2.0 for 24 h). The reaction depends on a Rh-based electron storage catalyst and proceeds at room temperature and in aqueous solution. The reaction mechanism we proposed involves the steps of four requirements (Fig. 1): 1) H_2-activation is performed in water, 2) electrons from H_2 are stored on the metal (M) center as a low-valent species, 3) the aryl halide is cleaved by oxidative addition to generate an M–C bond, and 4) radical transfer occurs due to the M–C cleavage. Furthermore, the fact that H_2 is inactive during the radical transfer step greatly reduces unwanted side reactions. *These results meet the short- and mid-term milestones "molecular modification of biological and synthetic H_2 and CO_2 catalysts" in Project 1 "Bio-inspired molecular catalysts for fuel and energy generation" of the Thrust's roadmap.*

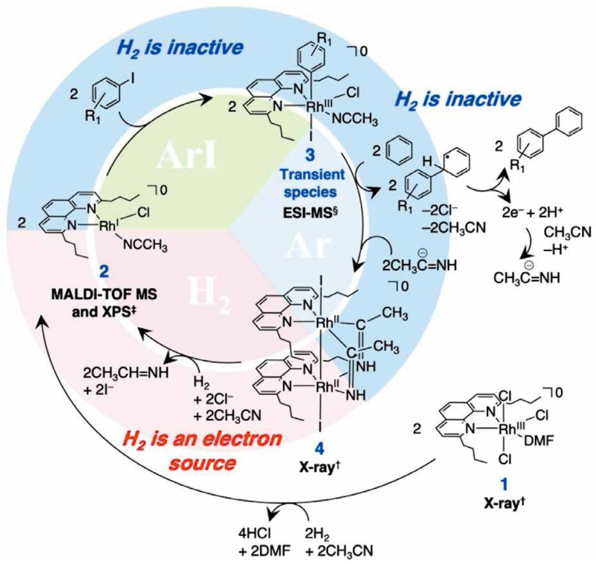


Fig. 1. A proposed reaction mechanism of the direct C–H arylation of benzene using H_2. The structures were determined by X-ray analysis. Complex **2** was characterized by MALDI-TOF MS and XPS. The thermally unstable transient species **3** was observed by ESI-MS.

2. Materials development for hydrogen service (Prof. Macadre)

In this work [2], we combine alloying and grain-refinement to obtain hydrogen-compatible low-Ni austenitic stainless steels. Figure 2 (left) shows that addition of nitrogen, by a process developed by Prof. Tsuchiyama, combined with microstructure refinement (grain size of 120μm after nitrogen addition, grain size of 15μm after refinement with cold-rolling and short normalizing) largely increases the strength of SUS304 and its hydrogen-compatibility. Nitrogen provides solid solution strengthening, grain boundary strengthening, and austenitic phase stabilization, thus replacing nickel to an extent. Grain refinement is an efficient method of increasing the yield stress without compromising ductility. As shown in Fig. 2 (Right), the hydrogen compatibility reaches the same range as stable austenitic steels such as SUS316L or SUS310S, which are recognized as some of the most resistant alloys to hydrogen embrittlement. The hydrogen compatibility is evaluated using two criteria: Nickel equivalent (Ni_{eq}), which is based on the austenite stability (calculated solely with the chemical composition and predicated on the principle that martensitic transformation leads to hydrogen embrittlement) and the Reduced Reduction of Area (*RRA*), obtained from the ratio of the reduction of area with and without hydrogen, which shows the decrease of ductility induced by hydrogen. The lines in Fig. 2. (Right) show the lower boundaries for both *RRA* and Ni_{eq} below which a steel is not hydrogen-compatible. *This effort is directed toward the short-term milestone "alloy design of low-Ni high-SFE austenitic stainless steels" in Project 4 "Material development for hydrogen service" of the Thrust's roadmap.*

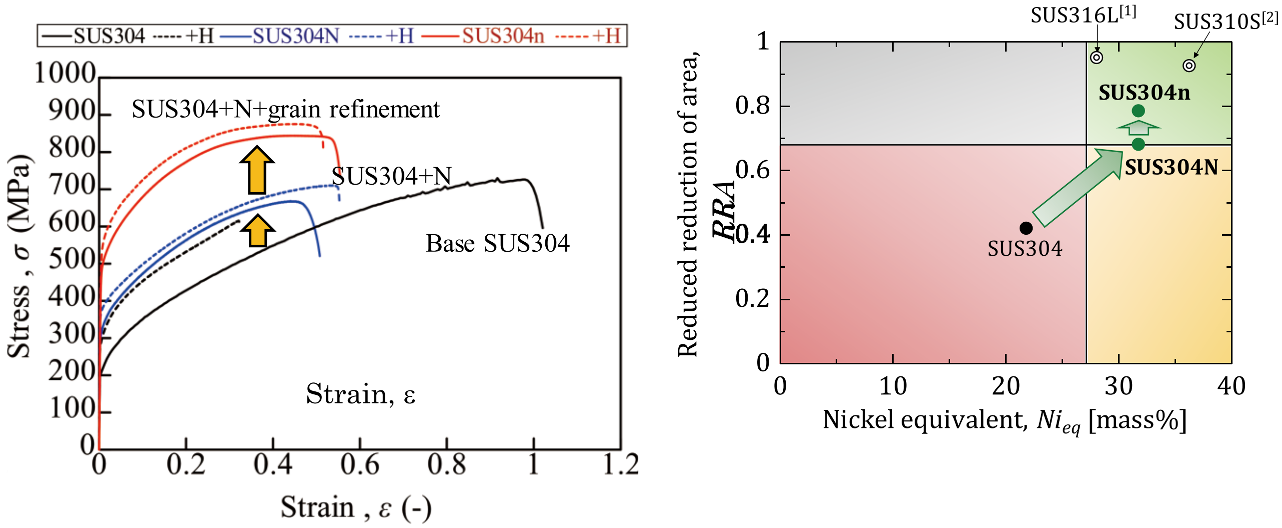


Fig. 2. Left: Tensile properties of SUS304 without hydrogen (straight line) and after exposure to 100 MPa hydrogen gas (dotted line). The addition of nitrogen and grain refinement greatly improve both the strength and the hydrogen compatibility (no hydrogen embrittlement). Right: Evaluation of the hydrogen compatibility with both chemical composition criterion (Nickel equivalent) and ductility criterion (Reduced reduction of area). The combination of nitrogen addition and grain refinement brings the compatibility in the range of SUS316L or SUS310S.

3. Ammonia mitigation and induction effects on hydrogen embrittlement of SCM440 low-alloy steel (PI Kubota and Prof. Komoda)

This work [3] reports two conflicting ammonia (NH_3) effects, namely mitigation of hydrogen embrittlement (HE) and induction of HE during fracture toughness testing of a low alloy steel in NH_3-added hydrogen and nitrogen gases, and the plausible underlying mechanisms of the effects (Fig. 3). The mitigation of HE by NH_3 was achieved by preferential adsorption of NH_3 on the Fe surface resulting in deactivation of catalytic action of the Fe surface for H_2 molecule dissociation into H atoms. In other words, NH_3 mixed in H_2 gas prevented hydrogen uptake in the material, and thus HE was mitigated. On the other hand, NH_3 adsorbed on the catalytic Fe surface was decomposed into hydrogen and other compounds such as NH_2. The created hydrogen induced HE. Whether mitigation or induction of HE is the case is determined by the reaction rates of NH_3 with Fe surface and NH_3 decomposition, respectively. The former is significantly faster than the latter. When the loading rate is high, the crack propagates only under only the NH_3 effect hindering hydrogen uptake, and HE is mitigated. When the loading rate is low, the NH_3 decomposition occurs and hydrogen is supplied during crack propagation resulting in HE. We also investigated the dependence of both effects on the NH_3 concertation. An increase in NH_3 concentration increased the HE mitigation effect by providing higher NH_3 coverage of the Fe surface. This is in contrast to the expectation that a higher NH_3 concentration may increase hydrogen supply, thus increasing the susceptibility to HE. This inverse dependence of HE on NH_3 concentration is due to the fact that vacant sites on the Fe surface adjacent to the NH_3-adsorbed sites are required for the NH_3 decomposition. Increased NH_3 surface coverage reduces the number of vacant sites, which results in less NH_3 decomposition. *This effort is directed toward the short-term milestone "Establish validated physical descriptions of effects of gas impurities on H_2 assisted cracking" in Project 3 "Predictive models of H_2-assisted cracking" of the Thrust's roadmap.*

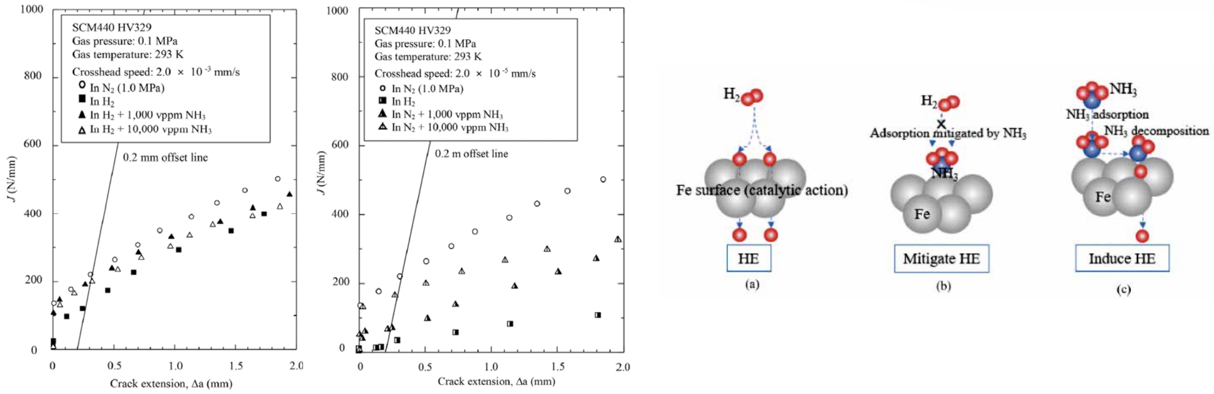


Fig. 3. Results of fracture toughness test in NH_3 mixed H_2 (Left) and NH_3 mixed N_2 (Middle) gases. Reduction in fracture toughness in hydrogen (H_2) gas (■) is mitigated by NH_3 (▲△). In contrast, reduction in fracture toughness is induced by NH_3 (▲△). The role of NH_3 in both conflicting NH_3 effects is graphically explained (Right). (a) Hydrogen embrittlement (HE) in H_2 gas is triggered by H_2 molecule dissociation into H atoms. (b) NH_3 is preferentially adsorbed on the Fe surface. Then, uptake of H_2 molecules by Fe surface is prevented. This results in mitigation of HE. (c) On the other hand, NH_3 adsorbed on the Fe surface is decomposed into H and other compounds such as NH_2. The created H induces HE.

4. The Contribution of textured surfaces to reducing friction in hydrodynamic lubrication (Prof. Yagi and PI Sugimura)

Reduction in friction is one of most crucial issues for energy savings in the field of tribology. The use of artificially textured surfaces is expected to improve lubrication characteristics in a wide range of lubrication regimes from boundary lubrication, elastohydrodynamic lubrication, and hydrodynamic lubrication. Yagi et al. [4] investigated the impact of textured surfaces on the lubrication performance in starved lubrication conditions. A friction test rig including an in-situ observation system was used with controlled lubricant quantity to create point contact between a convex glass lens and rotating steel disc. The in-situ observation system captures the meniscus pattern around the lubricated area as well as optical interferograms of the film thicknesses. Longitudinal or transverse grooves are created on discs, which improve lubricant supply into the lubricated area at high sliding conditions, compared to a flat disc. The results show that textured groove patterns created on the surface improve lubricant oil transport into the lubricated area even in starvation conditions. Mechanisms for improving the lubricant supply through textured patterns are also discussed based on the in-situ observation results. *These results contribute to the short-term milestone "Petroleum-based lubrication" in Project 5 "Low friction and wear technology by control of tribo-interfaces" of the Thrust's roadmap.*

5. Friction and wear of PTFE composites in hydrogen (Prof. Sawae and PI Sugimura)

Single-filler polytetrafluoroethylene (PTFE) composites are widely used as materials for seals and piston rings in hydrogen applications, and their tribological performance greatly affect reliability and durability of the components. Sawae et al. [5] have studied the dependence of friction and wear on salient factors including filler materials, sliding conditions including environmental gas, its purity and temperature, and the mechanisms of the relevant processes. The present study focused on different tribological behaviors with different filler materials in purity-controlled hydrogen. PTFE composites with different filler materials were prepared and their tribological characteristics were evaluated in gaseous hydrogen to investigate the tribological function of each filler material. The results indicate that glass fibers in hydrogen cause severe abrasion on the cast iron sliding counterface and hence increased wear in both the composite and counterface. The friction and wear characteristics of polyphenylene sulphide-filled PTFE in hydrogen are similar to those in ambient air because of the formation of a PTFE-based transfer film on the counterface regardless of the surrounding atmosphere. On the other hand, carbon fibre-filled PTFE exhibit excellent low friction and low wear in hydrogen. In this case, both the composite surface and sliding counterface are covered with carbon-rich tribofilms. *These results contribute to the understanding of the failure mechanism of polymer seals used in hydrogen infrastructure and meet the short-term milestone "Tribo-failure prevention" in Project 5 "Low friction and wear technology by control of tribo-interfaces" of the Thrust's roadmap.*

6. Elucidation of the mechanism for ammonia synthesis via hydrogenation of N_2 on Ru/MgO catalysts (PI Yamauchi and Prof. Noguchi)

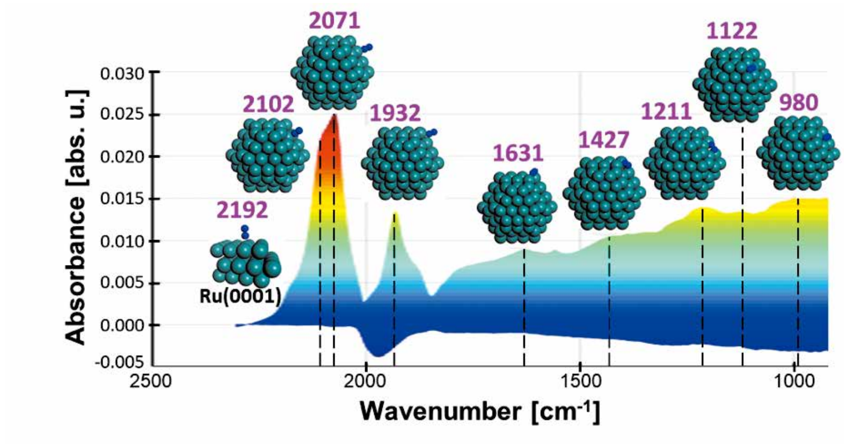
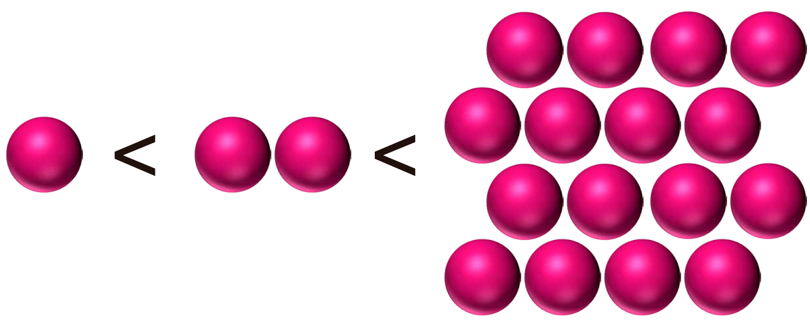


Fig. 4. IR absorbance differences observed for Ru/MgO in the period of 0–78 s after exposure to N_2 gas at 250 °C and the matching DFT-calculated configurations of N_2 chemisorbed on Ru153 and Ru (0001). Values in magenta and green correspond to experimental and DFT-calculated wavenumbers, respectively.

Ammonia is a promising hydrogen carrier, and hence ammonia synthesis catalysts which can efficiently combine nitrogen and hydrogen are highly sought. In this work, we achieved in situ observation of activated nitrogen molecules on a catalyst under reaction conditions for the first time, which would strongly support further improvement of catalytic performance. More specifically, this work [6] reports adsorption states of N_2 and H_2 on Ru nanoparticles supported on MgO under reaction conditions close to those of ammonia synthesis (1 atm, 250 ºC), which was revealed by modulation-excitation infrared spectroscopy and density functional theory calculations using nanoscale Ru particle model (Fig. 4). We first resolved several N_2 adsorption peaks, from which the two highest ones correspond to the molecules' vertical chemisorption on the top and bridge sites. Longer-term observation clearly showed the change in the population from the vertically adsorbed N_2 on the top to the bridge sites of the nanoparticle. Because of the site heterogeneity on the Ru nanoparticle, the remaining lower peaks were assigned to the horizontally adsorbed N_2 having a dipole moment. These peaks correspond to activated N_2 species exhibiting elongated bond distances, and bond orders that could correspond to a lesser double N-N bond caused by the increased charge transfer from the nanoparticle to the N atoms. After its adsorption on the nanoparticle's top sites, the H_2 molecule rapidly dissociates, leading to H atoms strongly binding to the surface and blocking the active sites of the Ru nanoparticle. *This achievement is toward the short-term milestone "R&D for power charge; Fuel regeneration by electroreduction: η=70 %" in Project 2 "Nanomaterials and nanodevices designed for efficient energy & materials conversion" of the Thrust's roadmap.*

7. Surface functionalization and hydrophobization of gold nanoparticles for efficient photoenergy conversion devices (Prof. Takahashi)



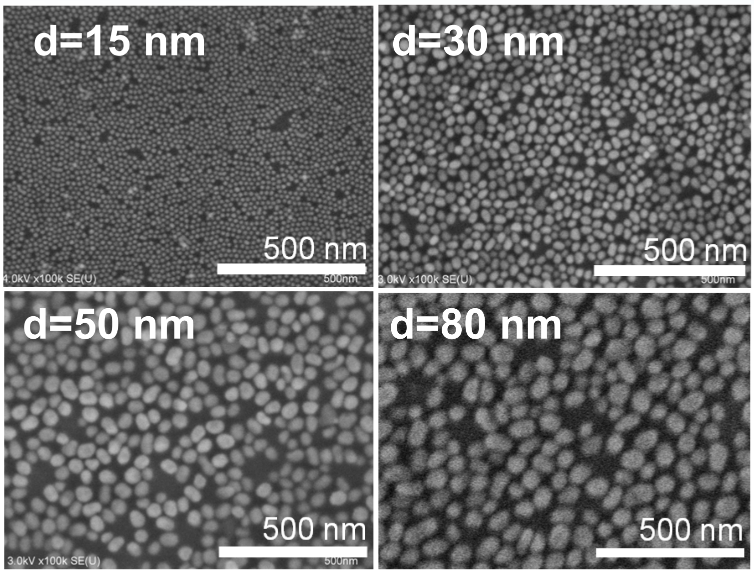


Fig. 5. Enhancement effects based on localized surface plasomon resonance depend on various factors, such as the size and the aggregation state of the plasmonic nanoparticles. A pair plasmonic nanoparticles exhibits larger enhancement effects than single ones. A 2D array of the nanoparticles exhibits much larger effects. 2D arrays of larger plasmonic nanoparticles so far are very effective for photoenergy harvesting.

Theoretical calculations show that order control of metal nanoparticles is an effective approach toward developing photoenergy conversion devices with high efficiencies [7]. This fabrication involving 80nm particles is the first reported worldwide; previous efforts involved nanoparticles only as large as 20nm. We also found localized electric fields of surface plasmon on Raman scattering and luminescence properties of porphyrin dye molecules which were anchored on the surface of ~50nm Au nanoparticles.

Our fabrication approach to controlling the arrangement of particles and dyes at the nano-level holds promise on effectively utilizing the photoenergy-harvesting effect of plasmonic metal nanoparticles (Fig. 5). *These results meet the short-term milestone "Establish novel photoenergy conversion system based on charge separation at the nanointerface" in Project 2 "Nanomaterials and nanodevices designed for efficient energy and materials conversion" of the Thrust's roadmap.*

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Advanced Energy Conversion Systems

1. Toward highly efficient solid oxide protonic electrolysis cells for large-scale hydrogen production (PI Matsumoto and Prof. Leonard)

Hydrogen plays a significant role in many future renewable energy strategies, and the process of steam electrolysis at moderate temperatures (400-600ºC) is a robust approach toward managing the degradation problem in high-temperature electrolysis devices (Fig. 1). The use of ceramic proton-conducting electrolytes provides a promising strategy for electrolysis within this temperature range. However, fabricating this type of electrolytes in a scaled-up manner for industrial use faces a number of obstacles. Fabrication of this class of devices is affected by stresses due to shrinkage mismatch and complications arising from sintering kinetics. Addressing these issues, we focused on fabricating multi-layered devices that can work with excellent efficiency via a cost-effective sequential tape-casting approach. We carefully controlled the starting powder properties and slurry formulation and successfully obtained single cells of dimensions up to 100 mm × 100 mm × 0.5 mm with diminished warping and no cracks during fabrication. In addition, the electrolytes in our half-cell are appropriately dense and gas-tight after co-firing at 1300ºC, which is about 200ºC lower than current sintering temperatures. Figure 1 presents a schematic illustration of a steam electrolysis cell with a proton conductor and a flat 50 × 50 mm^2 $BaZr_{0.44}Ce_{0.36}Y_{0.2}O_{2.9}$ electrolyte cell. The devices could perform excellently at 500 and 600ºC; electrolysis voltage as low as 1.3 V is attainable at a current density of 1 A/cm^2 at 600°C achieving ~83% current efficiency [1]. From this performance, the calculated amount of electricity required to produce 1 $N\text{-}m^3$ of hydrogen is ~3.5 kWh, lower than the 5 kWh necessary for the same amount of hydrogen using ordinary water electrolysis. *These results pave the way for low-cost fabrication of large-sized protonic electrolysis cells and are directed to the midterm milestone of Project 1 "Solid oxide cells for power and fuel generation (Development of highly efficient oxide-ion-conductor-based SOFC and SOEC)."*

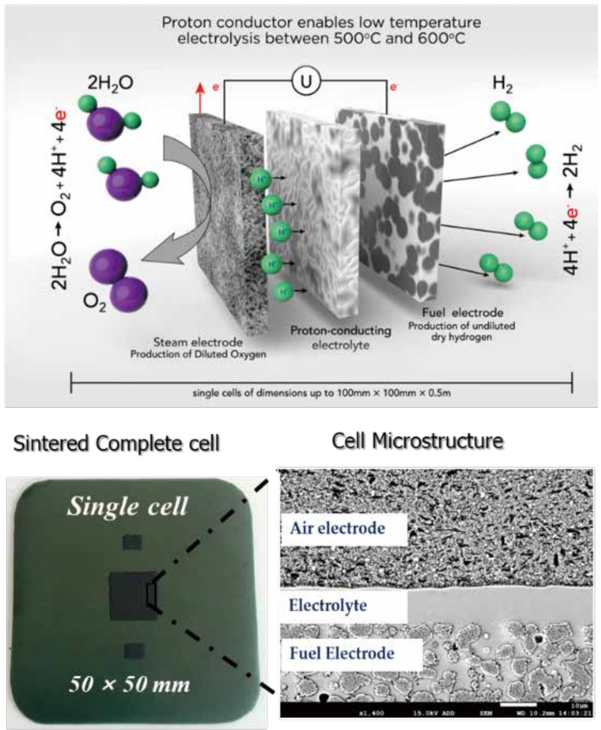

Fig 1. Schematic illustration of a steam electrolysis cell with a proton conductor and a flat 50 × 50 mm^2 electrolyte cell.

2. Tailor-made multi-resonance terminal emitters toward narrowband, high-efficiency, and stable hyperfluorescence organic light-emitting diodes (PI Adachi and Prof. Matsushima)

Recently, there has been a wide variety of studies on thermally activated delayed fluorescence (TADF)-based OLEDs since TADF can realize 100% electron-photon conversion using simple aromatic compounds, indicating the unlimited possibilities of TADF molecular design. Further, hyperfluorescence (HP)-OLEDs in which excitons are generated by TADF and all excitons are transferred to a terminal emitter (TE) have been developed since they can offer the compatibility of high efficiency and narrow spectral width, which is in strong demand for practical display applications. Here we succeeded in our recent cutting-edge HP-OLEDs demonstrating high OLED performance by optimizing host, TADF, and TE molecules [2, 3]. In particular, we focused on the blue emission, which is capable of showing narrow FWHM and high EL quantum yield (Fig. 2). Blue HP-OLEDs based on two new TEs are fabricated, resulting in high external quantum efficiency (EQE) of over 20%, high color purity, and high brightness. In this study, we established a designing principle for a TADF and TE in HP-OLEDs focusing on efficient FRET and no significant carrier trapping. Further, we will demonstrate the enhancement of device durability of HP-OLEDs based on the unique mechanism of active removal of triplets [4] and multi-component EML systems [5]. *These accomplishments represent our initial work in the space of blue OLEDs, under Project 6 for "Light-emitting system with low power consumption" in the Thrust's roadmap.*

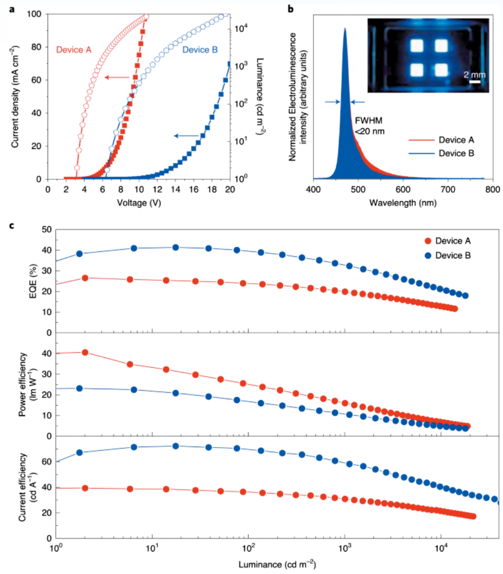

Fig 2. EL performance of hyperfluorescence based OLED.

3. Photo-enhanced ionic conductivity across grain boundaries in polycrystalline ceramics (PI Tuller)

Grain boundary conductivity limitations are ubiquitous in material science. We show that illumination with above-bandgap light can decrease the grain boundary resistance in solid ionic conductors [6]. Specifically, we demonstrate the increase of the grain boundary conductance of a 3 mol% Gd-doped ceria solid oxide electrolyte thin film by a factor approximately 3.5 at 250°C and the reduction of its activation energy from 1.12 to 0.68 eV under illumination (Fig. 3). The presented model predicts that photo-generated electrons decrease the potential barrier heights associated with space charge zones depleted in charge carriers between adjacent grains. The discovered opto-ionic effect could pave the way for the development of new electrochemical storage and conversion technologies operating at lower temperatures and/or higher efficiencies and could be further used for fast and contactless control or diagnosis of ionic conduction in polycrystalline solids. *This accomplishment progresses us toward achieving the short-term and mid-term milestones of Project 1 "Solid oxide cells for power and fuel generation" in the Thrust's roadmap.*

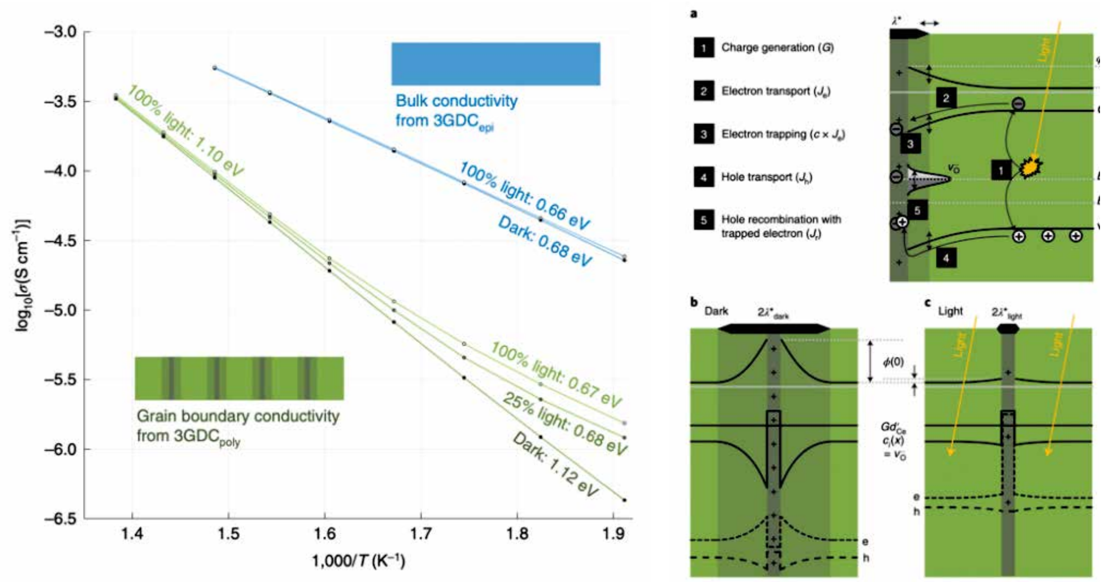

Fig 3. (a) Arrhenius dependence of the ionic conductivity obtained from epitaxial and polycrystalline samples of Gd doped CeO_2 solid electrolyte in the dark and under different levels of illumination; (b) Mechanism of the opto-ionic effect and the consequences for potential distribution and charge carrier concentrations.

4. Perovskite oxynitride semiconductors for photoelectrochemical (PEC) water splitting (PIs Ishihara and Lippert)

Perovskite oxynitride semiconductors have recently attracted significant attention, as promising photoelectrode materials for photoelectrochemical (PEC) water splitting, as demonstrated by the extensive studies of the PEC activity of oxynitride powder-based photoelectrodes and/or deposited thin film electrodes. High crystalline quality, oxynitride thin films grown by physical vapor deposition are ideal for PEC water splitting. Our team studied the fundamental physical and chemical properties of the surface of these materials, including their evolution. In particular, using a combination of high-sensitive low-energy ion scattering (LEIS) and X-ray photoelectron spectroscopy (XPS), we monitored the surface evolution of LaTiOxNy (LTON) and CaNbOxNy (CNON) thin films (Fig. 4) [7]. *These results directly address the short- and mid-term milestones under Project 4 for "Catalyst design for photochemical water splitting" in the Thrust's roadmap.*

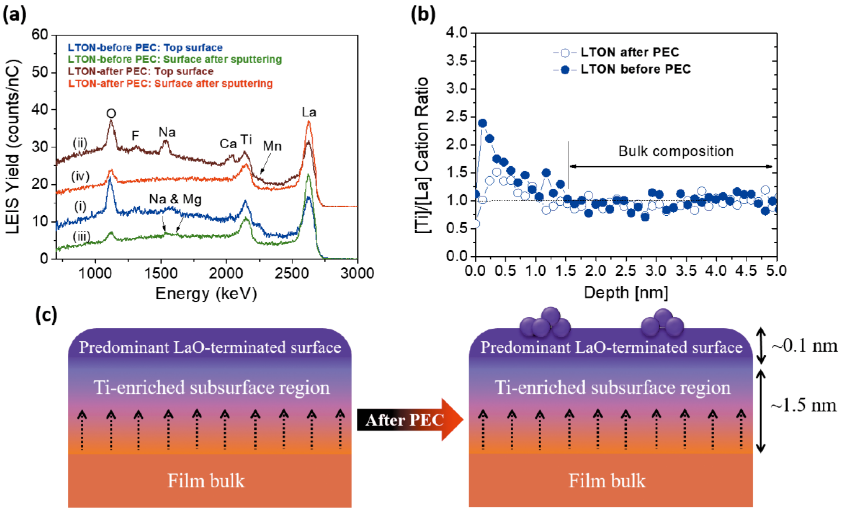

Fig 4. (a) LEIS energy spectra of LTON-(001) epitaxial films, measured by a 3 keV He+ analysis beam on the outer surface of the samples before (i) and after PEC (ii) and after depth profiling of both samples by Ar sputtering. (b) comparison of cation (Ti:La) ratios as a function of depth for LEIS spectra of LTON-(001) films before PEC and after PEC. (c) schematic illustration of compositional variations in near-surface region of the LTON-(001) films before and after PEC measurement.

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Multiscale Science and Engineering for Energy and the Environment

1. Direct air capture by nanomembrane (PI Fujikawa and Prof. Selyanchyn)

Climate change caused by emissions of greenhouse gases into the atmosphere is arguably one of the most important issues for our society. Direct capture of the carbon dioxide (CO_2) from the air (direct air capture, DAC) is one among a variety of negative emission technologies that are expected to keep global warming below 1.5°C, as recommended by the Intergovernmental Panel for Climate Change (IPCC). Current DAC technologies are mainly based on sorbent-based systems where CO_2 is trapped in the solution or on the surface of porous solids covered with compounds with high CO_2 affinity. These processes are currently rather expensive, although the cost is expected to go down as the technologies are developed and deployed at scale.

We discuss the potential of membrane-based DAC (m-DAC) by taking advantage of the state-of-the-art performance of organic polymer membranes [1]. Based on process simulation, we showed that targeted performance for the m-DAC is achievable with competitive energy expenditure. It is shown that application of a multi-stage separation process can enable the preconcentration of atmospheric CO_2 (0.04%) to 40% (Fig. 1). This possibility and combination of the membranes with advanced CO_2 conversion may lead to realistic means for opening a circular CO_2 economy.

This achievement directly addresses the short-term milestone "Development of nanomembrane materials with high CO_2 permeance," in the Project "Capture of CO_2 at multiple concentration levels" of the Thrust's roadmap.

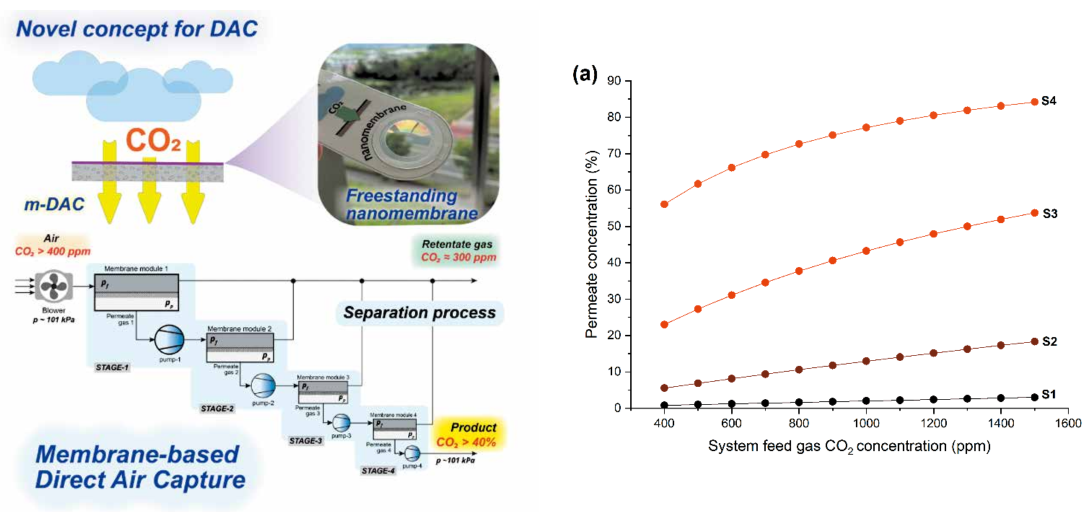


Fig 1. (a) Proposed strategy of direct air capture by 4-stage membrane separation process, (b) Influence of CO_2 content in a surrounding atmosphere (feed gas) on the CO_2 concentration in the product gas at each separation step.

2. Continuous monitoring of injected CO_2 (PI Tsuji and Prof. Ikeda)

Active-source time-lapse (4D) seismic surveys are commonly used to monitor reservoirs of CO_2 storage with high spatial resolution on the basis of variations in seismic velocity. However, the high cost of conventional time-lapse (4D) seismic monitoring (Fig. 2a) typically limits the use of 4D techniques to long time intervals (e.g. 5 years), making it difficult to identify unexpected and rapid changes such as leakage in CO_2 storage reservoirs. To continuously monitor the stored CO_2, we have developed a new continuous monitoring system based on small seismic sources. The source system generates continuous waveforms with a wide frequency range. Because the signal timing is accurately controlled, stacking the continuous waveforms enhances the signal-to-noise ratio, allowing the use of a small seismic source to monitor extensive areas. An active-source system with dimensions of ~1m based on an oscillating mass of ~10 kg (Fig. 2b) has produced a monitoring signal that was detected at a distance of ~80 km and enabled temporal variations of seismic velocity to be identified with an error of <0.01% [2]. The long signal propagation achieved by the permanent active-source monitoring systems allowed us to greatly downsize the source system for monitoring smaller subsurface volumes of kilometer scale. Recently, we have developed minimal (cm-scale) seismic source system [3] for reservoir-scale monitoring (Fig. 2c) and found that the monitoring signal derived from the small seismic source can propagate to 1 km. Therefore, we can use the cm-scale seismic source system for the continuous monitoring of CO_2 storage with low cost. Because of the low cost of the cm-scale seismic source, we can deploy a large number of seismic sources and obtain high-spatial resolution monitoring. Toward this end, we collaborated with four private companies to commercialize this monitoring system.

This achievement is directed toward the short-term milestone "Develop effective monitoring system using continuous source system and fiber optic cable (DAS)" in the Project "Monitoring of CO_2 saturation and pore pressure" of the Thrust's roadmap.

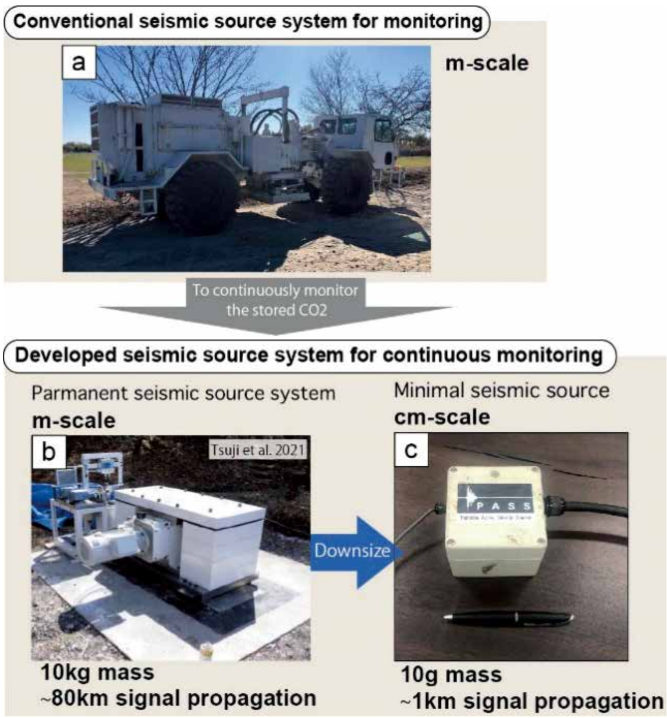


Fig 2. Continuous seismic source system for continuous monitoring. (a) Conventional seismic source system commonly used in the onshore monitoring. Seismic source system for continuous monitoring of CO_2 storage reservoirs in (b) meter-scale [2] and (c) centimeter-scale [3].

3. Modeling of CO_2 leakage for sub-seabed CO_2 storage (PI Tsuji and Prof. Jiang)

A risk associated with sub-seabed CO_2 storage is leakage of the stored CO_2 due to unpredictable reasons such as earthquakes. For such a situation, understanding the hydrodynamics and the complex phase interactions of three-phase systems (CO_2 gas, water, and sediment) is important for estimating the environmental impact on the deep ocean ecosystem due to CO_2 leakage. We developed a sophisticated numerical method to simulate the process of upward migration of leaked gas bubbles through a brine-filled sediment column at the seafloor and elucidate the influence of leak flow rate and interfacial tension on the phenomena. The dimensionless Eötvös (EO) and Weber (WE) numbers can characterize the three different flow regimes (connected finger flow, transition flow, dispersed bubbly flow) during CO_2 leakage (Fig. 3). We found that the surface tension force and the buoyancy force play a major role in determining the CO_2 leakage behavior [4].

This achievement is part of our research in the project titled "Monitoring of CO_2 saturation and pore pressure."

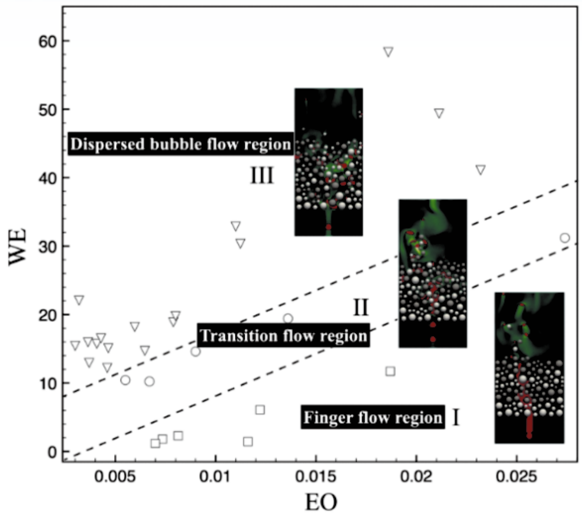
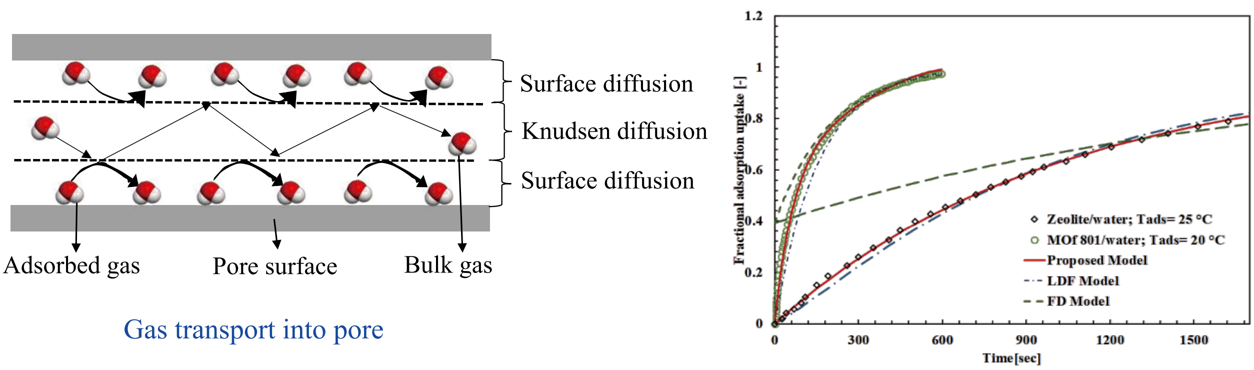


Fig 3. Flow regimes of rising CO_2 bubbles in sediment. The different regions are connected finger flow (square, Region I), transition flow (circle, Region II), and dispersed bubble flow (triangle, Region III). The dashed line indicates the transition boundary, and EO and WE denote respectively the Eötvös and Weber numbers.

4. New model for gas-solid adsorption kinetics (PI Saha)

In achieving carbon neutrality, utilizing energy efficiently is as important as the usage of renewable energy. The gas-solid adsorption phenomenon has been utilized in many applications because it allows for utilization of waste heat as driving force. The two most important features in gas-solid adsorption are the sorption uptake and kinetics. Although there are many models for predicting adsorption isotherms, there is hardly any proper kinetics model which can accurately predict the sorption kinetics. The most significant drawback of traditional kinetics models such as Fickian diffusion, linear driving force, and semi-infinite model has been their time-dependent deviation from experimental data. Based on the widely used linear driving force model, we have developed a new mathematical model [5] which can correlate the experimental adsorption kinetics data more precisely than any other previously published models. The proposed model (Fig. 4) can predict the adsorption dynamics accurately both during the initial unsaturated condition as well as during the later period when the adsorbent is near its saturated condition. Thus, one can use this model for predicting the adsorption system performance for both short and long cycle times. *This effort directly addresses the short-term milestone "Clear understanding of adsorption/desorption process of functional adsorbents" in the Project "Heat mass transfer: adsorption" in the Thrust's roadmap.*



$$\phi(t) = \phi(0) + \{\phi(\infty) - \phi(0)\}\left\{1 - \exp\left(-\left[\frac{t}{(R_p^2/F_0 D_s)}\right]\right)^{mt^2+nt+p}\right\}$$

Time-adapted linear driving force model

Figure 4. Proposed kinetics model and comparison with main-stream models.

5. Lubrication type model for wetting dynamics of multicomponent liquids (PI Takata and Prof. Wang)

Wetting dynamics of multicomponent liquids is crucial in liquid-based energy systems, including absorption heat pumps/transformers as well as desalination and water harvesting systems. Due to the system complexity rooted in multiphase and multicomponent characteristics, the wetting dynamics of these application-oriented working fluids remains poorly understood. Based on the lubrication theory, which has been successfully utilized for the simulation of single component liquids, we developed a comprehensive and efficient model [6] for describing the wetting dynamics of multicomponent liquids (droplets and thin films) with interfacial phase change. We focused on the dynamics of hygroscopic aqueous solution droplets and analyzed the interplay between different physical processes (Fig. 5). Specifically, under the assumption of a precursor film in front of the three-phase contact line, the model is in qualitative agreement with our experimental results, quantitatively with respect to the initial spreading rates and qualitatively with respect to the overall behavior. Depending on the droplet state and the ambient condition, evaporation or vapor absorption occurs. The evaporative/absorptive mass flux varies both spatially and temporally as the droplet approaches equilibrium. It is demonstrated that the dominating mechanisms, i.e. capillary, thermal Marangoni, and solutal Marangoni compete with each other, and lead to diverse droplet dynamics at different stages of evaporation or vapor absorption. The findings shed light on the physical processes within droplets with both positive and negative interfacial mass fluxes and provide rational explanations for the experimental observations. The work paves a methodological base for fully understanding the dominating mechanisms and for optimizing the fluid behaviors, indicating great potentials in efficiency enhancement of liquid-based energy systems. *This effort addresses the short-term milestone "Clear understanding of wettability effects in liquid-vapor phase change" in the Project "Phase change heat transfer" of the Thrust's roadmap.*

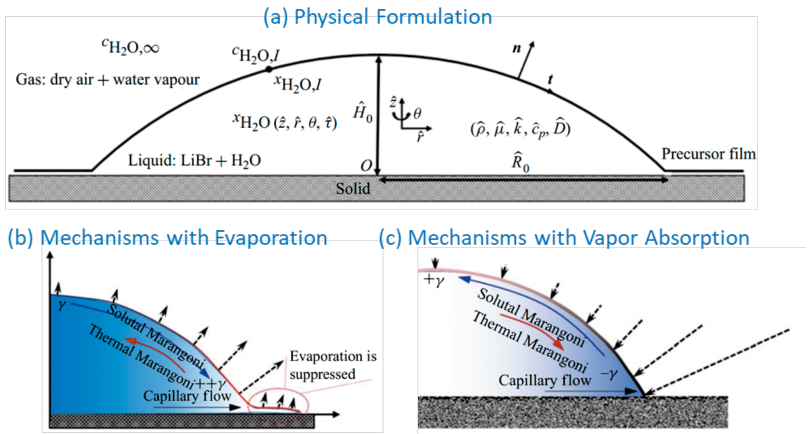


Fig 5. Proposed lubrication-type model for multicomponent droplets with interfacial phase change

6. Global evaluation of the impact of low-carbon energy transitions on social equity (PI Chapman)

A shift toward renewable energy is generally considered positive toward advancing the energy transition, however, very little research has been undertaken to uncover the lifestyle related impacts. Also, it is well known that different nations with different endowments of natural resources and different levels of development will advance their transition at different speeds and using a variety of policy instruments. Even with this understanding, renewable energy deployment is often undertaken under a 'one-size-fits-all' policy approach. By evaluating low-carbon energy transitions in 99 nations, each with a different starting point and trajectory for their transition, over a period of 26 years, we begin to quantify the social impacts of transitions (Fig. 6) and to suggest evidence-based policies, appropriate to each nation's needs. Using indicators relevant to energy policy and the energy transition, five critical social equity impacts of environmental improvement, health, employment, participation, and energy cost are investigated from the viewpoint of an 'equitable' energy transition. We investigate the correlation between quantitative social equity impacts and the shift toward new renewable energy-based electricity (i.e., wind, photovoltaic, geothermal, tidal, biomass etc.) from 1990 to 2015, for 99 nations with differing development levels, energy resources and policies. We find that increased levels of new renewable energy deployment generally accompany social equity improvement, however geography, national income level and complementary energy policies are also important [7]. This study's holistic evaluation of energy transitions and social equity outcomes could be used as an input to proactive policy development contributing to the realization of a more equitable energy transition.

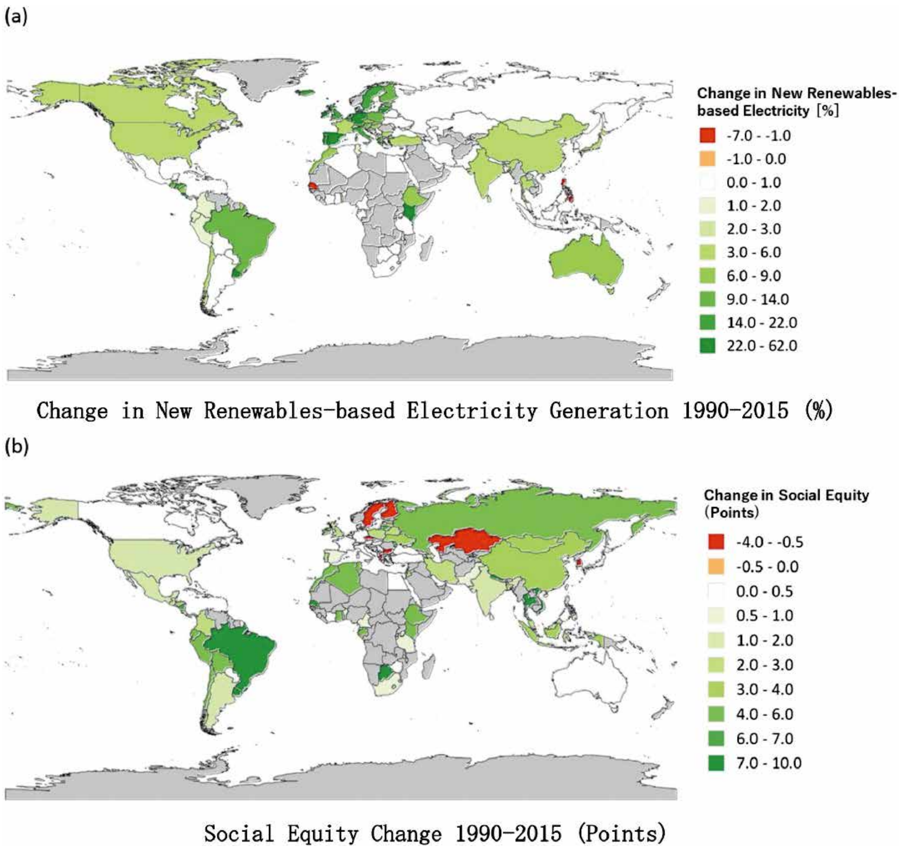


Fig 6. Contrasting (a) the change in RE-based electricity generation and (b) social equity outcomes.

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Advanced Energy Materials

1. Non-conventional octameric structure of C-phycocyanin (PI Ogo and Prof. Yoon)

This work provides the first experimental finding of a new type of light-harvesting protein complex, which has the potential as light-harvesting pigment for a model system of photosynthesis. C-phycocyanin (CPC), a blue pigment protein, is an indispensable component of giant phycobilisomes, which are light-harvesting antenna complexes in cyanobacteria that transfer energy efficiently to photosystems I and II. X-ray crystallographic and electron microscopy (EM) analyses have revealed the structure of CPC to be a closed toroidal hexamer by assembling two trimers. In this study [1], the structural characterization of non-conventional octameric CPC is reported for the first time (Fig. 1). Analyses of the crystal and cryogenic EM structures of the native CPC from filamentous thermophilic cyanobacterium *Thermoleptolyngbya* sp. O-77 unexpectedly illustrated the coexistence of conventional hexamer and novel octamer. In addition, an unusual dimeric state, observed via analytical ultracentrifugation, was postulated to be a key intermediate structure in the assembly of the previously unobserved octamer. These observations provide new insights into the assembly processes of CPCs and the mechanism of energy transfer in the light-harvesting complexes.

Fig 1. Crystal models of hexameric and octameric phycocyanin from a filamentous thermophilic cyanobacterium *Thermoleptolyngbya* sp. O-77. The structural chains of hexameric and octameric phycocyanins are represented by green and cyan ribbon models, respectively. The phycocyanobilins of light harvesting-pigment are represented by gray lines.

Disciplines: Biology, biochemistry, structural biology

2. Effect of gas pressure on hydrogen environment embrittlement of carbon steel A106 in carbon monoxide mixed hydrogen gas (PIs Kubota and Staykov)

In this work, through fracture toughness testing, we characterized the carbon monoxide (CO) effect on the mitigation of hydrogen embrittlement (HE) in conjunction with the hydrogen gas pressure effect for the case of A106 pipeline steel in hydrogen (H_2), nitrogen (N_2), and CO mixed H_2 gases [2]. Mitigation of HE by CO was experimentally confirmed and a critical CO concentration at which HE was suppressed was identified as a function of partial H_2 gas pressure. The critical CO concentration increased with increasing H_2 partial pressure (Fig. 2. Left). Molecular dynamics (MD) simulations based on surface chemistry were conducted to interpret this trend. The MD simulations revealed that the dissociation rate of H_2 molecules to atomic hydrogen on the Fe surface significantly increases with increasing gas pressure, whereas the adsorption rate of CO on the Fe surface was almost independent of the gas pressure (Fig. 2, Middle and Right). These results indicate that the increase in the gas pressure promotes hydrogen uptake in the material, which accounts for the experimental results showing that the CO concentration at which complete HE prevention is achieved increases with the elevation of the gas pressure.

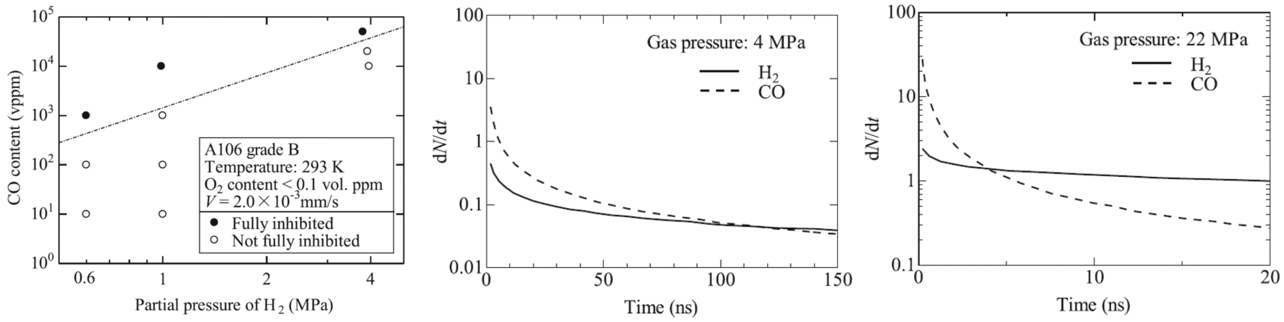

Fig 2. Critical CO concentration required for HE mitigation (Left). Higher CO concertation is needed to achieve mitigation of HE when H_2 partial pressure increases. Results of molecular dynamics simulations that show the changing of reaction rate (d*N* /d*t*) of H_2 or CO (Middle and right) with the change in environmental gas pressure are shown in the figures on the middle and right. The crossing point of CO and H_2 lines moves to the left with increasing gas pressure. This means that CO mitigating effect is weakened with an increase in gas pressure.

Disciplines: Hydrogen embrittlement, mechanics of materials, surface chemistry, theoretical chemistry

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Advanced Energy Conversion Systems

1. Electro-chemo-mechanics (PI Tuller)

Understanding complex chemo-mechanical relationships is crucial for understanding and avoiding failures in any solid-oxide-cell-based electrochemical devices. Electro-chemo-mechanics studies at I²CNER and MIT by the team of PI Tuller previously identified the atomistic origins of chemical expansion and discovered factors that can be used to tailor it. This has led to rational design of energy conversion materials with enhanced durability and innovation of new characterization techniques (surface science, optical spectroscopy, crystallography, high temperature electrochemistry, and computational materials science). PI Tuller and his team investigated the impact of strain on ion migration [1] in solid oxide electrolytes with the ultimate objective of determining if this approach can be used to further improve electrolyte conductivity and therefore performance [2].

Disciplines: electrochemistry, mechanics, materials science, surface science, crystallography, microstructural characterization

References

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Multiscale Science and Engineering for Energy and the Environment

1. Mechanical strengthening of membrane (PI Fujikawa)

Nanometer-thick films are promising technology on enhancing the performance of membrane gas separation. However, membrane thinning decreases the mechanical toughness and leads to membrane breaking and crack formation. Improvement of mechanical properties of nanomembranes has been pursued in I²CNER and industrial partners by PI Fujikawa and Dr. Kunitake. It has been found that incorporation of cellulose nanofibers under a nanomembrane enhances its mechanical durability [1]. Robust, nanometer-thick, permselective membranes were developed by composite formation from poly(dimethylsiloxane) (PDMS) and cellulose nanofibers (CNF).

Their unique behavior is discussed in relation to that of a single-component PDMS nanomembrane. In the absence of the CNF component, the PDMS nanomembrane with a thickness of 34 nm displays ultrahigh permeability of CO_2 gas, which is only ca. one order of magnitude smaller than that of free-flowing gases through a porous poly(acrylonitrile) support film (PAN, thickness 150 μm). The constant CO_2/N_2 selectivity observed for the whole range of membrane thickness (34 nm–10 μm) suggests that in the single-component membrane, the kinetic process at the membrane surface determines the permselective behavior. Multilayered composite membranes are obtainable by repeated spin coating. The mechanical weakness of the single-component PDMS membrane is improved by complexation with CNF, as confirmed by the bulge test and the ease of macroscopic handling. Such a robust PDMS–CNF nanomembrane gives superior permeation of 50,000 GPU with a defect-free PDMS layer of ca. 17 nm thickness. Interestingly, the permeation characteristics of the composite membrane are strongly affected by the asymmetric arrangement of PDMS and CNF layers, and the gas permeation from the side of the CNF layer is drastically reduced. The PDMS composite membrane is expected to provide practically useful systems as a means of direct air capture.

Disciplines: Polymer chemistry, surface science, nanomaterial chemistry

2. Perovskite-based bidirectional optical wireless power transfer systems (Profs. Hoa and Matsushima, PI Adachi)

Optical power transfer provides a way of transmitting power through long distances without using wires. This is done by means of optical waves, in which solar cells serve as optical receivers converting optical energy to electricity (Fig. 1). In our proposed novel system of bidirectional optical wireless power transfer, solar cells are employed as optical transceivers, i.e. devices capable of both absorbing and emitting light. To achieve that, perovskite solar cells are selected owing to their numerous advantages including small Stokes shift that make them suitable to be optical transceivers.

In this work, a novel optical wireless power transfer was proposed [3], for the first time, where a single device – an optical transceiver – was used for both absorption and emission of light. As a result, the system structure, weight, size, and cost can be reduced. This optical transceiver was made from metal halide perovskite fabricated by the groups of Matsushima and Adachi. Various characteristics of this perovskite transceiver were measured including the absorbance, photoluminescence spectra, time-resolved transient photoluminescence curve, quantum yield, I-V curve and luminance-voltage curve in the light emitting mode, quantum efficiency, and incident photon-to-electron conversion efficiency (IPCE). The overlapped electroluminescence and IPCE curves show that our perovskite device can indeed work in both light receiving and emitting modes, i.e. the proposed system is viable. This was again experimentally verified by using two perovskite devices put in parallel at a distance of 1 cm, with one worked in the pulse light emitting mode while the other worked in the light absorption mode. The measured output of the perovskite receiver had the same form with that of the perovskite transmitter, hence experimentally validated our proposed system. Lastly, a mathematical model for representing the overall system power conversion efficiency (PCE) was developed.

The proposed novel system in [3] was then further analyzed in [4] to test the system's performance and the mathematical model's prediction of the system's PCE under various working conditions. It turned out that PCE predictions were satisfactory even when the two perovskite transceivers were misaligned or rotated but predictions were not accurate if collimating lens was used to focus the light emitted from one perovskite cell. Accordingly, a data-driven mathematical model in the form of a ratio of polynomials was proposed and validated to capture the system PCE when a collimating lens was utilized and when perovskite transceivers were misaligned or rotated.

This research is at the intersection of materials science, photonics, and power and energy systems. It has a great potential to be used in a vast number of applications including internet of things (IoT) devices, wearables and consumer electronics, transportation electrification, and wireless power networks.

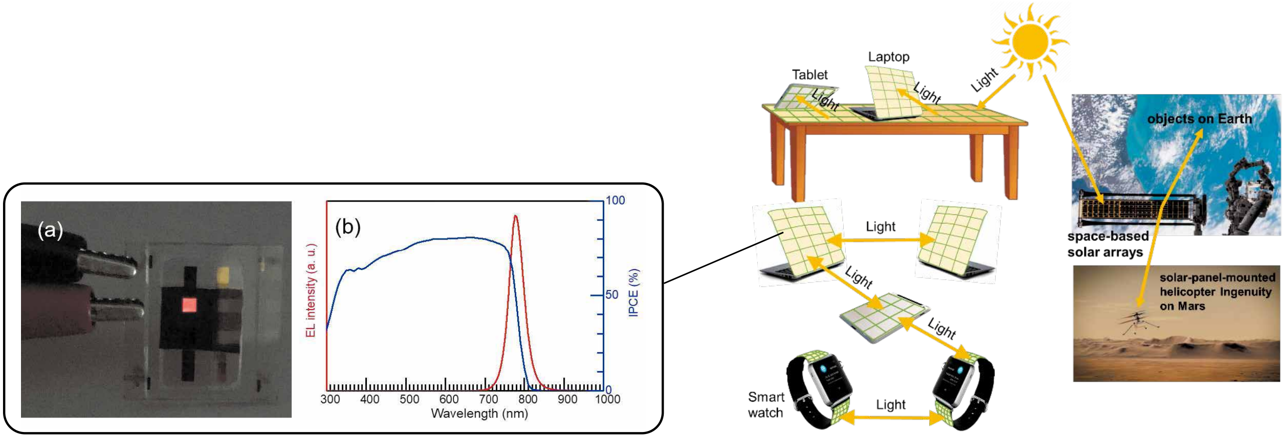
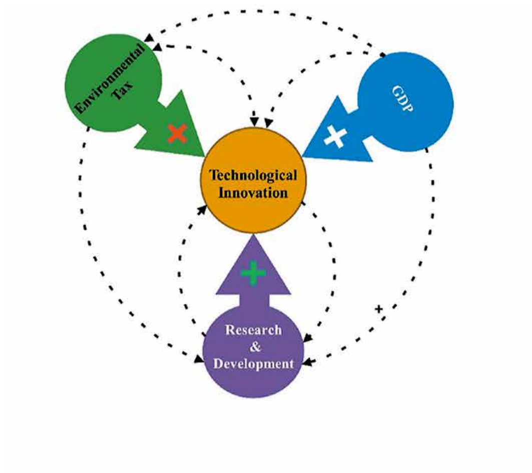


Fig 1. Illustration for perovskite-based bidirectional optical wireless power transfer systems.

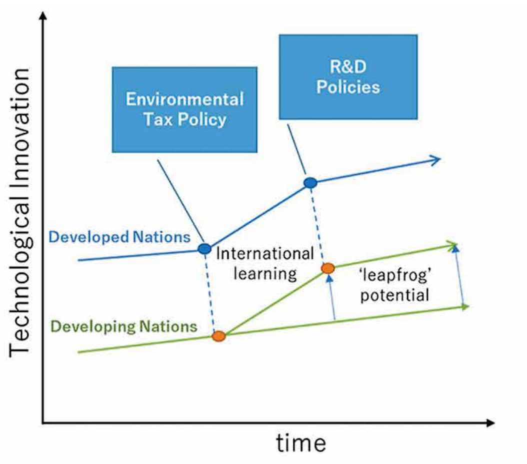
Disciplines: Photochemistry, mathematics

3. Econometric evaluation of environmental taxes on innovation (PIs Chapman and Saha)

Several studies have investigated the effect of environmental taxes on economic growth and carbon emissions. However, limited studies have quantitatively identified the connection between environmental taxes and technological innovations. In this collaboration between energy analysis and energy economics thinking, robust statistical methods are applied to this issue to identify the positive linkage between environmental taxes and innovation, especially in developed economics.



Long-run relationship between technological innovation and environmental taxes



Potential innovation 'leapfrog' benefits for developing nations

Fig 2. Long run relationships on technological innovation (left) and the desired leapfrog effect for developing nations (right).

Toward this goal, we developed a model [5] which consists of panel cointegration analysis considering the cross-sectional dependence, applied to quantify the effects of environmental taxes on environment-related technological innovation in high and middle-income 42 countries from 1995 to 2018 (Fig. 2, left). The long-run results suggest that environmental taxes stimulate technological innovation; for example, a 1% increase in environmental taxes was found to increase environment-related technological innovation by 0.57 and 0.78% on average for high and middle-income countries using the common correlated effects mean group (CCEMG) and augmented mean group (AMG) techniques, respectively. The policy implications of this study suggest that imposing environmental taxes can accelerate the advancement of environmental-related technologies for reducing carbon emission and sustainable development in high and middle-income nations, with possible applications in a broad range of nations, particularly as an evidence base for developing nations to shorten energy transition timelines (Fig. 2, right). It is hoped that these findings can be applied to developing economies to enable a 'leap-frog' impact on furthering the energy transition.

Disciplines: Energy Analysis, Econometrics

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Returning Results to Society

The relevance of I²CNER's research efforts and objectives in FY2021 toward enabling the green innovation initiative of the government of Japan is evidenced through 20 new collaborative projects with industry as well as 4 new or continued projects that resulted in technology transfer events. A detailed list of all the I²CNER Technology Transfer Events is outlined in the report "Technology Transfer Summary: I²CNER's Interaction With and Impact on Industry." During the calendar year 2021, I²CNER filed for 17 patents, and was granted 16, bringing the total number of patent applications since inception to 355 and patents awarded to 118.

The technology transfer that occurred in FY21 includes:

1. PI. S. Fujikawa provided consulting services to several companies on the development of technologies for mass-production of CO_2 separation nanomembranes.

The I²CNER research team of PI Fujikawa has developed the world's thinnest CO_2 separation nanomembranes with ultrahigh gas permeance. This technology underlies the development of CO_2 capture systems at scale and it is an essential tool in combating global warming. To accelerate the societal implementation of these nanomembrane-based CO_2 capture systems, I²CNER has established collaborative relationships with a number of industrial partners for the development of roll-to-roll mass production processes for CO_2 capture membranes.

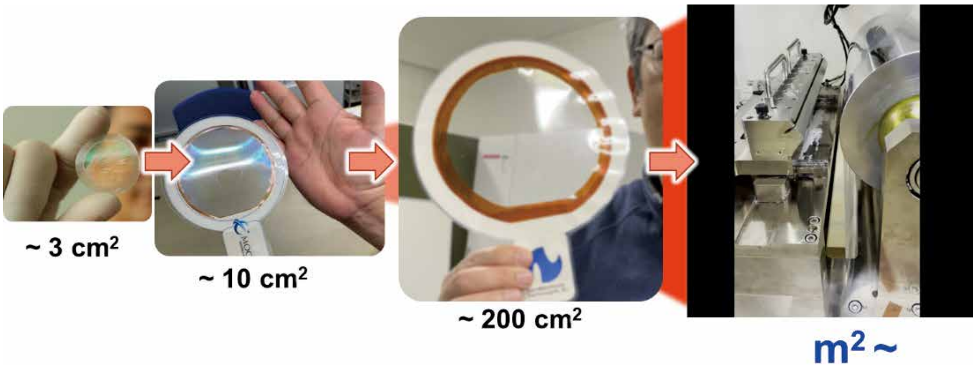


Fig 1. Enlargement of CO_2 separation membranes toward mass-production of nanomembranes.

2. Scaled-up production of polymer-wrapped carbon-based catalyst for industrial fuel cell application (PI T. Fujigaya).

The technology gap between lab-scale synthesis and industrial-scale production is always an issue for the insertion of advanced new catalysts into practical fuel cell applications. By optimizing the synthesis process, we succeeded in scaling-up the process of production of the polymer-wrapped catalysts from 10 mg/day to 0.1 kg/day. This production rate is sufficient for real-world fuel cell applications and the production protocols have been shared with a number of industrial partners who are participating in our pilot program.

Fig 2. Polymer-wrapped catalyst prepared from industry-scale production (left: 0.1 kg) vs lab-scale synthesis (right: 10 mg).

3. Preparation of Tubular Solid Oxide Reversible Cell for CO_2 reduction transferred to IHI (PI. Ishihara)

Fabrication method of tubular type solid oxide cells using LSGM thin film by dip coating was transferred to IHI. Measurement procedure for steam and CO_2 high temperature electrolysis was also provided. This collaboration is continued in FY22 for reduction of CO_2 from power generator.

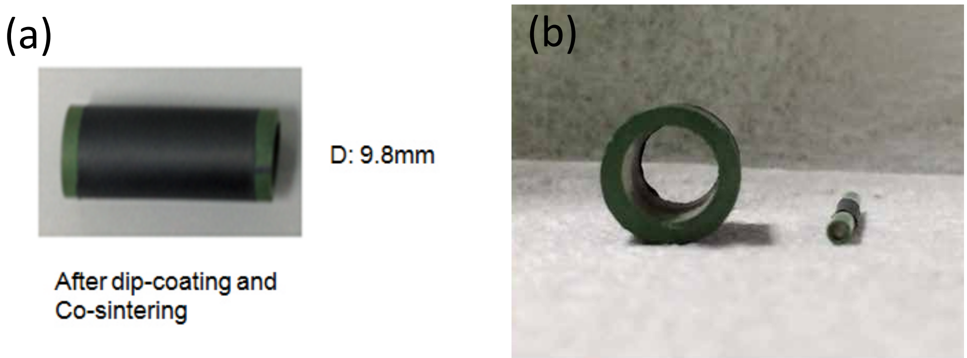


Fig 3. Photograph of the fabricated tubular type SORC for CO_2-H_2O or CO_2 high temperature electrolysis by dip coating: (a) view from above, and (b) side view.

4. PI A. Staykov and Professor Y. Fukumoto (Institute of Mathematics for Industry) with DAICEL corporation for automatized discovery of polymers with desired functionality.

Prof. Staykov (I^{2}CNER) and Fukumoto (IMI) continued their industrial collaboration with DAICEL on design and development of AI-based ML algorithm for fully automatized polymer design based on ring opening reaction of lactone monomers. In the earlier years of this collaboration, optimization of the monomers was achieved. In 2022 the entire polymer design was addressed. The project is in its final phase with the algorithm being successfully designed and tested in DAICEL in October 2022. At this stage we are finalizing the automatization of the software which is expected to be transferred to DAICEL in 2023. Our algorithm (summarized in Fig. 4) could successfully predict reaction rates of compounds synthesized in the DAICAL laboratory with very good agreement with the industrial data. In the next stage, our algorithm will be applied to generate new monomers with expected high reaction rate which will be used in the research and development department of DAICEL and proposed to the industrial facilities. Upon competition of the current project, the joint research of Profs. Staykov and Fukumoto with DAICEL will continue and plans are already underway.

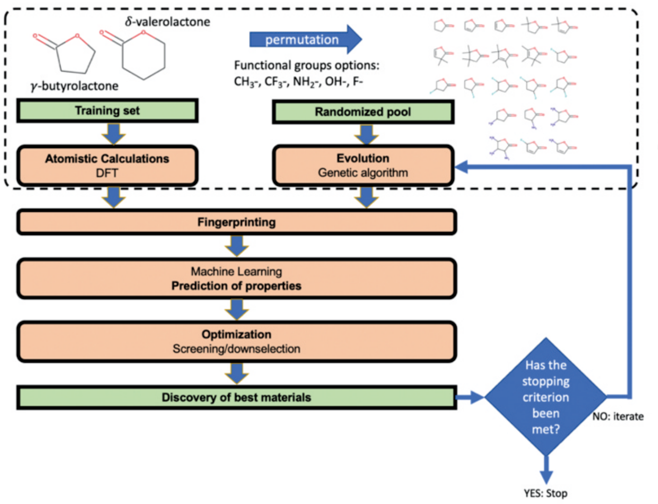


Fig 4. Block diagram of the artificial intelligence machine learning applied on lactone molecules. The algorithm contains autonomous DFT simulation engine, evolutionally tool for selective molecule breeding, machine learning tool for molecular screening, and iterative procedure for structure optimization.

Network of International Collaborations

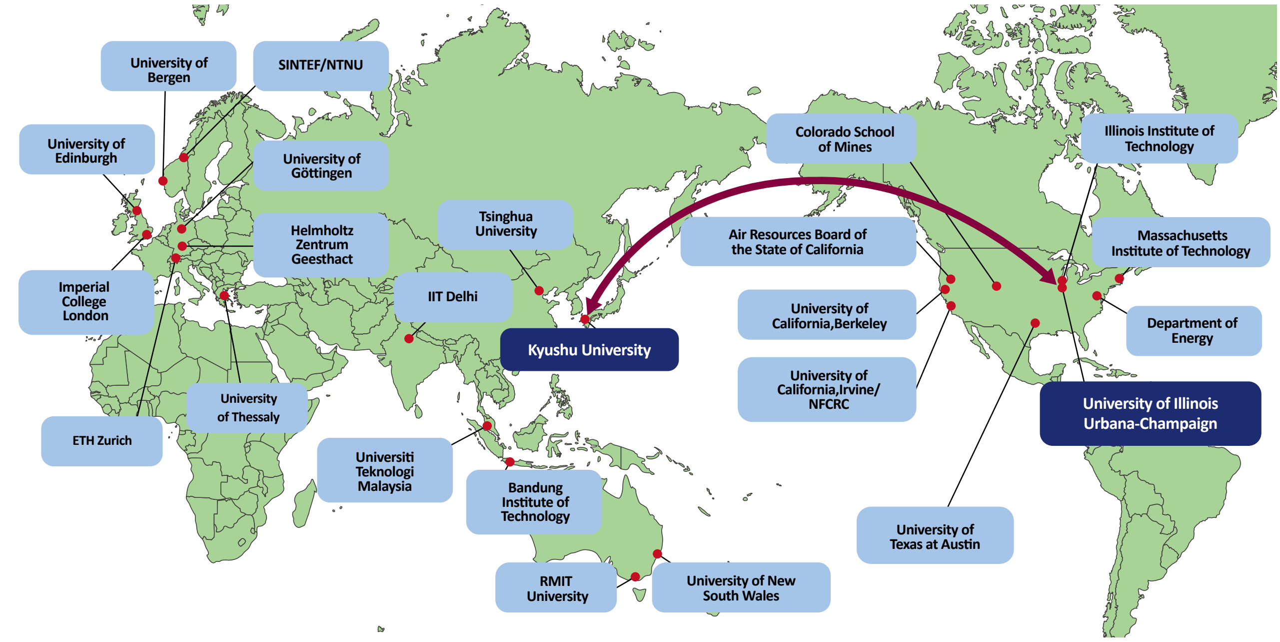
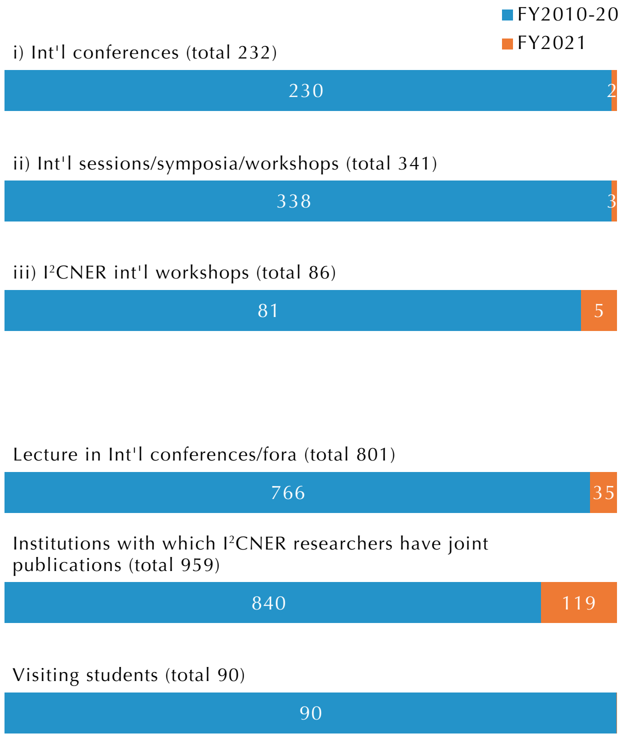


Figure 9. This map includes the home institutions of I²CNER's foreign WPI faculty as well as those institutions with which I²CNER has academic agreements.

Globalization by the Numbers

In FY2021, despite the limitations of the COVID-19 pandemic, there were a significant number 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 2 international conferences (232 in total since inception); 3 international conference sessions/symposia or workshops (341 since inception); and 5 I²CNER international workshops (86 since inception).
- Our researchers have given 35 keynote, plenary, and invited presentations in international conferences and fora (801 since inception).
- Our researchers have joint publications with researchers from 119 new institutions (959 in total since inception).
- Between its inception and March 31, 2022, the Institute has hosted a total of 90 graduate and undergraduate students from various institutions around the world, including Illinois. The numbers of visiting students each year include: 1 (FY2010), 9 (FY2011), 6 (FY2012), 7 (FY2013), 7 (FY2014), 6 (FY2015), 10 (FY2016), 17 (FY2017), 10 (FY2018), and 17 (FY2019). Of these, 63 stayed for more than a month at KU. Of the 90 total visiting students, 44 students were from Illinois and 29 stayed for more than one month. *In FY2020 and 2021, due to COVID-19, there were no students visiting from overseas.*



The international collaborations that occurred with each Thrust during FY21 include:

Advanced Energy Conversion Systems Thrust:

A. Clausthal University of Technology, Institute of Energy Research and Physical Technologies, Goslar, Germany (PI Tuller, H. Fritze): Demonstrated ability to investigate chemical expansion in oxides in a non-contact mode at elevated temperatures on the pico-meter scale.

- H. Wulfmeier, D. Kohlmann, T. Defferriere, C. Steiner, R. Moos, H. L. Tuller, and H. Fritze, "Thin-Film Chemical Expansion of Ceria based Solid Solutions: Laser Vibrometry Study," *Zeitschrift für Physikalische Chemie*, 41pp (2021). DOI: https://doi.org/10.1515/zpch-2021-3125.

B. Huazhong University of Science and Technology, School of Environment and Science Engineering (PI Ishihara, L. Guo): Development of CO_2 hydrogenation catalyst as well as VOC oxidation catalyst, and analysis of surface composition and reaction mechanism.

- Yu Wang, Ji Wu, Gang Wang, Dengyao Yang, Tatsumi Ishihara, Limin Guo, "Oxygen vacancy engineering in Fe doped akhtenskite-type MnO2 for low-temperature toluene oxidation," *Applied Catalysis* B: Environmental, 285, 119873, (2021).

C. University of Illinois Urbana-Champaign, Imperial College London, and UC Berkeley (PI Ishihara, L. Martin): Preparation of oriented perovskite film with laser ablation method and surface outmost layer composition was analyzed with low energy ion scattering.

- Ran Gao, Abel Fernandez, Tanmoy Chakraborty, Aileen Luo, David Pesquera, Sujit Das, Gabriel Velarde, Vincent Thoréton, John Kilner, Tatsumi Ishihara, Slavomír Nemšák, Ethan J. Crumlin, Elif Ertekin, and Lane W. Martin, "Correlating Surface Crystal Orientation and Gas Kinetics in Perovskite Oxide Electrodes," *Advanced Materials*, 33, 2100977, (2021) DOI: 10.1002/adma.202100977.

Advanced Energy Materials Thrust:

A. University of Gottingen (C. Volkert, R. Kirchheim, M. Kubota, P. Sofronis): Study of crack initiation in a low alloy steel. Following the joint publication in 2020 on macroscopic mechanical testing of hydrogen embrittlement (Proc. ISOPE 2020, ISBN 978-1-880653-84-5), we continued on with microscopic mechanical testing in a transmission electron microscope and in-situ observation of crack initiation. This series of studies aims to bridge the hydrogen embrittlement mechanisms as they are observed at the microscale and manifested at the macroscale toward the development of predictive models of H_2-assist cracking.

- Lin Tian, Christine Borchers, Masanobu Kubota, Petros Sofronis, Reiner Kirchheim, Cynthia A. Volkert, "A study of crack initiation in a low alloy steel," *Acta Materialia*, 223, 117474, (2022).

B. Universiti Teknologi Malaysia (L. Shahira, Y. Sawae): Fundamental studies of the reinforcing effect of graphene-based materials filled into ultrahigh molecular weight polyethylene for orthopedic applications. We aim to develop novel high-performance UHMWPE-based polymer composites with high mechanical strength, high wear resistance and low friction coefficient by using graphene-based materials as reinforcing nano-fillers. We defined the orthopedic implant as a target application of developed composites and used a multidirectional sliding tester and diluted bovine serum to simulate the tribological condition of artificial hip joints and evaluate friction and wear characteristics of composites.

- N.H. Shahemi, S. Liza, Y. Sawae, T. Morita, K. Fukuda, Y. Yaakob, "The relations between wear behavior and basic material properties of graphene-based materials reinforced ultrahigh molecular weight polyethylene," *Polymers for Advanced Technologies*, 32(11), 4263-4281, (2021).

C. Slovak Academy of Sciences (F. Lofaj, H. Tanaka, Y. Sawae): Fundamental studies of the tribological performance of HiPIMS W-C:H coatings in various environments. We aim to understand tribo-chemical reactions between HiPIMS W-C:H coatings and gaseous environments during sliding, and their effects on the transfer film formation on the sliding counterface and the associated tribological performance of coatings.

- F. Lofaj, H. Tanaka, R. Bureš, Y. Sawae, M. Kábatová, K. Fukuda, "The effect of humidity on friction behavior of hydrogenated HIPIMS W-C:H coatings," *Surface and Coating Technology*, 428, 127899, (2021).
- F. Lofaj, R. Bureš, M. Kábatová, H. Tanaka, Y. Sawae, "Modelling of tribo-chemical reactions in HiPIMS W-C:H coatings during friction in different environments," *Surface and Coating Technology*, 434, 128238, (2022).

D. Indian Institute of Technology Delhi (S.K. Sinha, Y. Sawae): Development of novel bio-lubricant-filled wear resistant and high strength polymer composite. This international collaboration was financially supported by a JSPS bilateral program from June 2018 to March 2020. We aim to develop novel high-performance epoxy-based polymer composites with high mechanical strength, high wear resistance and low friction coefficient by using biological lubricants which were inferred from biotribology studies on synovial joint lubrication. We defined the orthopedic implant as a target application of developed composites and used a multidirectional sliding tester and diluted bovine serum to simulate the tribological condition of artificial hip joints and evaluate friction and wear characteristics of composites.

- J.K. Hirwani, R. Nishimura, H. Shinmori, T. Morita, Y. Sawae, S.K. Sinha, "Epoxy (SU-8) polymer composites with Ultra-high molecular weight polyethylene and Hyaluronic acid fillers for hip prosthetic implant application," *Tribology International*, 167, 107399, (2022).

E. SINTEF and Norwegian University of Science and Technology (V. Orden, R. Johnsen, H. Matsunaga, and M. Kubota): The main goal of the project is to continue, strengthen and expand the collaboration in education and research between Norway and Japan in the field of hydrogen-materials interaction. The partnership involves development of joint courses, researcher exchange and creation of arenas for competence sharing. Student and young researcher exchange has been suspended this year due to Covid-19 pandemic.

Multiscale Science and Engineering for Energy and the Environment Thrust:

A. University of Waterloo (S. Mitra, K. Takahashi): Development of a 3D measurement method for probing the condensation dynamics of low surface tension droplets. This aims at the short-term milestone. "Clarification of the best suitable adsorbent and refrigerant combination for adsorption heat pump and refrigeration systems," of project "Thermal Energy Systems 1: Heat-driven adsorption heat pump/ refrigeration system" in the Thrust's roadmap.

- Irshendu Misra, Hideaki Teshima, Koji Takahashi, Sushanta K. Mitra, "Reflected Laser Interferometry: A Versatile Tool to Probe Condensation of Low-Surface-Tension Droplets," *Langmuir*, Vol. 37, pp. 8073-8082, 2021.

B. Osaka University (Y. Yamaguchi, H. Teshima): Fundamental understanding of interfacial tensions of surface nanobubbles. This effort aims at the short-term milestone "Clarification of the best suitable adsorbent and refrigerant combination for adsorption heat pump and refrigeration systems," of project "Thermal Energy Systems 1: Heat-driven adsorption heat pump/ refrigeration system" in the Thrust's roadmap.

- Hideaki Teshima, Hiroki Kusudo, Carlos Bistafa, Yasutaka Yamaguchi, "Quantifying interfacial tensions of surface nanobubbles: How far can Young's equation explain?" *Nanoscale*, Vol. 14, pp. 2446-2455(2022).

C. National Renewable Energy Laboratory (Taichi Kuroki, Naoya Sakoda): Themodynamic modeling of hydrogen tank. This effort aims at the short-term milestone "Optimization of H_2 station deployment considering user preference," of project "Hydrogen Fuel Station Research" in the Thrust's roadmap.

- Taichi Kuroki, Kazunori Nagasawa, Michael Peters, Daniel Leighton, Jennifer Kurtz, Naoya Sakoda, Masanori Monde, Yasuyuki Takata, "Thermodynamic Modeling of Hydrogen Fueling Process from High-Pressure Storage Tank to Vehicle Tank", *International Journal of Hydrogen Energy*, Vol. 46, pp. 22004-22017(2021).

D. Tsinghua University (Weigang Ma, Naoya Sakoda): Review of thermophysical property. This effort aims at the short-term milestone "Understanding of turbulent-chemistry interaction by experiment and numerical examination," of project "High Efficiency Power Generation System" in the Thrust's roadmap.

- Siyuan Cheng, Fengyi Li, Fei Shang, Weigang Ma, Hui Jin, Naoya Sakoda, Xing Zhang, Liejin Guo, "A Review of Experimental Researches on the Thermophysical Properties of Hydrogen-Containing Mixtures at High Temperatures and High Pressures," *Journal of Chemical and Engineering Data*, Vol. 66, pp. 3361-3385, 2021.

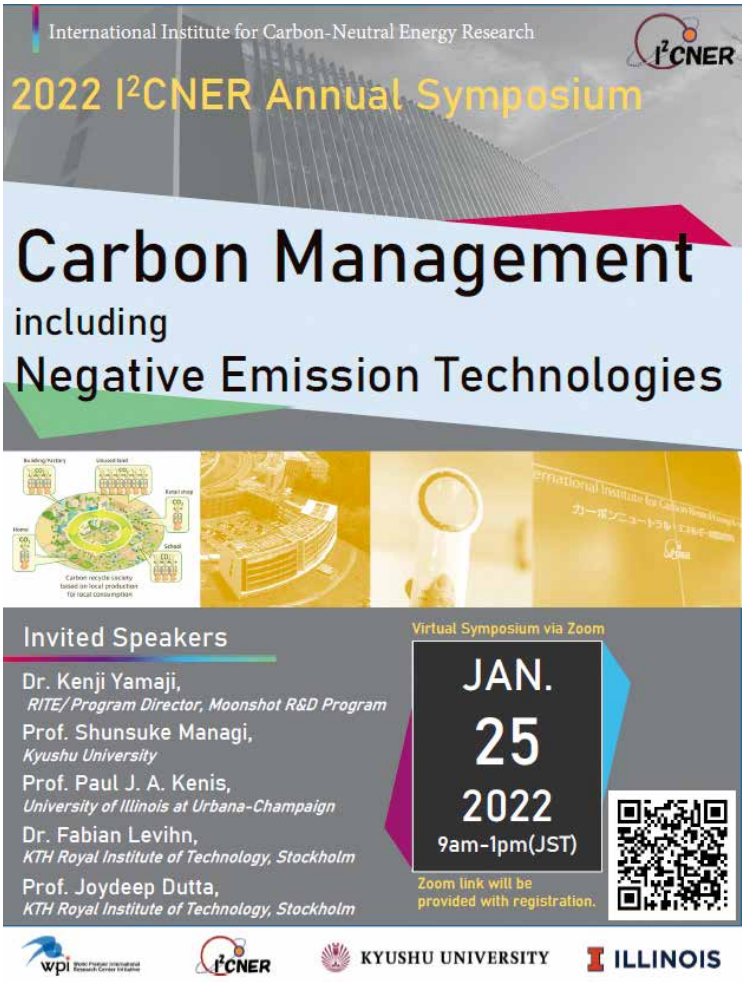
E. University of Edinburgh (K. Sefiane, Zhenying Wang): Fundamental understanding of wetting and evaporation of multicomponent droplets. This effort aims at the short-term milestone "Clarification of the best suitable adsorbent and refrigerant combination for adsorption heat pump and refrigeration systems," of project "Thermal Energy Systems 1: Heat-driven adsorption heat pump/ refrigeration system" in the Thrust's roadmap.

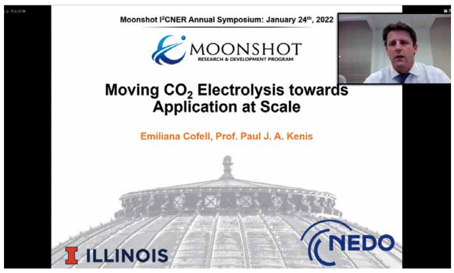
- Zhenying Wang, Daniel Orejon, Yasuyuki Takata, Khellil Sefiane, "Wetting and evaporation of multicomponent droplets." *Physics Reports*, Vol. 960, pp. 1-37, 2022.

F. University of Illinois Urbana-Champaign (J. Stubbins, C. Brooks, K. Huff): This effort aims respectively at the the short- and long-term milestones "Theoretical and quantitative evaluation of national and global transitions" and "Engendering a sustainable energy transition incorporating emerging technologies" of the project "Energy transitions," (iv) Socio-techno-economic and Policy Analysis in the Thrust's roadmap.

- Andrew Chapman, Yosuke Shigetomi, Shamal Chandra Karmaker, Bidyut Baran Saha, Kathryn Huff, Caleb Brooks, James Stubbins, "The cultural dynamics of energy: The impact of lived experience, preference and demographics on future energy policy in the United States." *Energy Research and Social Science*, Vol. 80, pp. 102231, 2021.

Carbon Management including Negative Emission Technologies
(2022 I²CNER Annual Symposium)





(photos, from top)
1. Tatsuro Ishibashi, President, Kyushu University
2. Dr. Akira Ukawa, WPI Program Director
3. Mr. John C. Taylor, Principal Officer at the U.S. Consulate in Fukuoka
4. Prof. Paul J. A. Kenis, University of Illinois Urbana-Champaign

Since its inception, I²CNER has held an annual symposium, which has evolved over time from an event that celebrates the current research achievements of its thematic research areas (three thrusts) to an exploratory forum that focuses on a single research topic that is highly relevant to I²CNER's research portfolio and the international community. Additionally, to explore new ways to best represent their thematic research areas, I²CNER's three thrusts jointly hold an international workshop with several researchers and engineers.

This year's I²CNER Annual Symposium, "Carbon Management including Negative Emission Technologies," held on January 25, 2022, welcomed Japanese and U.S. government officials as well as world-class researchers to engage in discussions on CO_2 management, starting with CO_2 capture directly from the air, followed by CO_2 conversion and storage. Five invited lectures on various perspectives of CO_2 management were presented. Academics, industry researchers, and members of the public were in attendance.

Dr. Kenji Yamaji

President and Director-General, Research Institute of Innovative Technology for the Earth (RITE)/ Program Director, Moonshot Research and Development Program/ Moonshot Goal 4

Dr. Kenji Yamaji outlined the R&D concept of Moonshot Goal No. 4 "Realization of sustainable resource circulation to recover the global environment by 2050." Dr. Yamaji stated that the goal aims to solve the problem of global warming (the Cool Earth) and to solve the problem of environmental pollution (the Clean Earth) through realizing sustainable resource circulation, aiming to deploy commercial plants or products utilizing circulation technology globally by 2050. He also expressed his expectations for Prof. Fujikawa's Moonshot project.

Prof. Shigenori Fujikawa

I^{2}CNER, Kyushu University

Prof. Shigenori Fujikawa offered an overview of his Moonshot project "Development of Global CO_2 Recycling Technology towards 'Beyond-Zero' Emission." Based on the innovative separation nanomembranes with world-leading CO_2 permeability and nanomembrane technology, Prof. Fujikawa aims to develop a CO_2 capture unit consisting of CO_2 separation nanomembranes with high CO_2 selectivity, and a highly efficient CO_2 conversion unit that converts the captured CO_2 into carbon fuel. This innovative DAC-U system will enable the ubiquitous capture of CO_2 from the atmosphere and the recycling of CO_2 as a carbon fuel. Prof. Fujikawa stressed that the goal is not only to solve the problem of climate change, but also to contribute to the realization of a carbon-recycling society based on Local Production Local Consumption.

Prof. Shunsuke Managi

Distinguished Professor, Director of Urban Institute, Kyushu University

Prof. Shunsuke Managi explained the Inclusive Wealth (IW) Index provides important insights into long-term economic growth and human well-being. The index measures the wealth of nations through a comprehensive analysis of a country's productive base and wealth in terms of progress, well-being and long-term sustainability. It measures all of the assets upon which human well-being is based in particular, produced, human and natural capital to create and maintain human well-being over time. Finally, he emphasized the importance of emerging technologies such as carbon direct capture and utilization systems and target setting of both national and regional plans.

Program *January 25, 2022*

MC: Prof. Roman Selyanchyn, I^{2}CNER

9:00 a.m.	Opening Remarks **Dr. Tatsuro Ishibashi,** President, Kyushu University **Mr. John C. Taylor,** Principal Officer at the U.S. Consulate in Fukuoka **Dr. Akira Ukawa,** WPI Program Director
9:25 a.m.	Introduction **Prof. Petros Sofronis,** Director, I^{2}CNER, Kyushu University
9:30 a.m.	Invited Lecture A "Carbon Management Projects in the Moonshot Goal 4" **Dr. Kenji Yamaji,** President and Director - General, Research Institute of Innovative Technology for the Earth (RITE)/ Program Director, Moonshot Research and Development Program/ Moonshot Goal 4
9:55 a.m.	I^{2}CNER Lecture "Development of Global CO_2 Recycling Technology towards "Beyond - Zero" Emission" **Prof. Shigenori Fujikawa,** I^{2}CNER, Kyushu University
10:20 a.m.	Invited Lecture B "Energy for sustainability: Analysis with Inclusive Wealth" **Prof. Shunsuke Managi,** Distinguished Professor, Director of Urban Institute, Kyushu University
11:00 a.m.	Invited Lecture C "Advancing CO_2 Electrolysis towards Application at Scale" **Prof. Paul J. A. Kenis[1] and Emiliana R. Cofell[2],** [1]Elio Eliakim Tarika Endowed Chair in Chemical Engineering, University of Illinois Urbana - Champaign (UIUC), [2]Materials Science and Engineering, UIUC
11:40 a.m.	Invited Lecture D "Electrochemical Separations for Energy and Sustainability" **Prof. Xiao Su,** Chemical and Biomolecular Engineering, UIUC
12:10 p.m.	Invited Lecture E "Green CO & CO_2 Removal" **Prof. Joydeep Dutta,** Chair of Functional Materials at KTH Royal Institute of Technology, Stockholm *pre - recorded
12:30 p.m.	Closing Remarks

Distinguished Visitors

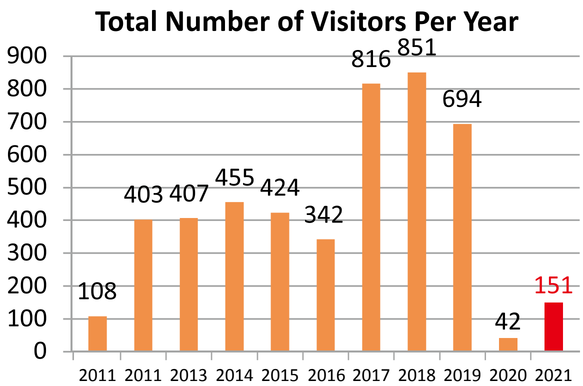
July 19, 2021 Mr. Eiichi Nakamura (left), Deputy Mayor of Fukuoka City

October 21, 2021 Mr. Osamu Hashimoto (center), President & CEO, Mitsui Chemicals Inc.

November 19, 2021, Ms. Katherine Rafaniello (right), Consulate Political Economic Officer at the U. S. Consulate in Fukuoka

November 29, 2021, Mr. Gianluigi Benedetti (center), the Italian Ambassador to Japan

March 10, 2022, Chairman and board members of KEIDANREN, Japan Business Federation



Although COVID-19 pandemic still persisted, the number of visitors increased in 2021 compared to the previous year.

October 1, 2021-June 25, 2022, PI Ishihara hosted Associate Prof. Yuanyuan Sun, College of Chemistry and Chemical Engineering, Hainan Normal University, Haikou, China. Profs. Sun and Ishihara worked on developing a new zeolite photocatalyst for conversion of CO_2 as well as water splitting.

Seminars

The I²CNER Seminar Series (ISS)

One of the most important goals of the I²CNER Seminar Series is to engage key members of the international community from academia, national laboratories, industry, and government agencies (policy makers). In FY2021, the Institute hosted 8 speakers (6 non-Japanese) for I²CNER Seminars. Cumulatively, 179 speakers have presented at 176 I²CNER Seminars. Under the circumstances of the COVID-19 pandemic, the I²CNER Seminar Series was held virtually as I²CNER Webinars and attracted participants not only from Japan but from around the world.

Selected ISS speakers

August 18, 2021

Prof. Tsutomu Miyasaka
Professor, Toin University of Yokohama, Japan
Title: Interfacial material engineering for high performance perovskite solar cells

January 12, 2022

Prof. Thomas Lippert
Professor, Paul Scherrer Institute (PSI), Switzerland
Title: Thin Films prepared by PLD: model systems for studies using large facilities techniques

October 6, 2021

Prof. Angus Rockett
Professor, Colorado School of Mines, USA
Title: Current Status and Research and Technology Opportunities in Photovoltaics

February 9, 2022

Prof. Nenad Miljkovic
Associate Professor, University of Illinois at Urbana - Champaign, USA
Title: Understanding the Fundamental Degradation Mechanisms of Hydrophobic Interfaces and Surface Structures Enables the Development of Enhanced Two-Phase Heat Transfer Processes

Institute Interest Seminar Series (IISS)

Since the inception of the Institute, young researchers have been presenting lectures 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. Cumulatively, 351 speakers have presented at 215 seminars. In FY2021, 19 speakers presented at 19 Institute Interest Seminars. Even during the pandemic, Zoom seminars effectively reached 404 attendees.

Selected IISS speakers

April 13, 2021

Assoc. Prof. Stephen Lyth
Advanced Energy Conversion Systems Thrust
Title: Fuel Cells: Powered by Hydrogen, Inspired by Nature

July 6, 2021

Prof. Katsuhiko Hirose
Multiscale Science and Engineering for Energy and the Environment
Title: Hydrogen in the Carbon Neutral Sustainable Society

August 31, 2021

Assoc. Prof. Aleksandar Tsekov Staykov
Advanced Energy Conversion Systems
Title: Oxygen Reduction Reaction and Electronic Properties on PrO and LaO Terminated Surfaces of Pr2NiO4 and La2NiO4

November 30, 2021

Prof. Atsushi Kurosawa
Multiscale Science and Engineering for Energy and the Environment
Title: Carbon-Neutral Energy System in 2050 – System Analysis

December 14, 2021

Prof. Masanobu Kubota
Advanced Energy Materials
Title: Activation of Catalyst by Friction

March 15, 2022

Dr. Seiichiro Kimura
Advanced Energy Conversion Systems Thrust
Title: Contribution of Think Tanks in the Formulation of Japan's Energy Policy

Conferences and Symposia

I²CNER Thrust Workshop: Toward Carbon Neutrality

January 28, 2021
Online meeting co-organized by Prof. Masanobu Kubota, Prof. Hiroshige Matsumoto and Prof. Takeshi Tsuji. The symposium was organized by PIs from three thrusts, Advanced Energy Materials thrust (AEM), Advanced Energy Conversion Systems thrust (AEC), and Multiscale Science and Engineering for Energy and the Environment thrust (MSEEE) to showcase I²CNER's interdisciplinary research on energy for carbon neutrality.

International Hydrogen Energy Development Forum 2022

January 27, 2022
Hybrid meeting (On-site and online), organized by Prof. Joichi Sugimura. This forum discusses research, development, and policy for the introduction of hydrogen technology and has been held for 16 years in a row in Fukuoka. The topics are in direct alignment with the objectives of the Advanced Energy Materials Thrust.

46th International Conference and Expo on Advanced Ceramics and Composites (ICACC 2021)

January 24-28, 2022, virtual
Symposium 6: Solid Electrolytes for Batteries/Diagnostics organized by PI Ishihara.

HYDROGENIUS, I²CNER, HydroMate and SINTEF Joint Research Symposium 2022 on Hydrogen-Materials Interactions

January 27-28, 2022
Online meeting co-organized by Prof. Hisao Matsunaga, Dr. Brian Somerday, Prof. Junichiro Yamabe, and Prof. Masanobu Kubota. This topical and impactful hydrogen embrittlement symposium has been continuously organized once a year from 2007 to 2022. The symposium attracts researchers from academia, industry, and government from around the world.

HYDROGENIUS & I²CNER Tribology Symposium

January 28, 2022
Hybrid meeting (On-site and online), organized by Prof. Yoshinori Sawae. The aim of this symposium was to discuss recent advances in tribology research for hydrogen energy systems. The topics are in direct alignment with the objectives of the Advanced Energy Materials Thrust. Due to COVID-19, the forum was held in a hybrid format.

7th National and 1st International Conference on Refrigeration and Air Conditioning (NCRA 2022)

February 24-26, 2022 in Guwahati, India
Saha, B.B., Co-Chairman

7th International Conference on Micro and Nano Flows (MNF2021)

May 24-26, 2021 in London, UK
K. Takahashi, Organizing Committee

23rd International Conference on Solid State Ionics (SSI-23)

July 17-22, 2022, in Boston
Co-organized by PI Tuller. The International Conference on Solid State Ionics is a major event in the field, attracting a worldwide audience every two years. It provides an unparalleled opportunity to gather leading international scientists and engineers, top-level industrial, management and business executives, as well as students and young scientists, to discuss all aspects of the science, technology and applications of ion-conducting materials. The Conference facilitates the exchange of ideas between people with different backgrounds and fosters the development and professional growth of both young and experienced researchers alike.

Asian Union of Thermal Science and Engineering (AUTSE)

Y. Takata, President
https://autse-asia.org/

Plenary and Keynote Presentations

S. Fujikawa, "Negative Emissions Technologies for a Beyond Zero Society," Opening memorial ceremony of Kyushu University, May 11, 2021

M. Yamauchi, "Inorganic nanocatalysts for efficient electrochemical material conversion," 20th Science Council of Asia Conference, Science Council of Asia (SCA) and China Association for Science and Technology (CAST), Guangzhou Nansha Garden Hotel, Guangzhou, China, May 14, 2021

K. Takahashi, "Gas molecules at solid-liquid interfaces," The 7th International Conference on Micro and Nano Flows (MNF2021) (Online), keynote lecture, May 25, 2021

S. Ogo, "Hydrogen activation in water," International Symposium on Bioorganometallic Chemistry 2021 (Digital ISBOMC21-Webinar 2), June 16, 2021

Y. Takata, "On the Quench of Water Spray: When does it occur?" ASME Summer Heat Transfer Conference 2021 (Online), June 18, 2021

S. Fujikawa, "Ubiquitous CO_2 capture directly from air by nanometer-thick membranes," Guest Lecture in KTH Climate Action Centre, online, October 16, 2021

A. Chapman, Bridgeland, R. McLellan, B., "The Energy Infrastructure Nexus: Hydrogen Penetration Potential and Infrastructure Issues for the USA," Ecodesign 2021, December 1-3, 2021

A. Chapman, "Evaluating the Hydrogen Economy: Modeling of Production, Consumption and Potential Penetration," JCCP Kuwait Hydrogen Symposium, invited presentation. December 6, 2021

M. Kubota, "Effect of hydrogen on creep properties of austenitic stainless steels and pure iron," 3rd International Forum on Hydrogen Codes, Standards and Safety in the United Nations Development Programme (UNDP) Hydrogen Industry Conference 2021, Nanhai Qiaoshan Cultural Center, Foshan, China, December 9, 2021

B.B. Saha, "Strategy and achievements of carbon-neutral energy research," 3rd International Conference on Recent Advancements in Mechanical Engineering (ICRAME) 2022, keynote lecture, Silchar, Assam, India, February 4-6, 2022

T. Tsuji "Geophysical imaging and monitoring for resource exploration and CO_2 reduction," 1st International Symposium on Earth Resources and Geo-environmental Technology 2022, (EraGET2022), keynote lecture, online, February 18, 2022

B.B. Saha, "Adsorption science and technology toward achieving carbon neutrality," 7th National and 1st International Conference on Refrigeration and Air Conditioning 2022, keynote lecture, Guwahati, India, February 24-26, 2022

B.B. Saha, "Functional adsorbent materials for carbon-neutral energy conversion systems," 4th International Conference on Advances in Mechanical Engineering, plenary lecture, Tamil Nadu, India, March 24-26, 2022

T. Tsuji "CO_2 reduction and managements using the earth: New concept of storage of CO_2 derived from the membrane-based DAC," Lecture in The Engineering Academy of Japan, online, November 5, 2022

Selected Awards

Date	Recipient's name	Name of award
2021/2/21	Hisao Matsunaga	Acta Materialia and Scripta Materialia, Outstanding Reviewer Award 2020
2021/1/1	Tatsumi Ishihara	Catalysis Society of Japan Award (Academic field)
2020/12/9	Toshinori Matsushima, Chuanjiang Qin, William J. Potscavage Jr, Atula S. D. Sandanayaka, Matthew R. Leyden, Fatima Bencheikh, Kenichi Goushi, Fabrice Mathevet, Benoît Heinrich, Go Yumoto, Yoshihiko Kanemitsu, and Chihaya Adachi	IDW 2020 Best Paper Award, International Display Workshops
2020/11/3	Takeshi Tsuji	Nishinippon Cultural Award, Nishinippon Shimbun
2020/10/29	Naoya Sakoda, Yukihiro Higashi	Best Paper Award, Japan Society of Thermophysical Properties
2020/9/14	Ryosuke Komoda	Division Award (Category: Encouragement Presented Paper), The Japan Society of Mechanical Engineers M & P Materials and Processing Division
2020/9/8	Toshinori Matsushima, Chihaya Adachi	Best Paper Award, The Japan Society of Applied Physics
2020/7	Elif Ertekin	2020 Dean’s Award for Excellence in Research, Grainger College of Engineering, UIUC
2020/6/20	Yutaku Kita	Young Researcher Award, Heat Transfer Society of Japan
2020/5	Nicola Perry	NSF CAREER Award
2021	Chihaya Adachi	Japan Society of Applied Physics Outstanding Achievement Award
2022	Harry Tuller	Elected Fellow of the Materials Research Society
2021	Xing Zhang	International Achievement Award, Thermal Engineering Division of the Japan Society of Mechanical Engineers
2021/5	Qinyi Li, Koji Takahashi, Xing Zhang	Academic Award, The Heat Transfer Society of Japan
2021/5	Zhenying Wang	Young Researcher Award, The Heat Transfer Society of Japan
2022/2	Hideaki Teshima	Inoue Research Award for Young Scientists, Inoue Foundation for Science
2021	Yutaku Kita	Young Researcher Award, Japan Society of Mechanical Engineers

Outreach Activities

Outreach Events

WPI seminar series for high school teachers (July 3, 2021)

6 WPI centers jointly hosted an online seminar series for high school teachers in FY 2021. On July 3, 2021, Prof. Yoon from I^{2}CNER gave a lecture titled "Research Strategy for Carbon Dioxide Reduction Using Hydrogen Enzymes" along with Prof. Nakajima from the Institute for Chemical Reaction Design and Discovery (WPI-ICReDD), Hokkaido University. Following the lectures, a crosstalk was held between two researchers and both researchers engaged in a lively question and answer session.

WPI Symposium for High School Students (December 18, 2021)

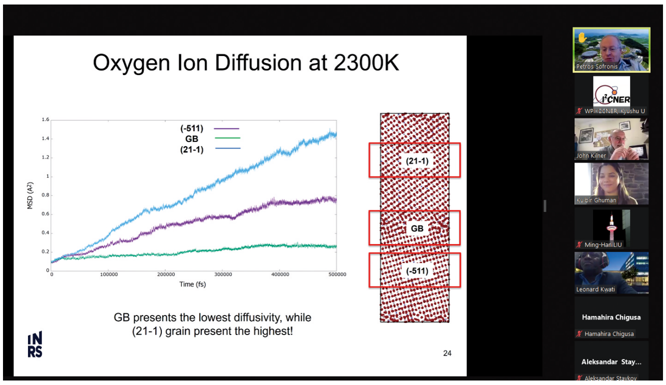
An online symposium "Nano world toward the Future" was held on December 18, 2021 hosted by the Nano Life Science Institute Kanazawa University (WPI-NanoLSI). The symposium was mainly targeted at high school students and teachers. Prof. Takahashi from I^{2}CNER gave a keynote lecture, titled "Control of metal nanostructures for highly efficient use of light energy" along with three other speakers representing institutions of WPI. At the research presentation by high school students in the afternoon, Profs. Kubota and Watanabe participated online and gave feedback and encouragement to high school students.

Energy Week 2022 (January 28 - February 4, 2022)

Kyushu University Energy Week 2022 was held January 28–February 4, 2022, featuring symposia concerning energy on the theme of "Energy Intelligence Beyond Borders: Aiming for the Future of Green Innovation." For this year's online symposium, Kyushu University's energy-related departments came together to organize international workshops and those between industry, academia, and government as well as other events around the theme of "future energy," which served as a forum for exchange and an international hub for energy researchers. The I^{2}CNER Annual Symposium, I^{2}CNER Thrust Workshop, I^{2}CNER-HYDROGENIUS Joint Research Symposium and I^{2}CNER-IMI Joint International Workshop, were all held during Energy Week. During the workshops, there were many questions and discussions that showed the enthusiasm from participants, academics, and researchers from institutions and industries across Europe, Asia, U.S., and Japan.

WPI seminar series for high school teachers

WPI Symposium for High School Students



I^{2}CNER Thrust Workshop during Energy Week 2022

Press Releases and Media Coverage

Press Releases in FY2021

DATE	DESCRIPTION
Jun. 4, 2021	**Profs. Shigenori Fujikawa and Takeshi Tsuji** (Multiscale Science and Engineering for Energy and the Environment Thrust) Underground storage of carbon captured directly from air -- green and economical
Jun. 22, 2021	**Prof. Ikuo Taniguchi** (Multiscale Science and Engineering for Energy and the Environment Thrust) Assembly of Defect-Free Microgel Nanomembranes for CO_2 Separation
Jun. 25, 2021	**Profs. Hajime Nakanotani and Chihaya Adachi** (Advanced Energy Conversion Systems Thrust) Direct Observation of Photoexcited Electron Dynamics in Organic Solids Exhibiting Thermally Activated Delayed Fluorescence via Time-resolved Photoelectron Emission Microscopy
Oct. 7, 2021	**Prof. Takeshi Tsuji** (Multiscale Science and Engineering for Energy and the Environment Thrust) Low-cost, continuous seismic monitoring system to support emission reduction efforts
Oct. 28, 2021	**Profs. Petros Sofronis and Tatsumi Ishihara** (Advanced Energy Conversion Systems Thrust) Mitsui Chemicals, Inc. – Carbon Neutral Research Center Established at Kyushu University's I^2CNER
Nov. 2, 2021	**Prof. Ki-seok Yoon** (Advanced Energy Materials Thrust) Non-conventional octameric structure of C-phycocyanin
Nov. 8, 2021	**Prof. Takeshi Tsuji** (Multiscale Science and Engineering for Energy and the Environment Thrust) Temporal changes in anthropogenic seismic noise levels associated with economic and leisure activities during the COVID-19 pandemic
Nov. 26, 2021	**Prof. Chihaya Adachi** (Advanced Energy Conversion Systems Thrust) Organic long-persistent luminescence stimulated by visible light in p-type systems based on organic photoredox catalyst dopants
Dec. 16, 2021	**Prof. Hiroshige Matsumoto** (Advanced Energy Conversion Systems Thrust) Future efforts as a Designated National University Corporation -Latest research efforts on "decarbonization"-
Feb. 9, 2022	**Prof. Shigenori Fujikawa** (Multiscale Science and Engineering for Energy and the Environment Thrust) Kyushu University and Sojitz Conclude Memorandum for Implementation of Membrane-based Direct Air Capture Technology and Related Technology Solutions to Capture Carbon Dioxide from the Atmosphere

Media Coverage in FY2021

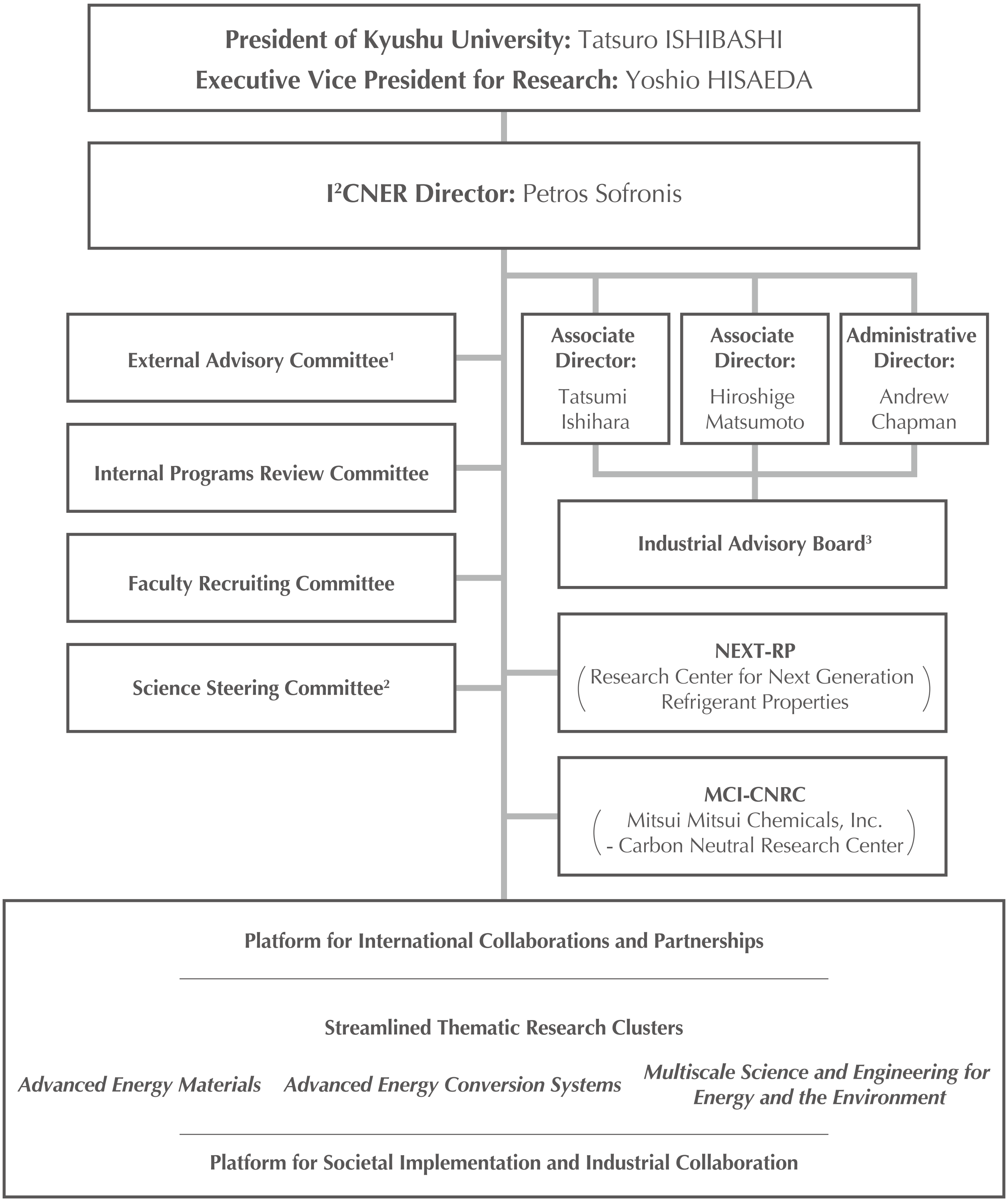
DATE	MEDIA OUTLET	DESCRIPTION
Jul. 19, 2021	JARN (Japan Air conditioning, Heat & Refrigeration News)	**Prof. Yukihiro Higashi** Daikin Develops a New Refrigerant for EV Air Conditioning
Aug. 31, 2021	Nikkan Kogyo Shimbun	**Prof. Shigenori Fujikawa** Save the Earth! NEDO Moonshot program
Oct. 18, 2021	Nihon Keizai Shimbun	**Prof. Takeshi Tsuji** Continuous monitoring system of underground CO_2
Oct. 29, 2021	Nihon Keizai Shimbun, Nikkan Kogyo Shimbun	**Prof. Tatsumi Ishihara** Mitsui Chemicals, Inc. – Carbon Neutral Research Center Established at Kyushu University's I^{2}CNER
Nov. 12, 2021	University Journal Online	**Prof. Takeshi Tsuji** Declining social activity due to the corona crisis, visualized with a "Seismometer"
Nov. 28, 2021	NHK	**Prof. Shigenori Fujikawa** Science ZERO "Front-runners for decarbonization"
Feb. 9, 2022	Nihon Keizai Shimbun	**Prof. Shigenori Fujikawa** Kyushu University and Sojitz Corporation have signed a memorandum

Press conference on the Mitsui Chemicals, Inc. – Carbon Neutral Research Center Established at Kyushu University's I^{2}CNER (Oct. 28, 2021)

Prof. Matsumoto in the KU press conference on the Designated National University Corporation (Dec. 16, 2021)

I²CNER Structure (as of April 1, 2022)

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, 2022 is as follows:

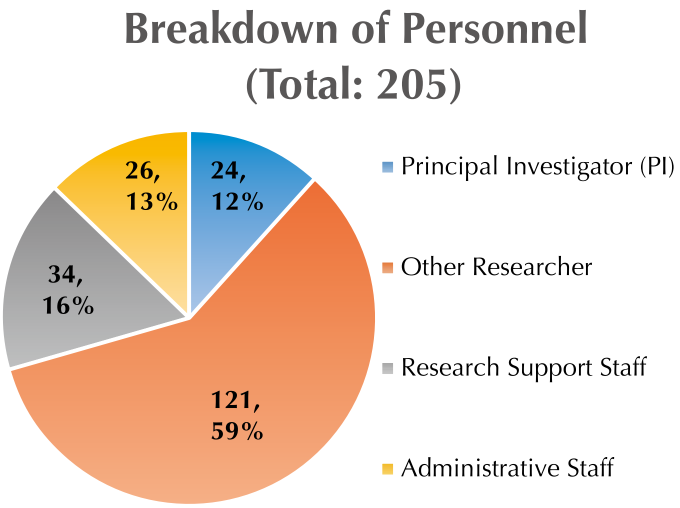
- Dr. Deborah Myers (Chair), Argonne National Laboratory, USA
- Dr. Kevin Ott (Vice-Chair), Retired, Los Alamos National Laboratory, USA
- Prof. Ronald J. Adrian, Arizona State University, USA, *National Academy of Engineering (NAE)*
- Prof. Fraser Armstrong, University of Oxford, UK, *Fellow of the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

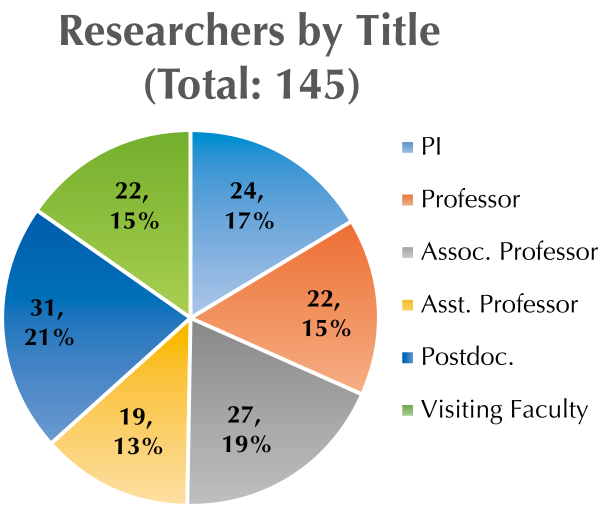
2) The **Science Steering Committee (SSC)** is chaired by the Director, and its members are the two Associate Directors and the lead PIs of the thrusts. The SSC is the body that reviews and advises on all matters of the Institute, e.g. planning and operation of research activities, budget implementation,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

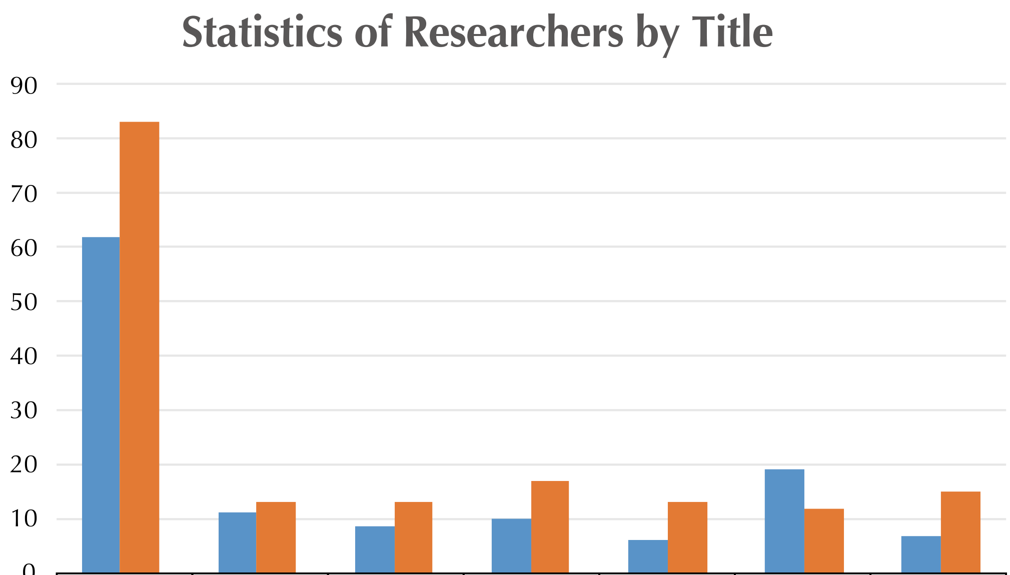
3) In FY2017, I^{2}CNER established the **Industrial Advisory Board (IAB)**, whose members are prominent executives from industry, government agencies, and national laboratories that advise I^{2}CNER on opportunities for interactions with industry and technology transfer. The first IAB meeting was held on February 1, 2018 and was attended by 9 out of 10 IAB members. The meeting provided invaluable inputs to I^{2}CNER researchers on areas that industries would have interest for promoting the development of new technologies. The full list of members as of April 1, 2022 is as follows:

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

Personnel (as of April 1, 2022)



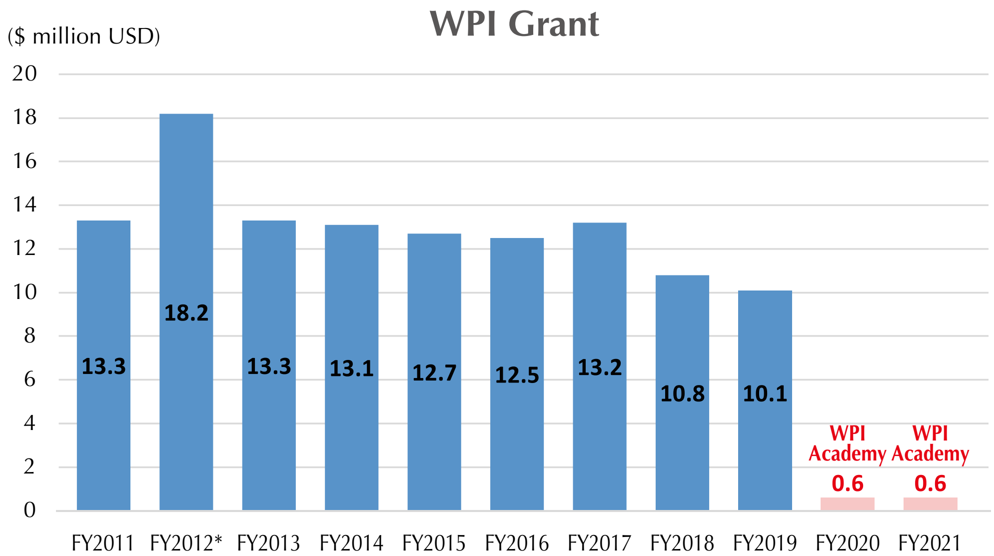




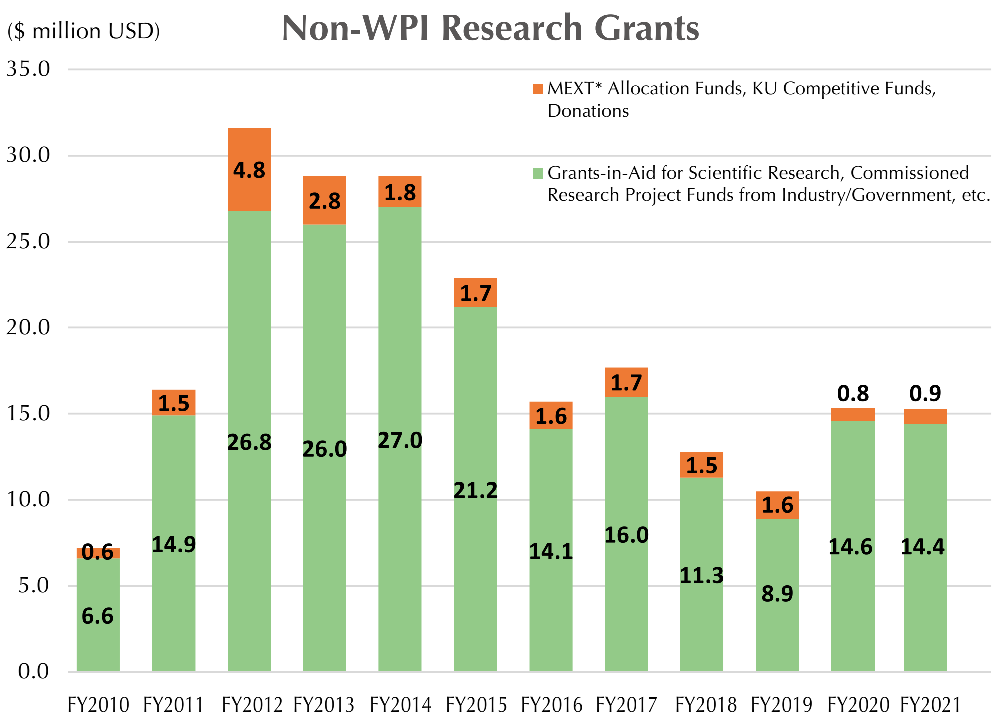
	Total	PI	Prof.	Assoc. Prof.	Asst. Prof.	Postdoc	Visiting Faculty
Overseas	62	11	9	10	6	19	7
Japanese	83	13	13	17	13	12	15
% Overseas	43%	46%	41%	37%	32%	61%	32%
% Female	10%	4%	0%	11%	26%	5%	5%

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, 2022)

Administration

Director
Prof. Petros Sofronis

Associate Directors
Prof. Tatsumi Ishihara
Prof. Hiroshige Matsumoto

Principal Investigators

Advanced Energy Conversion Systems Thrust
Prof. Hiroshige Matsumoto (Thrust Lead PI)
Prof. Chihaya Adachi
Prof. Tsuyohiko Fujigaya
Prof. Andrew A. Gewirth, University of Illinois Urbana-Champaign, USA
Prof. Tatsumi Ishihara
Prof. John A. Kilner, Imperial College London, UK
Prof. Thomas Lippert, Paul Scherrer Institut, Switzerland
Prof. Kazunari Sasaki
Assoc. Prof. Aleksandar Tsekov Staykov
Prof. Harry L. Tuller, Massachusetts Institute of Technology, USA

Advanced Energy Materials Thrust
Prof. Masanobu Kubota (Thrust Lead PI)
Prof. Reiner Kirchheim, University of Göttingen, Germany
Prof. Seiji Ogo
Prof. Petros Sofronis
Dr. Brian Somerday, Southwest Research Institute, USA
Prof. Joichi Sugimura
Prof. Miho Yamauchi

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Prof. Shigenori Fujikawa (Thrust Lead PI)
Assoc. Prof. Andrew Chapman
Prof. Bidyut Baran Saha
Prof. James Stubbins, University of Illinois Urbana-Champaign, USA
Prof. Koji Takahashi
Prof. Takeshi Tsuji, University of Tokyo, Japan
Prof. Hiroaki Watanabe

Full-time Faculty & Postdoctoral Associates

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Dr. Miho Isegawa
Dr. Sovann Khan
Dr. Wu Kuan Ting
Assoc. Prof. Toshinori Matsushima
Dr. Yutaka Osaki
Dr. Veeramani Vediyappan
Assoc. Prof. Motonori Watanabe

Advanced Energy Materials Thrust
Assoc. Prof. Yukina Takahashi
Prof. Toshihiro Tsuchiyama
Assoc. Prof. Ki-Seok Yoon

Multiscale Science and Engineering for Energy and the Environment Thrust
Dr. Sumitomo Hidaka
Asst. Prof. Nguyen Dinh Hoa
Prof.Yasuyuki Takata

Platform for International Collaborations and Partnerships
Assoc. Prof. Kaveh Edalati (AECS Thrust)
Asst. Prof. Leonard Kwati (AECS Thrust)
Asst. Prof. Mai Tomisaki (AECS Thrust)

Research Center for Next Generation Refrigerant Properties
Prof. Yukihiro Higashi
Dr. Frantisek Miksik

Mitsui Chemicals, INC. -Carbon Neutral Research Center
Dr. Sharif Md Hossain
Dr. Md. Amirul Islam
Dr. Ming-Han Liu
Dr. Mohammad Moniruzzaman
Dr. Tomoaki Nakaishi
Dr. Debashis Sahu
Prof. Toshihiro Takai
Dr. Thinh Nguyen Van

Satellite Faculty & Postdoctoral Associates

Advanced Energy Conversion Systems Thrust
Assoc. Prof. Elif Ertekin
Prof. Nenad Miljkovic
Asst. Prof. Nicola Helen Perry
Prof. Angus Rockett
Prof. Hong Yang

Advanced Energy Materials Thrust
Prof. Paul J. A. Kenis

Multiscale Science and Engineering for Energy and the Environment Thrust
Prof. Kenneth Christensen
Assoc. Prof. Kathryn Huff

Part-time Faculty & Postdoctoral Associates

Advanced Energy Conversion Systems Thrust
Asst. Prof. Kenichi Goushi
Prof. Kohei Ito
Dr. Nuttavut Kosem
Assoc. Prof. Stephen Lyth
Asst. Prof. Masashi Mamada
Assoc. Prof. Junko Matsuda
Assoc. Prof. Hajime Nakanotani

Assoc. Prof. Tomohiro Shiraki
Asst. Prof. Juntae Song
Assoc. Prof. Atsushi Takagaki
Asst. Prof. Naoki Tanaka
Prof. Kazunari Yoshizawa

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Dr. Masaki Donoshita
Assoc. Prof. Hirokazu Kobayashi
Asst. Prof. Takuro Masumura
Assoc. Prof. Takahiro Matsumoto
Prof. Hisao Matsunaga
Asst. Prof. Takehiro Morita
Dr. Tomohiro Noguchi
Assoc. Prof. Hironobu Ozawa
Prof. Yoshinori Sawae
Asst. Prof. Hiroyoshi Tanaka
Assoc. Prof. Tatsuya Uchida
Assoc. Prof. Kazuyuki Yagi
Asst. Prof. Kosei Yamauchi
Asst. Prof. Takeshi Yatabe
Dr. Akina Yoshizawa

Multiscale Science and Engineering for Energy and the Environment Thrust
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Dr. Rasha Afmed Hanafy Bayomi
Dr. Chao-Hung Cheng
Dr. Ramadan M. M Eljamal
Asst. Prof. Tatsunori Ikeda
Dr. Kenshi Itaoka
Asst. Prof. Yutaku Kita
Prof. Masamichi Kohno
Assoc. Prof. Ken Kojio
Asst. Prof. Kaname Matsue
Assoc. Prof. Jin Miyawaki
Prof. Takahiko Miyazaki
Prof. Shoji Mori
Asst. Prof. Takeo Nakano
Dr. Adchara Padermshoke
Assoc. Prof. Qin-Yi Li
Assoc. Prof. Naoya Sakoda
Assoc. Prof. Roman Selyanchyn
Assoc. Prof. Atsuomi Shundo
Dr. Feng Sinan
Prof. Yuichi Sugai
Prof. Atsushi Takahara
Asst. Prof. Hideaki Teshima
Assoc. Prof. Kyaw Thu
Dr. Nutthon Yokachuksuse
Dr. Panlong Yu
Asst. Prof. Zhenying Wang

Visiting Professors & Scholars

Advanced Energy Conversion Systems Thrust
Prof. Limin Guo, *Huazhong U. of Science and Technology*
Prof. Stephen John Skinne, *Imperial College London*
Dr. Seiichiro Kimura, *Renewable Energy Institute, Japan*
Kenshi Mitsuishi, *Mitsui Chemicals, Inc., Japan*
Prof. Ken Okazaki, *Tokyo Institute of Technology*
Asst. Prof. Helena Tellez-Lozano

Advanced Energy Materials Thrust
Prof. Nikolaos Aravas, *University of Thessaly, Greece*
Asst. Prof. Mohsen Dadfarnia, *Seattle University*
Asst. Prof. Ryosuke Komoda, *Fukuoka University, Japan*
Dr. Kinya Kumazawa, *Japan Institute for Promoting Invention and Innovation*
Assoc. Prof. Arnaud Macadre, *Yamaguchi University, Japan*
Dr. Akihide Nagao, *Air Liquide Laboratories, Japan*
Prof. Robert O. Ritchie, *University of California, Berkeley, USA*

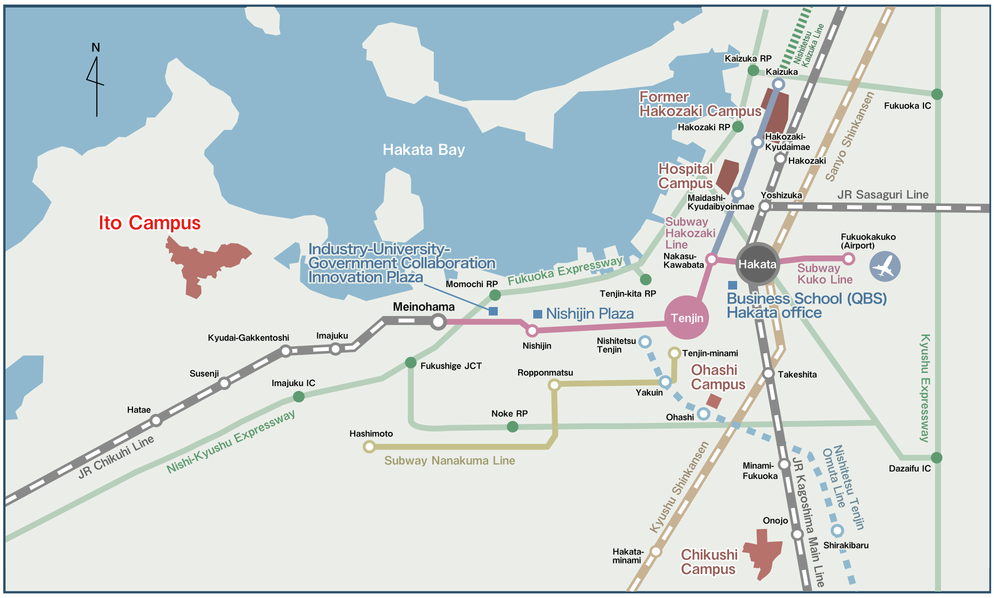
Multiscale Science and Engineering for Energy and the Environment Thrust
Prof. Makoto Akai, *National Institute of Advanced Industrial Science and Technology*
Asst. Prof. Jiang Fei, *Yamaguchi University, Japan*
Prof. Benny Freeman, *University of Texas at Austin, USA*
Prof. Yasumasa Fujii, *University of Tokyo, Japan*
Prof. Katsuhiko Hirose, *Toyota Motor Corporation, Japan*
Prof. Kuniaki Honda
Asst. Prof. Jihui Jia, *China University of Petroleum*
Prof. Toyoki Kunitake, *Kitakyushu Foundation for the Advancement of Industry Science and Technology, Japan*
Prof. Atsushi Kurosawa, *Institute of Applied Energy, Japan Science and Technology, Japan*
Prof. Sushanta Mitra, *University of Waterloo, Canada*
Assoc. Prof. Daniel Orejon, *University of Edinburgh, UK*
Prof. Khellil Sefiane, *University of Edinburgh, UK*
Asst. Prof. Biao Shen, *University of Tsukuba*

Platform for Societal Implementation and Industrial Collaboration
Dr. Munetaka Higuchi, *Mazda Motor Corp., Japan*
Assoc. Prof. Suguru Ikeda, *Mazda Motor Corp., Japan*
Dr. Soichiro Ikeda, *Mazda Motor Corp., Japan*

Research Center for Next Generation Refrigerant Properties
Prof. Ryo Akasaka, *Kyushu Sangyo University, Japan*
Prof. Chieko Kondo, *Nagasaki University, Japan*
Prof. Akio Miyara, *Saga University, Japan*

Access Map

Map of Fukuoka City



Fukuoka Airport → 5min. → Hakata Station → 5min. → Tenjin Station → 14min. → Meinohama Station → 10min. → Kyudai gakkentoshi Station → 15min. → Kyudai Big Orange-mae/ Central Library

From Fukuoka Airport,Hakata Station, or Tenjin Station:
Take a train on the Fukuoka City Subway bound for "Meinohama" or "Chikuzen-Maebaru/Karatsu/Nishi-Karatsu."

At Meinohama Station:
If your train's destination is "Meinohama," transfer to a JR Kyushu train bound for "Chikuzen-Maebaru/Karatsu/Nishi-Karatsu."

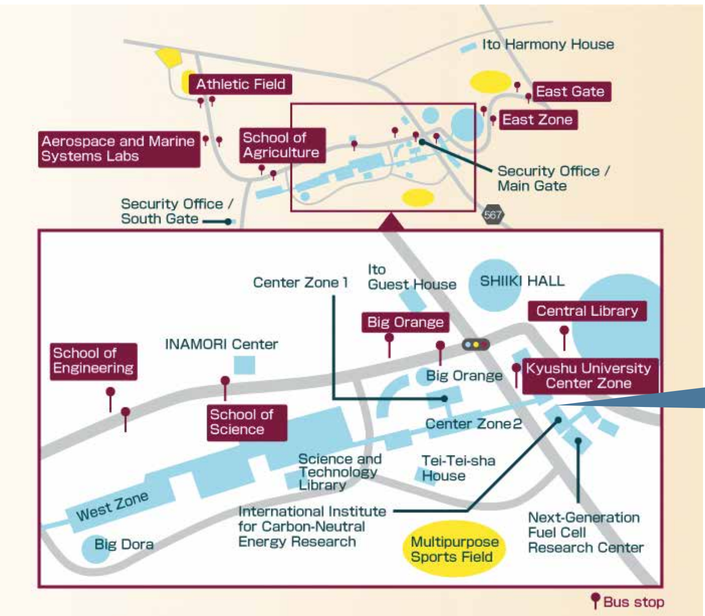
If your train's destination is "Chikuzen-Maebaru/Karatsu/Nishi-Karatsu," no transfer is required at Meinohama Sta.

34min.

At Kyudaigakkentoshi Station:
Transfer to Showa bus bound for Kyushu University's Ito Campus.

15min.

Campus Map



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Twitter: twitter.com/I2CNER

I²CNER Annual Report 2021

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The overhead view of the I²CNER building portrays the *Keeling Curve, which rises over time, to indicate that I²CNER'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_2) 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.

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